User Manual of the Deft incompressible flow solver

Guus Segal

Marcel Zijlema

Ronald van Nooyen

Charles Moulinec

version 1.1

August 16, 2000

Contents

Chapter 1

Introduction

The information about the Deft Navier-Stokes solver is distributed over three different documents. This User Manual contains all information needed to run the program for an arbitrary problem on a given grid. The Deft Programmers Guide [40] explains the internals of the program and discusses program installation and maintenance. The Mathematical Manual [38] discusses the mathematical details and the discretization. The user manual deals with these subjects only insofar as they are relevant to the program options.
In addition to the above mentioned documents you may need the manuals of your chosen grid generator and display program. At the moment the following pre- and postprocessing packages are supported:

- SEPRAN 2D and 3D grid generation [39]
- LISS 2D grid generation [3]
- SEPRAN 2D and 3D postprocessing [39]

Please note that this manual describes the Unix version of Deft and SEPRAN, other implementations may behave differently.

1.1 Purpose and motivation

The purpose of the program is the solution of the 2D and 3D Navier-Stokes equations (incompressible or incompressible) coupled with an arbitrary number of convection-diffusion equations (also known as transport equations) on fairly general grids by the boundary fitted finite volume method. The main goal is to solve these equations in an accurate and fast way. During code development emphasis was placed on speed of execution on vector and parallel computers. This resulted in a restriction on the way in which the region can be decomposed into blocks. Only blocks that are topologically equivalent to a a rectangle or a cube are allowed. More specifically, each block must be simply connected (no holes) and preferably have at least four corners in R^2 and eight in R^3. Some

examples of single block grids are shown in Figure 1.1.1; Figure 1.1.2 shows an example of a grid consisting of four single blocks.

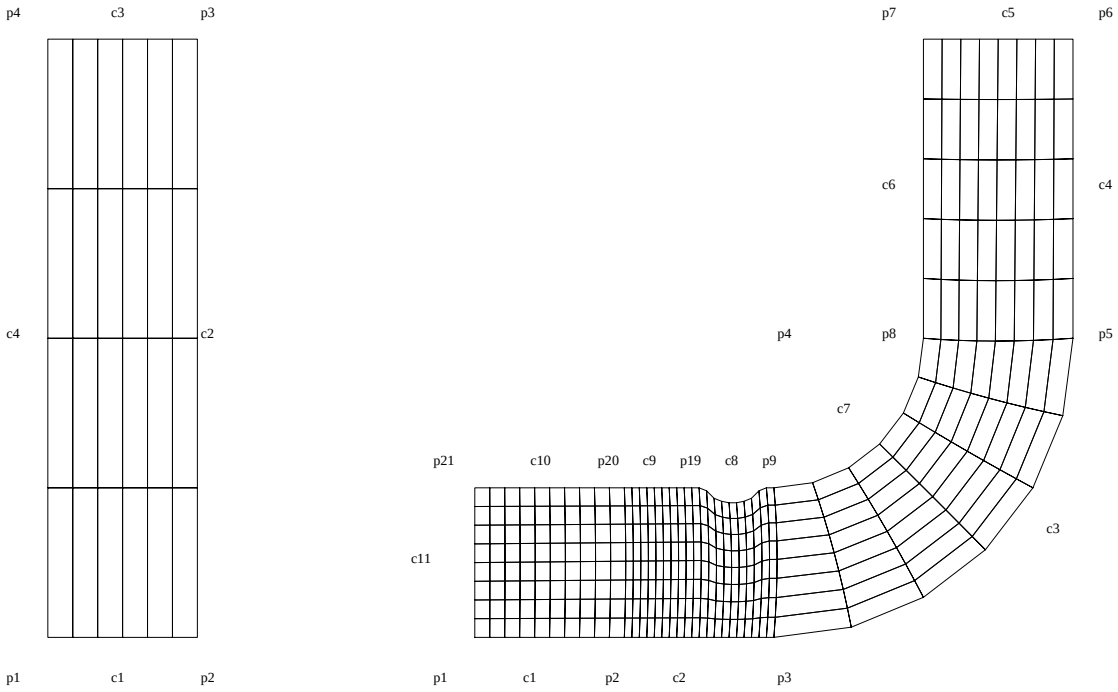


Figure 1.1.1: Two possible single block grids

Note that, for computations, blocks are actually mapped onto rectangles or their 3D equivalents.

1.2 Limitations

The program can deal with the Navier-Stokes equations, coupled with a number of transport equations or alternatively a set of convection diffusion equations for a given velocity field.
The region must be such that it can be subdivided into a number of blocks, each of which can be mapped onto a rectangle or a cube. The grid on the rectangle or cube must be rectangular. In the original region, the grids are allowed to be curvilinear.
Here is the current state of the package. Concerning the 2-D method, three discretizations are available: the standard staggered scheme based on a total

transformation of the equations and accurate on smooth grids only, the Wesseling and Van Beek [48] staggered scheme accurate on non-smooth grids also and the Wesseling and Van Beek collocated scheme, which is currently used only to compute incompressible laminar flows. Note that the staggered approach follows a coupled treatment of the momentum equation whereas the collocated approach follows a decoupled treatment of it. Concerning the 3-D method, two discretizations are available: the standard staggered scheme and the Wesseling and Van Beek staggered scheme. The mapping of the domain onto a rectangle or cube divides the boundary of the domain into parts that correspond to the sides of that rectangle or cube.
While the coefficients may depend on time, place and the solution of the system of equations, the solution used to compute them is always the "old" solution. i.e. the solution obtained in the last time step.
The solution procedure per time step is always an iterative one and the equations are decoupled, i.e. first the momentum equations are solved with a pressure correction step, and then each of the transport equations is dealt with.
Always remember that the mesh should be such that a piecewise linear interpolation on the mesh contains all aspects of both the solution and the boundary conditions.

1.3 Hardware and software requirements

The program needs at least 4Mb of memory and 20Mb of hard disk space to run. Run time depends on problem size and complexity.
To add user-defined functions to the program, a fortran 77 compiler and a linker are needed. On a Unix system the standard fortran 77 compiler and linker may be used.

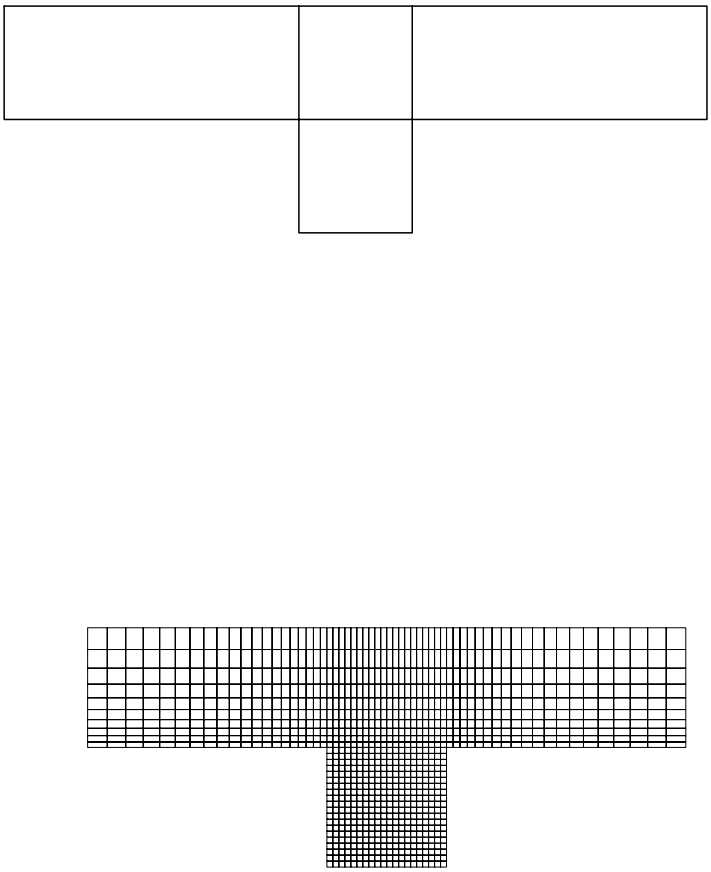


Figure 1.1.2: Grid consisting of four single blocks

Chapter 2

Theory

In this chapter we shall give an overview of the equations that can be solved by the Deft program for compressible and incompressible flow. The boundary conditions allowed will be specified as well as the available turbulence models. Mathematical details, in so far they are not necessary for the user, will not be treated. We refer to the Mathematical Manual [38] for a complete description. However, if the user has the opportunity to choose between various possibilities the consequences will be indicated in this chapter.

2.1 Physics

In this section we formulate the equations for compressible and incompressible viscous fluid flow as they are solved by Deft. The user definable parameters will be indicated.
The Deft incompressible program has been developed to solve the momentum equations in combination with the incompressibility condition. In the compressible case of course there is no incompressibility condition, but the same types of methods are applied. The flow may be laminar or turbulent. Both stationary and time-dependent flows are allowed.
The momentum equations may be coupled with an arbitrary number of transport equations (convection-diffusion equations). Hence, flows with heat transfer are included. Since it is possible to skip the momentum equations, in fact Deft may also be used to solve stand-alone convection-diffusion equations. Either the convection or the diffusion term may be set equal to zero.

2.1.1 Momentum equations

The two basic equations that describe an incompressible viscous fluid are: the continuity equation (2.1) and the Navier-Stokes equation (2.2) for an incompressible fluid.

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = \rho f_i \tag{2.2}$$

where $\boldsymbol{\tau}$ is the deviatoric stress tensor, defined as

$$\tau_{ij} = \mu(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}) \tag{2.3}$$

Here, we have used the assumption $D\rho/Dt = 0$ (total derivative of ρ is zero). We use the Einstein summation convention, i.e. if an index occurs twice in a term, a summation over that index is implied. Summations run from 1 to the dimension of the space in which we work. If an index occurs once, the equation represents a set of equations, one for each space dimension.
In the above formulae ρ is the density of the fluid, $\boldsymbol{u}$ is the velocity field, p the pressure and $\boldsymbol{x}$ are the space co-ordinates. The coefficient μ represents the dynamical viscosity. f_i represents the i^{th} component of some external force given in Cartesian co-ordinates.
The coefficients ρ, μ and f_i may all depend on space, time and of all the unknowns $(\boldsymbol{u}, p, T \ ... \ )$.

The stress tensor has the form:

$$\sigma_{ij} = \tau_{ij} - p\delta_{ij} \tag{2.4}$$

If the viscosity μ is zero, these equations are known as the Euler equations.

The compressible Navier-Stokes equations read:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{2.5}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = \rho f_i \tag{2.6}$$

These equations must be extended with an equation of state (See Section 2.1.8) and an extra energy equation, usually the enthalpy equation (See Section 2.1.9).

The deviatoric stress tensor for the compressible equations contains an extra term, compared to the incompressible case:

$$\tau_{ij} = \mu(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}) - \frac{2}{3}\mu\delta_{ij}\frac{\partial u_k}{\partial x_k}, \tag{2.7}$$

where δ_{ij} is the Kronecker delta.

2.1.2 Boundary conditions for the momentum equations

In order to solve the momentum equations uniquely it is necessary to prescribe boundary conditions at the complete outer boundary of the domain. In R^2 exactly two boundary conditions for the velocity in two independent directions

are necessary, in R^3 exactly three boundary conditions are required. The types of boundary conditions may vary for each part of the boundary.
A boundary condition of the form p is given is ill-posed, but there may be boundary conditions that involve the pressure, for instance σ^{nn} given. Whenever u_n is given, however, no other boundary condition may involve the pressure.

The following types of boundary conditions for the velocity are available in Deft, for a staggered arrangement of unknowns. For the collocated scheme, only Dirichlet boundary conditions are available at this moment.

Dirichlet boundary conditions These boundary conditions indicate that the complete velocity at a part of the boundary is prescribed. Typical examples are the no-slip boundary conditions $\boldsymbol{u} = 0$ and the fully developed inflow conditions, where the tangential velocity is zero and the normal velocity is parabolic.
In Deft the Dirichlet boundary conditions may be prescribed by giving noslip, inflow or explicitly giving the normal and tangential velocities or the Cartesian components.

Stresses prescribed A completely different possibility is to prescribe the normal (σ^{nn}) and tangential (σ^{nt}) stress components at a boundary.
Since the normal stress is equal to $-p + 2\mu\frac{\partial u_n}{\partial n}$ and in practical problems either μ, or the normal derivative of the normal velocity at boundary is small, prescribing the normal stress is more or less the same as prescribing the pressure.
A special case is the so-called outflow boundary condition which is defined as $\sigma^{nn} = 0$ and $\sigma^{nt} = 0$.

Normal velocity and tangential stress given This boundary condition is typical for free surface boundaries where we have $u_n = 0$ and $\sigma^{nt} = 0$ (tangential stress). This boundary condition is also indicated as free slip boundary condition.

Tangential velocity and normal stress given This boundary condition will for example be used at outflow. A typical example is parallel_outflow which means $u_t = 0$ and $\sigma^{nn} = 0$ or approximately $p = 0$.

Given pressure In the case of viscous flow the pressure can not be prescribed explicitly, but only by prescribing the normal stress. See "Tangential velocity and normal stress given".
In the case of the Euler equations one can not speak about stress boundary conditions. However, also in this case the pressure is prescribed by giving the normal stress. So for this special case the user must read "Tangential velocity and normal stress given" as "pressure given". The value of the pressure must be substituted as normal stress.

Law of the wall This wall law typically occurs in turbulent flow. It is used instead of a no-slip condition at a fixed wall, when a "high-Reynolds number" turbulence model is applied as explained in Section 2.1.5. The reason

to do this is to bridge the viscous sub-layer so that the number of cells in the neighbourhood of the fixed wall may be decreased considerably compared to a classical no-slip boundary condition. Hence the computation time will be strongly reduced. A disadvantage of this approach is that the law of the wall is only accurate in special situations.
With the log-law-based wall law a turbulent shear stress tangent to the wall τ_w is computed depending on smoothness or roughness of the boundary. The user defines only the roughness or smoothness. A free slip type boundary condition will be used in the following way: $u_n = 0$ and $\sigma^{nt} = \tau_w$
In Section 2.1.6 more information about the wall functions can be found.

2.1.3 Convection-diffusion or transport equations

In addition to the momentum and continuity equations given above, the program can solve several transport equations of the form

$$\frac{\partial c^* T}{\partial t} + \frac{\partial c^* u_j T}{\partial x_j} - \frac{\partial}{\partial x_j}\kappa_{ij}\frac{\partial T}{\partial x_i} + DT = f^* \tag{2.8}$$

It is possible to skip the momentum equations in which case only the transport equations are solved. Hence Deft is also able to solve a stand-alone convection-diffusion equation or even a pure convection or pure diffusion equation.
The coefficients c^*, κ_{ij}, D and f^* may depend on all dependent and independent variables.
For example, we consider the incompressible flow with heat transfer. The energy equation is thus given by

$$\frac{\partial \rho c_p T}{\partial t} + \frac{\partial \rho c_p u_j T}{\partial x_j} - \frac{\partial}{\partial x_j}(\lambda_T + \frac{c_p \mu_t}{\sigma_T})\frac{\partial T}{\partial x_i} = S_T \tag{2.9}$$

Here T is the temperature, c_p is the specific heat capacity at constant pressure, λ_T is the laminar thermal conductivity, μ_t is the turbulent viscosity specified by a two-equation turbulence model (see Section 2.1.5), σ_T is the turbulent Prandtl number as being of the order of 1, and S_T represents energy sources or sinks. In our applications we take $\sigma_T = 2$.

2.1.4 Boundary conditions for the transport equations

The following types of boundary conditions for the scalar T are available in Deft:

Dirichlet boundary condition: This boundary condition means that the unknown T is prescribed at a part of the boundary.

Neumann boundary condition: This boundary condition has the form:

$$\kappa_{ij} n_i \frac{\partial T}{\partial x_j} = h, \tag{2.10}$$

with h given and n_i the i^{th} component of the outward normal.

Mixed or Robbins boundary condition: This boundary condition has the form:

$$gT + \kappa_{ij} n_i \frac{\partial T}{\partial x_j} = h, \tag{2.11}$$

with g and h given.

Thermal boundary conditions may be specified in terms of temperature or heat flux.

2.1.5 Turbulence models

In modeling the flow a turbulence model may be used if this seems appropriate. Turbulence modeling capabilities are primarily based on two-equation eddy-viscosity models. These models are based on approximate constitutive laws which predict the unknown Reynolds stress tensor $\rho\overline{u_i' u_j'}$ that appears in the Reynolds-averaged Navier-Stokes equations (2.2), as follows

$$\tau_{ij} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) - \rho\overline{u_i' u_j'} \tag{2.12}$$

Through the introduction of an eddy-viscosity μ_t these models relate the Reynolds stresses to mean flow variables and to the turbulent velocity and length scales. Based on series-expansion arguments, a general relationship between stresses and mean strains can be written as

$$\begin{aligned} -\rho\overline{u_i' u_j'} \quad = \quad & -\frac{2}{3}\rho k\delta_{ij} + 2\mu_t s_{ij} - \frac{4\mu_t^2}{\rho c_\mu k}[c_{\tau 1}(s_{ik}s_{kj} - \frac{1}{3}s_{kl}s_{kl}\delta_{ij}) \\ & + c_{\tau 2}(\omega_{ik}s_{kj} + \omega_{jk}s_{ki}) + c_{\tau 3}(\omega_{ik}\omega_{jk} - \frac{1}{3}\omega_{kl}\omega_{kl}\delta_{ij})] \end{aligned} \tag{2.13}$$

where k is the turbulent kinetic energy, s_{ij} and ω_{ij} are the mean rate of strain and rotation tensors, viz.,

$$s_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}), \quad \omega_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}) \tag{2.14}$$

Both k and μ_t are predicted from the solution of two semi-empirical transport equations for two turbulence quantities to be presented later. Note that the constitutive relation (2.13) includes terms up to quadratic order in the velocity gradient. The common approach is to determine the closure coefficients c_μ, $c_{\tau 1}$, $c_{\tau 2}$ and $c_{\tau 3}$ so that agreement is achieved with a simple shear flow and with one other difficult class of flow. Several researchers have proposed anisotropic eddy-viscosity formulations, which can be cast into (2.13). These are summarized in Table 2.1.1.

The turbulent viscosity μ_t must be specified by the two-equation model. At the moment four types of two-equation models are dealt with: the standard $k-\varepsilon$ model [24], the RNG based $k-\varepsilon$ model [64], the extended $k-\varepsilon$ model [9] and the Wilcox's k-ω model [63]. All these models use transport equations for both

Model	c_μ	$c_{\tau 1}$	$c_{\tau 2}$	$c_{\tau 3}$	Approach
Boussinesq	0.09	0	0	0	Analog of Stokes' viscosity law (isotropic) [23]
Speziale Yoshizawa	0.09	0.1512	0.1512	0	Asymptotic expansion DIA technique [46]
Rubinstein-Barton	0.085	0.68	0.14	-0.56	RNG theory of Yakhot and Orszag [35]
Nisizima-Yoshizawa	0.09	-0.7881	0.1769	1.0675	Kraichnan's DIA technique [29]
Myong-Kasagi	0.09	0.275	0.2375	0.05	Relation from processes in high-Re k-budget [28]

Table 2.1.1: Numerical values of closure constants in stress-strain relation.

k and ε or ω, as follows

k-ε type model

$$\mu_t = \rho c_\mu \frac{k^2}{\varepsilon} \tag{2.15}$$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j k) - \frac{\partial}{\partial x_j}(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j} = P_k - \rho\varepsilon \tag{2.16}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j \varepsilon) - \frac{\partial}{\partial x_j}(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_j} = \frac{\varepsilon}{k}(c_{\varepsilon 1} P_k - c_{\varepsilon 2}\rho\varepsilon) \tag{2.17}$$

Wilcox's k-ω model

$$\mu_t = \rho \frac{k}{\omega} \tag{2.18}$$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j k) - \frac{\partial}{\partial x_j}(\mu + \sigma^* \mu_t)\frac{\partial k}{\partial x_j} = P_k - \beta^* \rho k \omega \tag{2.19}$$

$$\frac{\partial \rho \omega}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j \omega) - \frac{\partial}{\partial x_j}(\mu + \sigma \mu_t)\frac{\partial \omega}{\partial x_j} = \frac{\omega}{k}(\alpha P_k - \beta \rho k \omega) \tag{2.20}$$

Here ε stands for the dissipation rate of turbulent energy, ω is the ratio of dissipation to turbulent energy ($\equiv \varepsilon/k$) and P_k is the production rate of turbulent energy given by

$$P_k = -\rho \overline{u_i' u_j'} \frac{\partial u_i}{\partial x_j} \tag{2.21}$$

Using the Boussinesq eddy-viscosity approximation, we obtain

$$P_k = \mu_t S^2 \tag{2.22}$$

where $S = (2 s_{ij} s_{ij})^{\frac{1}{2}}$ is the magnitude of the mean rate of strain. In a stagnation flow, the very high levels of S produce excessive levels of turbulent energy

whereas deformation near stagnation point is nearly irrotational. Defining the magnitude of the mean rotation as $\Omega = (2\omega_{ij}\omega_{ij})^{\frac{1}{2}}$ and replacing (2.22) by

$$P_k = \mu_t S\Omega \tag{2.23}$$

leads to a marked reduction in energy production near the stagnation point, while having no effect in a simple shear flow [20]. In [8] a hybrid form is proposed in which (2.22) and Kato-Launder correction (2.23) are averaged:

$$P_k = \mu_t S((1-\alpha)S + \alpha\Omega) \tag{2.24}$$

with $0 \leq \alpha \leq 1$ a weight factor. This hybrid model is particularly used for stagnation flows. In that case the weight factor is chosen to be $\alpha = 0.85$, as recommended by [8].

The models contain some closure constants which are given as follows:

the standard k-ε model

$$c_\mu = 0.09, \quad c_{\varepsilon 1} = 1.44, \quad c_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3 \tag{2.25}$$

the RNG k-ε model

$$c_\mu = 0.085, \quad c_{\varepsilon 1} = 1.42 - \frac{\eta(1-\eta/\eta_0)}{1+\gamma\eta^3}, \quad c_{\varepsilon 2} = 1.68, \quad \sigma_k = 0.7179, \quad \sigma_\varepsilon = 0.7179 \tag{2.26}$$

the extended k-ε model

$$c_\mu = 0.09, \quad c_{\varepsilon 1} = 1.35 + c_{\varepsilon 3} c_\mu \eta^2, \quad c_{\varepsilon 2} = 1.9, \quad c_{\varepsilon 3} = 0.05, \quad \sigma_k = 0.75, \quad \sigma_\varepsilon = 1.15 \tag{2.27}$$

the k-ω model

$$\alpha = \frac{5}{9}, \quad \beta = \frac{3}{40}, \quad \beta^* = \frac{9}{100}, \quad \sigma = \frac{1}{2}, \quad \sigma^* = \frac{1}{2} \tag{2.28}$$

with

$$\eta = \frac{Sk}{\varepsilon}, \quad \eta_0 = 4.38 \text{ and } \gamma = 0.012 \tag{2.29}$$

The extended model in Deft employs slightly revised values for coefficients $c_{\varepsilon 1}$ and $c_{\varepsilon 3}$. Chen and Kim [9] recommended $c_{\varepsilon 1} = 1.15$ and $c_{\varepsilon 3} = 0.25$ which produce significantly wrong solutions over a wide range of flows. In [17], it was reported that this model give consistently better results, when $c_{\varepsilon 1} = 1.35$ and $c_{\varepsilon 3} = 0.05$.

The treatment of the wall is a crucial point when calculating turbulent flows. For most applications the use of wall functions is sufficient for reproducing the impact of the wall on the flow. This will be described in Section 2.1.6. Nevertheless, some flow problems need a more accurate treatment, especially when heat or mass transfer is involved. In such cases, viscous effects must be accurately represented, and Section 2.1.7 will discuss commonly used low-Reynolds-number corrections.

2.1.6 Wall function method

Near a solid wall, wall functions use empirical laws, to circumvent the inability of the k-ε model to predict a logarithmic velocity profile near a wall [24]. An important advantage of wall functions is that they allow inclusion of empirical information for special cases, such as, for example, wall roughness. For a rough wall, the wall shear stress τ_w is computed as follows:

$$\tau_w = \frac{\rho c_\mu^{1/4} \kappa \sqrt{k_{\mathrm{P}}}}{\ln(E_r Y_{\mathrm{P}}/h_{\mathrm{R}})} \boldsymbol{u} \cdot \boldsymbol{t}_{\mathrm{P}} \quad \text{if } h_{\mathrm{R}}^+ \equiv \frac{\rho c_\mu^{1/4} \sqrt{k_{\mathrm{P}}} h_{\mathrm{R}}}{\mu} > 11.6. \tag{2.30}$$

The subscript P denotes the grid point in the center of the wall-adjacent control volumes, which is assumed to be located in the log-law region, Y is the distance perpendicular to the wall, h_{R} denotes the average height of roughness elements, $\boldsymbol{u} \cdot \boldsymbol{t}$ is the tangential velocity along the wall, κ is the Von Kármán constant (approximately equal to 0.4) and E_r is a roughness parameter. For a very rough wall E_r should be approximately 30, as recommended by Schlichting [37]. For $h_{\mathrm{R}}^+ < 11.6$ the wall is considered to be smooth. In that case, wall functions for a smooth wall, as explained in [24], can be employed:

$$\tau_w = \frac{\rho c_\mu^{1/4} \kappa \sqrt{k_{\mathrm{P}}}}{\ln(E Y_{\mathrm{P}}^+)} \boldsymbol{u} \cdot \boldsymbol{t}_{\mathrm{P}} \quad \text{with } Y_{\mathrm{P}}^+ = \frac{\rho c_\mu^{1/4} Y_{\mathrm{P}} \sqrt{k_{\mathrm{P}}}}{\mu} \text{ and } E = 9.0. \tag{2.31}$$

The location of the cell center away from the wall must be such that $Y_{\mathrm{P}}^+ > 11.6$ for the wall law (2.31) to be valid. Otherwise, it is calculated from the viscous sublayer profile:

$$\tau_w = \frac{\mu}{Y_{\mathrm{P}}} \boldsymbol{u} \cdot \boldsymbol{t}_{\mathrm{P}} \tag{2.32}$$

The rapid variation of turbulence quantities also necessitates special measures in evaluating the production and dissipation rates of turbulent kinetic energy near the wall. The average production and dissipation rates used in the near-wall cells have the following form:

$$\overline{P}_k = \tau_w \frac{\boldsymbol{u} \cdot \boldsymbol{t}_{\mathrm{P}}}{Y_{\mathrm{P}}}, \tag{2.33}$$

$$\overline{\varepsilon} = \begin{cases} c_\mu^{3/4} k_{\mathrm{P}}^{3/2} \frac{Y_{\mathrm{P}}^+}{Y_{\mathrm{P}}}, & Y_{\mathrm{P}}^+ < 11.6 \text{ and } h_{\mathrm{R}}^+ < 11.6 \\ c_\mu^{3/4} k_{\mathrm{P}}^{3/2} \frac{\ln(E Y_{\mathrm{P}}^+)}{\kappa Y_{\mathrm{P}}}, & Y_{\mathrm{P}}^+ > 11.6 \text{ and } h_{\mathrm{R}}^+ < 11.6 \\ c_\mu^{3/4} k_{\mathrm{P}}^{3/2} \frac{\ln(E_r Y_{\mathrm{P}}/h_{\mathrm{R}})}{\kappa Y_{\mathrm{P}}}, & h_{\mathrm{R}}^+ > 11.6. \end{cases} \tag{2.34}$$

These expressions replace P_k and ε, respectively, which are source terms in the standard form of the equation for turbulent energy (2.16). Finally, the flux of turbulent energy through the wall is set to zero and the value of ε at the first grid point away from the wall is determined from

$$\varepsilon_{\mathrm{P}} = \frac{c_\mu^{3/4} k_{\mathrm{P}}^{3/2}}{\kappa Y_{\mathrm{P}}}. \tag{2.35}$$

Wall functions provide also the means of modeling the near-wall region for the temperature. The heat flux q at smooth walls is computed as follows ([24]):

$$q_w = \frac{\rho c_p c_\mu^{1/4} \kappa \sqrt{k_{\text{P}}}}{\sigma_T \ln(E Y_{\text{P}}^+)} (T_{\text{P}} - T_w) \quad \text{if } Y_{\text{P}}^+ > 11.6 \tag{2.36}$$

Here T_w is the temperature at the wall. In the viscous sublayer, we have

$$q_w = -\lambda_T n_j \frac{\partial T}{\partial x_j} \approx \lambda_T \frac{T_{\text{P}} - T_w}{Y_{\text{P}}} \tag{2.37}$$

2.1.7 Low-Reynolds-number modeling

Thus far, the turbulence models we have considered are restricted to high-Reynolds number applications, except the Wilcox's k-ω model. This means that they cannot be applied in the near-wall viscous-dominated regions. Many researchers have attempted to devise viscous corrections for the k-ε model to permit its integration through the viscous sublayer [34]. It is well known that a low-Reynolds-number approach imposes a very fine mesh normal to the wall, which can be prohibitive when dealing with large 3D applications.

When the low-Reynolds-number k-ε model is used the values of the closure constants c_μ, $c_{\varepsilon 1}$, $c_{\varepsilon 2}$, σ_k and σ_ε remain the same and the viscous damping functions are introduced into the constants, as follows:

$$c_\mu \leftarrow f_\mu c_\mu, \quad c_{\varepsilon 1} \leftarrow f_1 c_{\varepsilon 1}, \quad c_{\varepsilon 2} \leftarrow f_2 c_{\varepsilon 2} \tag{2.38}$$

The damping functions are chosen according to the model proposed by Lam and Bremhorst [22]:

$$f_\mu = (1 - e^{-0.0165 R_y})^2 \, (1 + \frac{20.5}{Re_T}) \tag{2.39}$$

$$f_1 = 1 + (\frac{0.05}{f_\mu})^3 \tag{2.40}$$

$$f_2 = 1 - e^{-Re_T^2} \tag{2.41}$$

with

$$R_y = \frac{\rho \sqrt{k} Y}{\mu}, \quad Re_T = \frac{\rho k^2}{\varepsilon \mu} \tag{2.42}$$

the local and turbulent Reynolds numbers, respectively. Boundary conditions for the momentum, k and ε equations are $\boldsymbol{u} = 0$, $k = 0$ and $n_j \partial \varepsilon / \partial x_j = 0$, respectively.

In the case of k-ω model, standard boundary conditions must be employed at a solid wall, i.e. for the momentum equations noslip conditions are imposed on the boundary, whereas for turbulent energy k a homogeneous Dirichlet condition holds (in order to avoid non-positive values of k, $k = 10^{-8}$ may be taken as

boundary condition on the wall). Due to the singular behaviour of ω at the wall, a special boundary condition for ω must be used, which is given by

$$\omega = \frac{N_\omega \nu}{Y_{\text{P}}^2}, \qquad Y_{\text{P}}^+ < 5.0, \tag{2.43}$$

where

$$N_\omega = \begin{cases} 6/\beta, & \text{without viscous corrections} \\ \\ 2/\beta^*, & \text{with viscous corrections.} \end{cases} \tag{2.44}$$

Even without viscous corrections the k-ω model correctly calculates the law-of-the-wall. Viscous corrections are needed in this model to predict the sharp peak of turbulent energy close to the wall accurately. More details can be found in [63].

2.1.8 Equation of state

For a compressible flow it is necessary to define the relation between density and pressure. This relation is known as equation of state.
For a perfect gas this equation is defined as:

$$\rho = \frac{\gamma}{\gamma - 1} \frac{p}{h}, \tag{2.45}$$

with p the pressure, h the enthalpy and γ the specific heat ratio.

2.1.9 Enthalpy equation

The energy equation for compressible flow is formulated in terms of the enthalpy by:

$$\frac{\partial h}{\partial t} + u_j \frac{\partial h}{\partial x_j} = -(\gamma - 1) h \frac{\partial u_j}{\partial x_j} \tag{2.46}$$

with u the Cartesian velocity, h the enthalpy and γ the specific heat ratio.
Mark that a non-conservative form for the energy equation is used. This form is used to get a greater efficiency in the pressure correction time stepping scheme. It could be replaced by a conservative form.

2.2 Discretization

In order to solve the momentum and transport equations a discretization procedure must be applied. We distinguish between the time integration and the space discretization. Besides that the incompressibility condition imposes extra problems with respect to the solution.
In Section 2.3 the time integration is treated, Section 2.4 deals with the incompressibility condition.
Compressible flows are computed by an adapted pressure correction scheme, see

Section 2.5

Space discretization is accomplished by a boundary-fitted finite volume method. A staggered grid arrangement is used. A collocated grid arrangement is available for incompressible laminar flows. The staggered arrangement means that not all unknowns are positioned in the same points, whereas the cell-center collocated arrangement means that all the unknowns are located in the same points. Both arrangements (staggering or non-staggering) introduce extra complications, but that is of no concern to the user. The output will always contain interpolated values in the vertices of the cells. Furthermore function subroutines for boundary conditions, coefficients and initial conditions are constructed such that the user has to evaluate these quantities only in certain points, without knowing what type of points it concerns. The mathematical details with respect to the discretization can be found in the Mathematical Manual [38].

Before we discretize the equations we need a grid. In Deft we restrict ourselves to so-called structured grids. For a structured grid the region must be mapped onto a rectangle (R^2) or a hexahedron (R^3). As a consequence each two-dimensional region must have four "sides" and each three-dimensional region have six "faces". The grid must be constructed such that it is a regular grid in the mapped region. Hence in R^2 the mapped grid consists of straight cells, nx in the x-direction and ny in the y-direction. A typical example of such a mapping is shown in Figure 2.2.1.

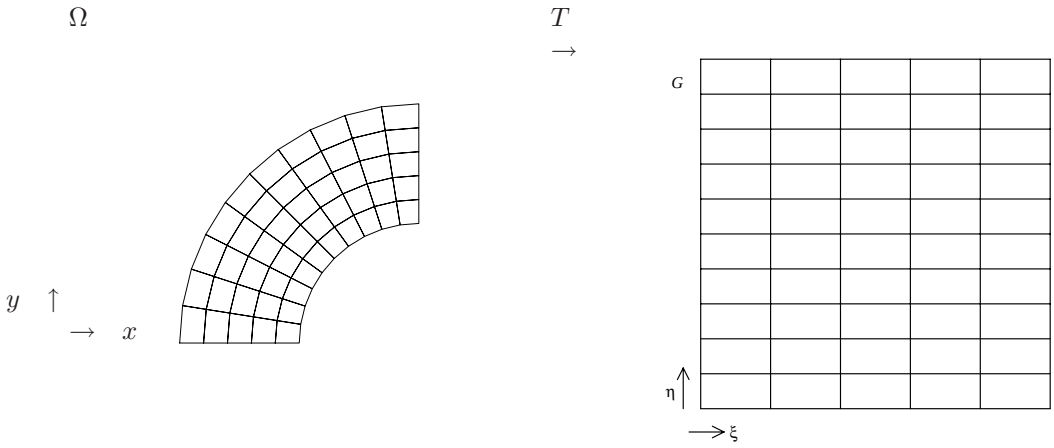


Figure 2.2.1: Boundary fitted co-ordinates and computational grid

A region that is mapped onto one such a rectangular domain will be called a block. Of course in practical problems the regions are often too complex to map onto one single block. In that case it is necessary to subdivide the domain into sub domains each of which can be mapped on a single block. Such an ensemble of blocks will be called a multi block configuration.
At this moment there is one restriction on the blocks in a multi block domain

and that is that grid lines in adjacent blocks must be continuous across block boundaries. Hence a grid line at the common boundary must be present in both blocks and intersect the boundary in one point. Figure 2.2.2 shows a subdivision of a domain in six blocks, the corresponding grid is given in Figure 2.2.3.

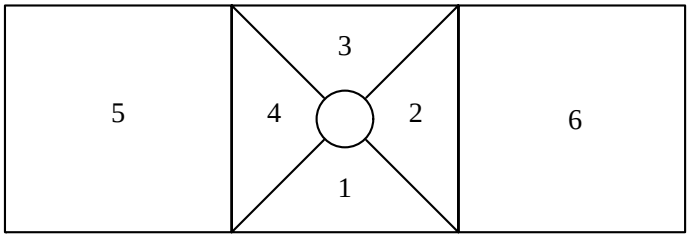


Figure 2.2.2: Decomposition of region into 6 blocks

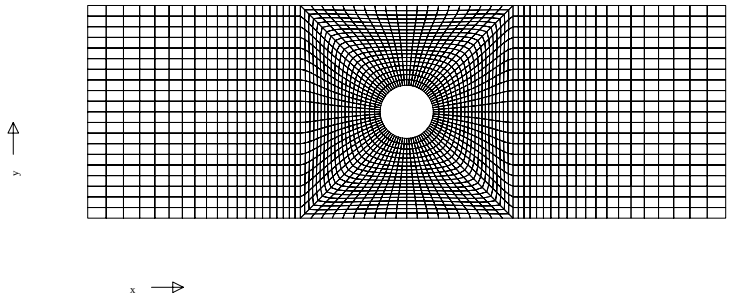


Figure 2.2.3: grid in multi block region

Once the grid has been defined, the finite volume method must be applied. The equations are discretized in the computational domain. Since the curved region has been mapped, the equations in the computational domain are complicated and the discretization is far from trivial. In this case there are several possibilities:

- The classical discretization, which is also the default discretization, is the discretization described in report 91-09 [51].

- Since the classical discretization is only applicable for fairly smooth grids an improved scheme has been developed by Wesseling and van Beek [48]. This scheme is more complicated but it is able to discretize the equations at rather non-smooth grids.

- Two schemes are available with a collocated arrangement of the unknowns (See [38]).The first one (see section 5.2), corresponding to the keyword discr_method=wesbeek naturally derives from the scheme developed by Wesseling and van Beek and the second one (see section 5.2) corresponding to the keyword discr_method=bilinear_interpolation, lays on an improvement of the previous method. It is based on bilinear interpolation.

All discretization schemes may be chosen by the user.

2.2.1 Restriction for the collocated scheme based on bilinear interpolation

In case of the collocated scheme improved by bilinear interpolation, quantities at the face center of the control volumes are given by bilinear interpolation. The bilinear function is built from quantities at the cell centers. Consider the $(1,0)$-face in Figure 2.2.4. To keep a compact nine-point molecule, we assume that $(1,0)$ is surrounded by the polygons defined by $(0,0)$, $(0,\pm 2)$, $(2,\pm 2)$, $(2,0)$. But that is not always possible (See Figure 2.2.4). Sometimes the grid is so skewed that point $(1,0)$ is lying in a polygon containing other centroids. In that case, the discretization is incorrect. A solution to remedy this problem is to refine the mesh.

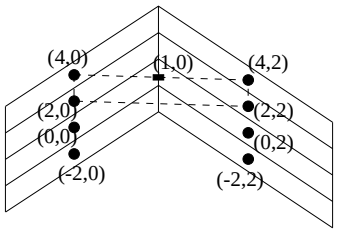


Figure 2.2.4: Configuration where $(1,0)$ is not surrounded by $(0,0)$, $(0,\pm 2)$, $(2,\pm 2)$, $(2,0)$

2.2.2 Upwind schemes

The finite volume method applied, may be considered as a type of central difference scheme. This implies that for convection-dominated flows it is possible

that wiggles in the solution arise. This is especially the case for the convection-diffusion equations, where the ratio convection/diffusion may be very large. In that case upwind discretization may be necessary. In fact in case of turbulence it is hardly possible to solve the turbulence transport equations without applying upwind discretization.

At this moment, four types of upwind schemes are implemented:

- the standard first order upwind scheme
- a hybrid central/upwind scheme
- higher order upwind schemes obtained with the κ-formulation
- TVD schemes with several classes of flux limiters:
  - Sweby Φ-limiter
  - R-κ limiter
  - MR-κ limiter
  - symmetric rational limiter
  - PL-κ limiter
  - MPL1-κ limiter
  - MPL2-κ limiter
  - symmetric PL-κ limiter

All upwind schemes are applied in each computational direction. Hence no stream line upwinding is used.
A short explanation and references of these schemes will be given below.

The standard first order upwind scheme This scheme is first order accurate, but it is unconditionally monotone. Details can be found in [44]. In skewed grids, the scheme generally produces numerical cross-flow diffusion, which may result in a large error in the solution.

A hybrid central/upwind scheme In an effort to combine the advantages of both central and first order upwind schemes Patankar and Spalding [33] have proposed a hybrid form of these schemes, which is based on the mesh-Péclet number, i.e. central differencing is employed for low Péclet and otherwise first order upwind differencing.

Higher order upwind schemes Using the so-called κ-formulation of Van Leer [53], it is possible to derive a higher order upwind scheme. Assuming that the velocity u_e as given in Figure 2.2.5 is positive, a general form of such a scheme may be written as

$$T_e = T_{\mathrm{C}} + \frac{1}{4}[(1+\kappa)(T_{\mathrm{E}} - T_{\mathrm{C}}) + (1-\kappa)(T_{\mathrm{C}} - T_{\mathrm{W}})] \tag{2.47}$$

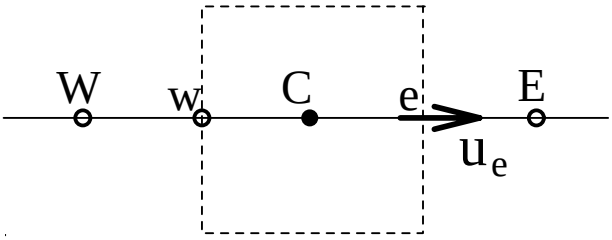


Figure 2.2.5: One-dimensional finite volume used to formulate the κ-scheme

where T is the unknown variable (both velocity components and scalars), the parameter $-1 \leq \kappa \leq 1$ indicates a specified scheme. The following often employed schemes can be obtained by setting κ as follows:

$$\kappa = -1 \rightarrow \text{one-sided linear upwind difference scheme (LUDS)} \tag{2.48}$$

$$\kappa = 0 \rightarrow \text{Fromm's scheme} \tag{2.49}$$

$$\kappa = \frac{1}{3} \rightarrow \text{Cubic upwind interpolation scheme (CUI)} \tag{2.50}$$

$$\kappa = \frac{1}{2} \rightarrow \text{QUICK} \tag{2.51}$$

$$\kappa = 1 \rightarrow \text{Central differencing scheme (CDS)} \tag{2.52}$$

For $\kappa \neq \frac{1}{3}$ the local truncation error is of second order and for $\kappa = \frac{1}{3}$ it is of third order.

TVD schemes All higher order schemes mentioned above are not monotone, i.e. they can give rise to un-physical numerical oscillations. To avoid non-monotone behaviour of the solution, a flux-limiting approach is employed [47]:

$$T_e = T_{\mathrm{C}} + \frac{1}{2}\Psi(r_e)(T_{\mathrm{C}} - T_{\mathrm{W}}) \tag{2.53}$$

with flux limiter Ψ. The limiter argument r_e is the upwind ratio of consecutive solution gradients:

$$r_e = \frac{T_{\mathrm{E}} - T_{\mathrm{C}}}{T_{\mathrm{C}} - T_{\mathrm{W}}} \tag{2.54}$$

Note that for $\Psi = 0$ the first order upwind scheme is recovered. Furthermore, the κ-scheme (2.47) is implemented in the flux-limiting form, i.e.,

$$\Psi_\kappa(r) = \frac{1}{2}(1+\kappa)r + \frac{1}{2}(1-\kappa) \tag{2.55}$$

Since no linear convection scheme of higher order accuracy can be monotone, nonlinear schemes or limiters should be employed for obtaining wiggle-free results, provided that

$$0 \leq \Psi(r) \leq \min(2r, M) \tag{2.56}$$

where $M \geq 1$ is a parameter that controls the resolution of sharp gradients, i.e. with a large value of M more accuracy near steep gradients can be obtained. The following classes of limiters are generalizations of the κ-scheme (2.55).

The so-called piecewise linear κ-based (PL-κ) class of limiters, proposed in [62], has been implemented:

$$\Psi_{\kappa,\mathrm{M},\alpha}(r) = \max[0,\, \min(M,\, \frac{1}{2}(1+\kappa)r + \frac{1}{2}(1-\kappa),\, (2+\alpha)r)], \quad M \geq 1,\; -1 \leq \alpha \leq 0 \tag{2.57}$$

The parameter α controls $\Psi'(0)$ and hence the amount of down-winding. This class brings together a number of flux limiters known in the literature. The Davis' limiter used in [1] is a member of the PL-κ class with the parameters $\kappa = -1$, $\alpha = 0$ and $M = 1$ and is identical to the BSOU scheme developed in [31]. The parameters $\kappa = \alpha = 0$, $M = 2$ give a scheme which was used by Van Leer in his MUSCL approach [52]. For $\kappa = \frac{1}{3}$, $\alpha = 0$ and $M = 2$ one obtains the so-called limited $\kappa = \frac{1}{3}$-scheme proposed by Koren [21]. The SMART scheme presented in [16] is obtained with $\kappa = \frac{1}{2}$, $M = 4$ and $\alpha = 0$. By taking $\kappa = 1$, $\alpha = -1$, $1 \leq M \leq 2$ the Chakravarthy-Osher limiter is recovered, discussed, for example, in [47] and [1], which also contains the Minmod limiter ($M = 1$) or SOUCUP scheme proposed in [66].

Another piecewise linear class is the symmetric PL-κ limiter presented in [62], that satisfies the symmetry condition $\Psi(r) = r\Psi(1/r)$:

$$\Psi_{\kappa,\mathrm{M}}(r) = \max[0,\, \min(M,\, \frac{1}{2}(1+\kappa)r + \frac{1}{2}(1-\kappa),\, \frac{1}{2}(1-\kappa)r + \frac{1}{2}(1+\kappa),\, Mr)] \tag{2.58}$$

of which UMIST [25] ($\kappa = \frac{1}{2}, M = 2$) and MUSCL ($\kappa = 0, M = 2$) are special ones. Here $1 \leq M \leq 2$.

In [70], it has been shown that the necessary and sufficient condition for second order accuracy at smooth extrema is

$$3\Psi(\frac{1}{3}) - \Psi(-1) = 2 \tag{2.59}$$

provided that such extrema are located at cell centers. In the same paper, two modifications of (2.57) have been proposed, which satisfy (2.59) and thus enhance the accuracy of the numerical solution. The first modified class, called the MPL1-κ limiter, is given by

$$\Psi_{\kappa,\mathrm{M},\alpha}(r) = \max[0,\, \min(2r, \frac{2}{3}),\, \min(M,\, \frac{1}{2}(1+\kappa)r + \frac{1}{2}(1-\kappa),\, (2+\alpha)r)] \tag{2.60}$$

where $M \geq 1$ and $-1 \leq \alpha \leq 0$. Observe that (2.60) and (2.57) are equivalent if $-1 \leq \kappa \leq 0$ and $\alpha = 0$. The other modified class, to be referred to as MPL2-κ class, obeys the so-called Spekreijse's monotonicity restriction [45]:

$$\exists\, \beta \in [-2, 0],\, \exists\, M > 0, \forall r \in I\!R: \quad \beta \leq \Psi(r) \leq M \quad \text{and} \quad -M \leq \frac{\Psi(r)}{r} \leq 2 + \beta \tag{2.61}$$

which is a less restrictive sufficient condition than (2.56) for a flux-limiting scheme (2.53) to be TVD. The modified limiter reads:

$$\Psi_{\kappa,\mathrm{M},\alpha}(r) = \max[0,\, \min(M,\, \frac{1}{2}(1+\kappa)r + \frac{1}{2}(1-\kappa),\, (2+\alpha)r)] + \min[0,\, \max(\alpha,\, -\alpha r)] \tag{2.62}$$

where $M \geq 1$ and $\alpha \in [-1, -\kappa] \cap [-1, 0]$. Clearly, the case with parameters $-1 \leq \kappa \leq 0$ and $\alpha = 0$ is identical to (2.60).

A class of piecewise linear limiters commonly used in the literature [47] is

$$\Psi_{\Phi}(r) = \max[\,0,\, \min(\Phi r,\, 1),\, \min(r,\, \Phi)\,], \quad 1 \leq \Phi \leq 2 \tag{2.63}$$

This so-called Sweby Φ-limiter class is not κ-dependent. Special members are Minmod ($\Phi = 1$) and Superbee ($\Phi = 2$) limiters.

The classes of limiters presented so far are piecewise linear. The next two classes of limiters are the so-called rational κ-based (R-κ) limiters which are more smooth. The R-κ limiter is given by

$$\Psi_{\kappa}(r) = \begin{cases} (r + |r|)\,(-r^2 + (3+\kappa)r - \kappa)/(1+r)^2, & r \leq 1, \;\; -1 \leq \kappa < 0 \\ ((2+\kappa)r - \kappa)/(1+r), & r \geq 1, \;\; -1 \leq \kappa < 0 \\ (r + |r|)\,((1+\kappa)r + 1 - \kappa)/(1+r)^2, & 0 \leq \kappa \leq 1 \end{cases} \tag{2.64}$$

and has been proposed in [68, 70]. For $\kappa = 0$ in (2.64) the resulting scheme is identical to the Van Leer's Harmonic limiter, discussed, for example, in [18], and to HLPA [65]. With $\kappa = \frac{1}{2}$ the ISNAS limiter, as presented in [69], is obtained which is identical to NOTABLE [32]. An alternative is the MR-κ limiter that may improve the accuracy of the numerical solution, by making use of condition (2.59), and is given by

$$\Psi_{\kappa}(r) = \begin{cases} r + |r|, & r \leq \frac{1}{3} \\ ((8+9\kappa)r^2 + (2-12\kappa)r + 2 + 3\kappa)/(3(1+r)^2), & \frac{1}{3} \leq r \leq 1, \;\; -1 \leq \kappa \leq 1 \\ ((2+\kappa)r - \kappa)/(1+r), & r \geq 1, \;\; -1 \leq \kappa < 0 \\ ((8+9\kappa)r^2 + (2-12\kappa)r + 2 + 3\kappa)/(3(1+r)^2), & r \geq 1, \;\; 0 \leq \kappa \leq 1 \end{cases} \tag{2.65}$$

A class of symmetric rational limiters that satisfy the monotonicity requirements (2.61) has been proposed in [62]:

$$\Psi_{\mathrm{M}}(r) = M\frac{r^2 + r}{r^2 + (M-1)r + 1}, \quad 1 \leq M \leq \frac{3}{2} \tag{2.66}$$

$M = 1$ recovers the Van Albada limiter, discussed, for example, in [18], and $M = \frac{3}{2}$ gives the OSPRE limiter, recently proposed in [62].

In conclusion, all limiters mentioned above are nonlinear. Therefore, a limited scheme is implemented in a defect correction manner:

$$\phi_{i+1/2} = \phi^{\text{LOS}}_{i+1/2} + (\phi^{\text{HOS}}_{i+1/2} - \phi^{\text{LOS}}_{i+1/2})^o \tag{2.67}$$

where $\phi^{\text{LOS}}_{i+1/2}$ stands for the approximation by a lower order scheme, for example, first order upwind, and $\phi^{\text{HOS}}_{i+1/2}$ is the higher order approximation. The term in brackets is evaluated explicitly using the values from the previous time step, which is indicated by the superscript 'o'.

2.3 Time integration

Since the equations to be solved are time-dependent it is necessary to use some time-integration scheme. Deft allows for three integration schemes, all of them based on the so-called θ method.

Suppose one wants to solve the ordinary differential equation:

$$\frac{dc}{dt} = f(x,t), \tag{2.68}$$

then the θ method can be written as:

$$\frac{c^{n+1} - c^n}{\Delta t} = \theta f(x, t^{n+1}) + (1-\theta) f(x, t^n) \tag{2.69}$$

where n denotes the time level and Δt the time-step. θ must be chosen in the range $0 \leq \theta \leq 1$.
For $\theta = 0$ the method reduces to the classical explicit Euler method, for $\theta = 1$ to the implicit Euler method. $\theta = \frac{1}{2}$ corresponds to the Crank Nicolson scheme. Explicit methods require a time-step restriction, since the method becomes unstable if the time-step is too large. At this moment $\theta = 0$ has not been implemented. Fully implicit methods ($\theta \geq \frac{1}{2}$), are unconditionally stable and hence any time-step may be used. However, an implicit scheme requires the solution of a system of linear equations at each time-step and as a consequence they are much more expensive per time-step than the explicit schemes.
The Crank Nicolson scheme is second order accurate and is preferred if a time-accurate method is required. However, a clear disadvantage of Crank Nicolson is that high frequency perturbations are not damped. For that reason a transient may be always visible if Crank Nicolson is applied. In order to damp the effect of the transient frequently values of θ greater than 0.5 are used. For example $\theta = 0.55$ is very popular.
The Euler implicit scheme may be less accurate but disturbances are damped very rapidly. Hence, if one is only interested in a stationary solution, this method is the one to use.
A disadvantage of the θ-method is the fixed θ. It could be advantageous to combine a number of different θ's per time step in such a way that second order accuracy is accomplished, and some damping is ensured as well. Two methods

that offer this opportunity are the fractional θ-method and the generalized θ-method. The latter is a generalization of the fractional θ-method, so we will restrict ourselves to the description of the generalized θ-method. We rewrite equation (2.69) as follows, letting $\Sigma_k = \sum_{i=1}^{k} \theta_i$:

$$\begin{aligned}
c^{n+\Sigma_2} &= c^n + \Delta t \left(\theta_1 f(x, t^n) + \theta_2 f(x, t^{n+\Sigma_2})\right) \\
c^{n+\Sigma_4} &= c^{n+\Sigma_2} + \Delta t \left(\theta_3 f(x, t^{n+\Sigma_2}) + \theta_4 f(x, t^{n+\Sigma_4})\right) \\
&\vdots \qquad\qquad \vdots \\
c^{n+\Sigma_{2k}} &= c^{n+\Sigma_{2k-2}} + \Delta t \left(\theta_{2k-1} f(x, t^{n+\Sigma_{2k-2}}) + \theta_{2k} f(x, t^{n+\Sigma_{2k}})\right)
\end{aligned}$$

There are two necessary conditions:

1. $\Sigma_{2k} = 1$ for a k-stage method. This gives a first order method, and is only a scaling requirement.
2. $\sum_{i=1}^{k} \theta_{2i-1}^2 = \sum_{i=1}^{k} \theta_{2i}^2$ to guarantee second order accuracy.

A third condition is optional, but guarantees some damping:

1. $\theta_{2i-1} = 0$ for at least one $i \in 1, \ldots, k$.

This condition includes at least one Implicit Euler step per time step.

The generalized θ-method is a 3-stage method, and is therefore 3 times as expensive as the Crank-Nicolson method. However, one may choose $\Delta t_{gen\theta} = 3 \cdot \Delta t_{CN}$ to accomplish similar results for both methods. A common choice for the generalized θ-method is the following 'optimum' for $k = 3$:

$$\begin{aligned}
\theta_1 = \theta_5 = \frac{\alpha}{2}, \quad \theta_3 = 0, \\
\theta_2 = \theta_6 = \alpha\frac{\sqrt{3}}{6}, \quad \theta_4 = \alpha\tfrac{\sqrt{3}}{3} \\
\alpha = \left(1 + \frac{2}{\sqrt{3}}\right)^{-1}.
\end{aligned}$$

A common choice for the fractional θ-method is the following:

$$\begin{aligned}
\theta_1 = \theta_5 = \beta\theta, \quad \theta_3 = \alpha(1 - 2\theta), \\
\theta_2 = \theta_6 = \alpha\theta, \quad \theta_4 = \beta(1 - 2\theta), \\
\alpha = \frac{1 - 2\theta}{1 - \theta}, \qquad \beta = \tfrac{\theta}{1-\theta}, \\
\theta = 1 - \frac{1}{2}\sqrt{2}.
\end{aligned}$$

With respect to the solution of the momentum equations coupled with some transport equations and or the turbulence equations, the situation is somewhat

more complex. In our present code we decouple the solution of momentum equations and transport equations. This means that in each time-step we start with the solution of the momentum equations coupled with the continuity equation. If coefficients depend on unknown variables at the new time level, the values at the previous time-level are used. After computing the velocity and pressure, the first transport quantity is computed, then the second and so on. Finally the turbulent quantities first k than ε or ω.
A consequence of this de-coupling is that the stability of the global system may be influenced. So due to the de-coupling it is possible that a smaller time-step may be necessary than one would expect if all equations would be solved simultaneously.

The turbulence equations may act on a much smaller time scale than the momentum equations. If that is the case the time step is limited due to the turbulence equations and a much smaller time step is required than one would need for the momentum equations itself.
In order to avoid a large overhead it is possible to perform a sub-stepping for the turbulence equations. This means that the turbulence equations are solved with a time step that is a fraction of the global time step. This sub-stepping is only implemented in combination with the Euler implicit scheme.

2.4 Aspects with respect to the incompressibility condition

One of the main problems of the incompressibility condition is that the continuity equation does not contain the pressure, where the equation itself is strongly related to the pressure computation. As a consequence the solution of the coupled momentum equations with the continuity equation is in general everything but simple. In fact it is always necessary to take precautions in order to be able to solve the coupled equations.
For time-dependent problems the pressure-correction method is one of the most popular methods to solve the problem with the continuity equation. At this moment it is the only method available in Deft.

Pressure-correction may be considered as type of splitting method. In the first step the velocity is estimated using the pressure at the previous time-level. In the next step the computed velocity is projected onto the space of divergence-free vector fields. In this step a type of Poisson equation for the pressure is solved and the velocity is adapted.

An important aspect of pressure correction is that during the time-stepping algorithm a term of the order of the truncation error in the time-integration scheme is neglected. Practical computations have shown that the time-step should be chosen relatively small if the solution changes rapidly, for example in case of a transient. Although, the pressure-correction method is stable if the

time-integration method is stable, the numerical solution may behave strangely if the gradient of the actual solution in time is large. The consequence is that the time-integration explodes (or the linear solver does not converge). The only remedy to solve this problem is to use small time-steps. However, once the solution becomes smooth in time, much larger time-steps are allowed.

The pressure correction method as described above is applied such that for each time step only one prediction and one correction step is carried out. Usually this is accurate enough, and if not, the time-step should be decreased. However, in some applications, it might be wise to perform more than one iteration per time step. Such an option is available in Deft, see the keyword TIME_INTEGRATION.

2.5 Aspects with respect to compressible flows

In this section certain aspects of the calculation of compressible flow, that require special attention, are explained.

boundary conditions

Care should be taken with the application of boundary conditions for compressible flow to have a well posed problem. We will only give an overview and refer to chapter 19 of [18] for a more elaborate discussion. We can distinguish five cases found in most common applications, where the application of the following boundary conditions leads to a well posed problem:

1. Sub-sonic inflow boundary: momentum, enthalpy prescribed
2. Supersonic inflow boundary: momentum, enthalpy and pressure prescribed
3. Sub-sonic outflow boundary: pressure, Neumann boundary condition for enthalpy prescribed
4. Supersonic outflow boundary: none prescribed
5. Solid wall boundary: freeslip or noslip for momentum, Neumann boundary condition for enthalpy prescribed

Upwind discretization of convective terms

In the case of compressible flow with discontinuities it is essential to use an upwind scheme for the convective terms in the momentum equation to avoid wiggles. This upwind scheme can be applied to m, as it where a convected quantity, or to the product of the quantities U and m as is commonly done in colocated schemes. It is found that the latter option gives better resolution of discontinuities.

Scaling of the unknowns

To be able to solve the equations uniformly in Mach a scaling is applied to the pressure [2]. The pressure in the computational process is effectively the scaled perturbation of the outflow pressure:

$$p = \frac{p^* - p^*_{\text{out}}}{\rho^*_0 w^{*2}_\infty} \tag{2.70}$$

where p^* and p^*_{out} denote the dimensional pressure and outflow pressure respectively and ρ^*_0 and w^*_∞ the stagnation density at the inflow and the velocity at the inflow boundary.

Furthermore all other quantities are non-dimensionalised with respect to the inflow quantities at stagnation condition [2]. These scaled quantities should be specified as boundary and initial conditions:

$$(\rho u)^1_\infty = \left(1 + \frac{\gamma - 1}{2} M^2_\infty\right)^{-\frac{1}{\gamma - 1}} \cos(\alpha_\infty) \tag{2.71}$$

$$(\rho u)^2_\infty = \left(1 + \frac{\gamma - 1}{2} M^2_\infty\right)^{-\frac{1}{\gamma - 1}} \sin(\alpha_\infty) \tag{2.72}$$

$$h_\infty = \left(1 + \frac{\gamma - 1}{2} M^2_\infty\right)^{-1} \tag{2.73}$$

$$p_{\text{out}} = 0 \tag{2.74}$$

$$\text{where} \tag{2.75}$$

$$M_\infty = \text{ Mach number at inflow} \tag{2.76}$$

$$\gamma = \frac{c_p}{c_v} \tag{2.77}$$

$$\alpha_\infty = \text{ angle of inflow with normal at inflow boundary} \tag{2.78}$$

Only for postprocessing purposes a reference pressure, density and velocity can be specified, which will scale the computational values back to the physical ones. If the Mach number is higher than 0.3 in the whole flow domain the scaling can be dropped and all initial and boundary conditions should be specified in a consistent dimensional form.

Density Bias

In the case of high Mach flow, it is essential that in the case of shocks the discretization will respect both the Rankine-Hugoniot jump relations and the entropy condition. The former is achieved by using a conservative discretization. For the latter it is necessary to introduce irreversibility in the flow. In the momentum equation this is accomplished by choosing a (higher order) upwind scheme, in the continuity equation by choosing a form of density upwind bias. In the case of Mach-based density bias, the density is upwinded when the Mach number exceeds 0.9. If the unconditional density bias is chosen, the density

is always upwinded. When a higher order (limited) upwind discretization is applied to the momentum equation, the gradient based density bias should be chosen to achieve second order accuracy away from steep gradients. All types of density bias can be applied in an implicit or explicit manner. When the implicit version is applied, the pressure correction equation becomes more expensive to solve. Hence for steady state calculations the explicit version is the proper choice.

2.6 Stationary problems

At this moment Deft does not contain any special methods to compute stationary solutions. If one wants to solve a time-independent problem, the only way is to solve the instationary Navier-Stokes equations and to choose the final time so large that steady state has been reached. Whether a stationary solution has been reached can be tested in Deft with the following stopping criterion:

$$\|u^{n+1} - u^n\|_{max} \leq \frac{1-\lambda}{\lambda} \left(relacc \|u^{n+1}\|_2 + absacc \right), \tag{2.79}$$

with

$$\lambda = \frac{\|u^{n+1} - u^n\|_2}{\|u^n - u^{n-1}\|_2}.$$

The values of *relacc* (relative accuracy parameter) or *absacc* (absolute accuracy parameter) can be defined by the user, the default value is zero.
It is advised to use the implicit Euler scheme in this case, since this allows for the largest time-steps. Unfortunately the combination with pressure correction may prevent the use of too large time-steps, since the solution may explode in case of a transient. The only way to solve this problem is to start with a small time-step and to enlarge the time-step after some time.

2.7 Linear solvers

After discretization of the incompressible Navier-Stokes equations various systems of linear equations have to be solved: the momentum and pressure equations and if necessary the transport and turbulence equations. In Deft these systems are always solved by iterative solution methods.

The data structure used and the structured grid are very well suited for iterative solution methods of Krylov subspace-type. In order to solve the system $Ax = b$ such a method searches for an element $x_k \in \{b, Ab, ..., A^{(k-1)}b\}$ such that $\|r_k\| = \|b - Ax_k\|$ is minimized in some norm. An attractive feature of these methods is that only matrix vector multiplications and basic linear algebra operations (inner products, vector updates etc.) are used.

If A is symmetric and positive definite, one of the best Krylov subspace methods

is the Conjugate Gradient method. However, all matrices which are used in the Deft package may be non-symmetric. For this class of matrices various Krylov subspace methods are known, where each method is optimal for a certain class of problems. For this reason several Krylov subspace methods are implemented to investigate which method should be used for a certain system.

Section 2.7.1 consists of an overview of the various Krylov subspace methods and their behaviour. In general the solver, which is used as default is robust and efficient. If a better method becomes available the default is changed.

It is well known that the Conjugate Gradient method only works well if a preconditioner is used. A preconditioner is a matrix P such that $P \approx A$ but $P^{-1}b$ is much cheaper to evaluate than $A^{-1}b$. In general P should be such that the number of iterations of the original iteration method decreases considerably. The same observation holds for the other Krylov subspace methods. Therefore various preconditioners are implemented, which are discussed in Section 2.7.2. For background information we refer to [58], [55], [57].

2.7.1 Solvers

The momentum, pressure, transport, and turbulence equations are solved by iterative methods of Krylov subspace-type. Below we give references and properties of the methods implemented.

LSQR [30]
The easiest way to circumvent the non symmetry of the coefficient matrix is to solve the normal equations $A^T Ax = A^T b$ by the Conjugate Gradient method. However this leads in general to an unstable and slow convergent method. LSQR is a stable version of the Conjugate Gradient method applied to the normal equations. For Poisson-like equations (pressure, or diffusion dominated-momentum, -transport, or -turbulence equation), LSQR is in general slow, but for convection dominated equations, which are discretized with central differences, this method can be fast. At this moment only a limited number of preconditioners are available for LSQR.

BI-CGSTAB: Bi-Conjugate Gradient Stabilized [49]
A generalization of the Conjugate Gradient method for non symmetric problems is the Bi-CG method. In this method two sequences of search directions are used, which are bi-orthogonal to each other. In CGS [43] one of these sequences is removed and the rate of convergence is (for many practical) examples two times as fast as Bi-CG. A more stable variant of CGS is the Bi-CGSTAB method proposed by [49]. Both methods are implemented. In general we prefer the Bi-CGSTAB method, so the CGS-method is mainly used for research reasons. An advantage of these methods is that only a limited amount of memory is required, and that no parameters have to be chosen.

GMRES-like methods Another generalization of the Conjugate Gradient method are GMRES-like methods. These methods have the same optimal properties with respect to the norm of the residual as the Conjugate Gradient method. However, due to the non-symmetry of the matrices all previous search directions should be stored in memory.

GMRES: Generalized Minimal Residual [36]
The first method in this class is the original GMRES method. Since the amount of memory increases linearly with the number of iterations it is necessary to stop the method after some iterations (in the sequel we call this number the restart value), form the approximate solution and restart the GMRES method. If the number of iterations is less than the restart value, GMRES is a very robust method. When the method is restarted, it can lose its fast convergence behaviour. A drawback is that the convergence depends critically on the restart value, so choosing the restart value too small leads to non convergence of GMRES.

GCR: Generalized Conjugate Residuals [14]
GCR is mathematically equivalent with GMRES. However, when unrestarted, it uses more memory than GMRES. If restarting is necessary it is possible to use other techniques (truncation) in GCR, which leads in general to a faster convergence than that of restarted GMRES. This alleviates the main drawback of GMRES.

GMRESR: GMRES-Recursive [50]
This method consists of an inner and an outer loop. The outer loop resembles GCR, whereas originally the inner loop consists of GMRES. Other iterative methods may be used in the inner loop. The properties of GMRESR are between that of GMRES and Bi-CGSTAB. It is a robust method and converges fast without requiring large amounts of memory. Note that GMRESR with GMRES(1) in the inner loop is equal to GCR. Finally this method is not very sensitive to variations in the restart value or the number of iterations in the inner loop. So the default values are reasonable for a wide range of problems.

Directions of use
For robustness the default solver is restarted GMRES for all equations. If the method is not convergent, the most robust choice is unrestarted GMRES. Another way to circumvent non convergence is to enlarge the maximal number of iterations and/or to lower the required accuracy. In many occurrences of non convergence, it appears something is wrong with the boundary conditions, coefficients or the time step used. For the pressure equation it is possible that Bi-CGSTAB is faster and/or uses less memory than the default choice. Finally the stopping criteria for the iterative methods are a compromise between efficiency and accuracy. Decreasing the required accuracy can save a considerable amount of CPU time.

2.7.2 The preconditioners

It appears that Krylov subspace methods are only fast converging when they are combined with a preconditioner. In this section a description is given of the preconditioners that are implemented in the Deft package. The requirements for a preconditioner P are: $P \approx A$ and $P^{-1}b$ is cheap to evaluate. The description starts with a very simple preconditioner P, namely P is the main diagonal of A, and finishes with a complicated preconditioner P which is an incomplete LU decomposition of A.

There are two different ways to use a preconditioner P. Firstly apply the method to

$$P^{-1}Ax = P^{-1}b,$$

which will be called preconditioning, and secondly

$$AP^{-1}y = b, x = P^{-1}y,$$

which will be called postconditioning. The convergence properties of the resulting preconditioned Krylov methods are approximately the same for both choices. However, when preconditioning is used the termination criterion is based on $\|P^{-1}(Ax_k - b)\|_2$, whereas if postconditioning is used the termination criterion is based on $\|Ax_k - b\|_2$. For this reason postconditioning is preferred, because then the termination criterion does not depend on the matrix P. We have observed examples where preconditioning needs less iterations than postconditioning, but the quality of the approximate solution was less than one may expect from the termination criterion. For background information see [58], [55], [57]. Below the implemented pre/postconditioners are specified.

Diagonal
If a diagonal preconditioner is used the matrix P is equal to the main diagonal of the original matrix A.

ILUD
The preconditioner P is an incomplete LU decomposition of the original matrix. Only the diagonal elements are adapted, the other elements of L and U are taken from the original matrix A. There are several methods to compute the diagonal elements. The original ILUD method can be modified (MILUD) in such a way that $Pv = Av$ for $v = [1, 1, ..., 1]^T$. MILUD is fast if the solution x is slowly varying. At this moment we use

$$RILUD = \alpha ILUD + (1 - \alpha)MILUD$$

where α is a given parameter.
The choice preconditioner = RILUD is implemented in the following way: suppose P is given by LL^T, the iterative method is applied to

$$L^{-T}AL^{-1}y = L^{-T}b, \;\; x = AL^{-1}y.$$

This enables us to use the efficient Eisenstat implementation.

ILU
The preconditioner is again an incomplete LU decomposition of the original matrix. Only the non-zero elements of the original matrix are adapted, so L and U have the same sparsity pattern as the original matrix. Again we use

$$RILU = \alpha ILU + (1 - \alpha)MILU$$

where α is a given parameter. This preconditioner cannot be used for the coupled momentum equations.

ILU_fill
This preconditioner consists of an incomplete LU decomposition with fill in. The parameter fill_in gives the number of diagonals allowed to become nonzero. In general the number of iterations decreases when fill_in increases, however every iteration becomes more expensive. For the case that the allowed fill in is equal to the bandwidth a full LU decomposition is made and the method converges in one iteration. This preconditioning can only be used for 2 dimensional problems. It cannot be used for the coupled momentum equations.

Multigrid
The multigrid method is implemented as a preconditioner. This increases its robustness, whereas the extra costs for the Krylov acceleration is negligible. The method consists of a multigrid V-cycle with alternating line Jacobi as smoother. This preconditioner can be used for every number of gridpoints, so it is not necessary that these numbers are multiples of 2. Multigrid preconditioning is not available for the coupled momentum equations.

Directions of use
The default preconditioners are a compromise between efficiency and robustness. For the momentum equations an MILUD preconditioner is used. Although this slightly influences the termination criterion, it is more efficient since we can use the efficient Eisenstat implementation [13]. In the other equations RILU is used as postconditioner. In the pressure equation the optimal choice of α depends on the boundary conditions of the momentum equations. If Dirichlet boundary conditions are used everywhere the default choice $\alpha = 0.975$ is optimal, but if on some parts of the boundary other conditions are used, then choosing α closer to one may lead to a faster convergence. For the transport and turbulence equations MILU postconditioning is the default.
For a large grid-size the multigrid post conditioner can lead to a considerable decrease of CPU time for the pressure equation.

2.8 Multi-block methods

In order to solve the incompressible Navier-Stokes equations on a complicated spatial domain it is a good idea to decompose the domain into a number of

smaller subdomains. The solution on the subdomains depend on each other. It is the task of the multi-block (domain decomposition) method to couple the solutions of the different subdomains in such a way that the correct solution on the whole domain is obtained. This leads to an iterative algorithm that requires the repeated of problems in the subdomains.

The multi-block algorithm is motivated above by geometrical reasons. Other reasons to use a multi-block approach are: parallelization or reduced memory requirements. A number of choices should be made to implement a multi-block algorithm. Below we give more details about the various choices. For background information we refer to [4].

2.8.1 Basic multi-block algorithm

In our algorithm we use non-overlapping blocks. To couple the subdomain solutions we use a Dirichlet-Dirichlet coupling. Special care is needed to handle the staggered arrangement of the unknowns. For the basic algorithm better couplings are available [4, 7]. Since we always combine the algorithm with a Krylov acceleration (where the influence of the coupling conditions is negligible) we have not implemented other coupling conditions.

The multi-block algorithm can be interpreted algebraically as a Block Gauss-Jacobi or Block Gauss-Seidel method. When the Dirichlet boundary conditions are obtained from the previous iteration we have Block Gauss-Jacobi and when the values are copied from one subdomain to another one obtains the Block Gauss-Seidel algorithm. In every multi-block iteration all subdomains are solved by an iterative method. To save CPU time it is a good idea to build the preconditioner only once and reuse it in the following multi-block iterations.

2.8.2 Subdomain solution

Two choices can be made: solve the subdomain problems accurately or inaccurately. When the subdomain problems are solved accurate enough the multi-block iteration can be applied to the interface equations. This leads to a large reduction of the vector lengths. However, this method is sensitive to the required subdomain accuracy. When the accuracy is too low the approximations do not converge to the exact solution.

When the subdomain problems are solved inaccurately the iteration vectors have the same length as the solution vector on the whole domain. In general this choice is robust and more efficient than accurate solution. A special case is the so-called ILU method. Then only one iteration is done per subdomain.

2.8.3 Acceleration method

From many experiments it appears that the basic multi-block algorithm is not robust. In some applications it costs many iterations or does not converge at

all. To enhance this the basic multi-block method is accelerated by a Krylov subspace method: GCR [14, 50, 6]. We choose GCR because this Krylov method can be used in combination with a variable preconditioner (multi-block) [60].

Since the amount of work and memory increases with the number of GCR iterations it is necessary to restart or truncate the method. For truncation we use the Jackson-Robinson technique and by restarting we use an optimized version of GCR [56]. To speed up convergence further it is a good idea to reuse search directions of previous time-steps. For the pressure equation this leads to a large reduction of CPU time [61].

2.8.4 Parallelism

The decomposition of the global domain into subdomains leads in a natural way to a number of problems which can be solved in parallel. A parallel implementation of the accurate multi-block algorithm is presented in [5]. Also a parallel implementation of the inaccurate method is available [15].

To compare the results on one and more computers it is a good idea to use the Block Gauss-Jacobi method also on one processor, otherwise the number of iterations are different. The default (Block Gauss-Seidel) is implemented such that on each processor Block Gauss-Seidel is used, but that of course over the various processors the Block Gauss-Jacobi method is used.

2.9 Restart

In many practical applications it is necessary to write the computed solution to a file for a later restart. Reasons to do this are for example:

- The necessary computation time is so long that it makes sense to save intermediate results in case of an abort.
- The user wants to change the time-integration method, for example he wants to use a different value of θ. A typical example is the flow around a cylinder in which the user wants to start with one time-step Euler implicit in order to suppress the transient and after that wants to resume with a generalized θ-method or with $\theta = 0.5$.
- The user has made a computation with a set of physical constants and wishes to perform the same type of computation with a different set. In that case the solution of the preceding set might be a good initial guess.
- The user has made a computation with a coarse grid and wants to do the same computation on a fine grid. The solution on the coarse grid interpolated to the fine grid may be a nice starting value, improving the convergence considerably.

The Deft program has its own "data-base" to store such set of solutions. Solutions of a specific run may be identified by a so-called session identifier. At this moment this identifier is restricted to an integer number.

Chapter 3

The global structure of an Deft session

In general the Deft session consists of four parts, which can be run separately. The four parts are

- Grid generation
- Pre-processing (reading and translation of the input file)
- Computation (solution of the flow problem)
- Post-processing (output of the results: plots and prints)

The sequence of the session is always:

grid generation followed by
pre-processing followed by
computation followed by
post-processing

In the Sections 3.1, 3.2, 3.3 and 3.4 the various stages are treated separately. The syntax of the input files is described in Section 3.7.

3.1 Grid generation

The first stage of an Deft job is to generate a grid. In that stage the user must decide whether he wants to use a single block approach or if multi block is necessary. Furthermore in the grid generation part it is also necessary to mark boundaries for example by a name or number in order to identify them in the pre-processing part. The reason for this is that boundary conditions must be prescribed at items that are known by some name.

Grid generation may be performed with any available package. However, Deft

requires a special file format to be made by this grid generator and hence some "file translator" may be necessary.

The present version of the Deft incompressible pre-processor expects that the grid has been made by the SEPRAN mesh generator SEPMESH, using the special option "isnas" or alternatively by the two-dimensional grid generator Liss.

In Section 3.1.1 the usage of SEPMESH is described.

3.1.1 Usage of SEPMESH

The generation of the mesh is performed by the program SEPMESH. At this moment only a batch version is available, which requires a file with data. This file must be created by the user for example with a text editor.

Program SEPMESH creates output in two ways:

- SEPMESH writes to the standard output device (usually the display from which you start the program, or a standard output file). This output consists of a copy of the input file, error messages if the input is incorrect and some messages from submesh generators.
- If the input is error-free and a mesh has been generated, then this mesh is written to a file named finvol.new. This file is used by the Deft pre-processor and the Deft main programs.

Chapter 4 describes how a mesh is generated.

SEPMESH must be used as follows:

```
sepmesh  inputfile
```

or

```
sepmesh  inputfile > outputfile
```

The inputfile is the file created by the user using the text-editor. If no outputfile is specified all information (including error messages) is written directly to the screen.
The output file may have any name except meshoutput, finvol.new and sepplot.** *, where * is any digit.

Example: sepmesh pipe.msh > pipe.out.

Remark: besides the file finvol.new sepmesh also creates files sepplot.001, sepplot.002, etc. which contain plot information.

So sepmesh creates output in 3 ways:

- a file finvol.new containing the complete description of the mesh;

- files sepplot.001, sepplot.002, etc. containing information of the plots to be made;
- output written to the screen or the outputfile (for example mesh.out). This output contains a hard copy of the input, error messages (if any) and some information about the mesh.

How the plot information may be translated into a plot is described in Section 3.5.

3.2 Pre-processing

Once the grid has been created, the physical, mathematical and solution parameters of the problem must be specified. This means for example specification of the viscosity, the density, the boundary conditions, the type of linear solver, time integration and the turbulence model.
This specification must be given with a text file. The Deft pre-processor reads this input file and interprets it. A number of possible errors in the input file is recognized by the pre-processor and in that case error messages are given. The pre-processor uses not only the input file but also the file finvol.new created by the grid generator. The Deft pre-processor has the name ISNASPRE.

Program ISNASPRE creates output in two ways:

- ISNASPRE writes to a file isnaspre.out. At the end of the run the tail of this file is echoed to the screen. The output file consists of a copy of the input file, and error messages or warnings if the input is incorrect.
- If the input is error-free ISNASPRE creates a so-called intermediate file isnasinp.cmp. This file contains a translation from the input file to a data structure recognized by the Deft main programs. For a description of the file isnasinp.cmp consult the Deft Programmers Guide [40].

Chapter 5 describes the isnas inputfile.

ISNASPRE must be used as follows:

```
isnaspre inputfile
```

'inputfile' must have been created by the user.

3.3 Computational part of Deft

If the pre-processing phase has been completed successfully, which means that also the grid has been generated, the Deft main program can be run. Depending on the input file used in the pre-processing part, the computational part may

take a large amount of computing time. It is also possible to run the Deft main program parallel at several computers provided the parallel environment PVM is available. Whether or not the parallel version will be used is specified in the input file.

For simple problems Deft provides a standard command: ISNASEXE. If the problem to be solved fits within the frame-work of ISNASEXE, there is no need to create or link your own main program. However, as soon as function subroutines are required to describe coefficients or boundary conditions, or if the grid is too fine to be solved by the standard program ISNASEXE it will be necessary to create and link a local program ISNASEXE.

After that type:

```
isnasexe
```

ISNASEXE uses the files finvol.new and isnasinp.cmp created by the grid generator and the pre-processor respectively. ISNASEXE creates output in two ways:

- Two files sepcomp.inf and sepcomp.out that will be used by the SEPRAN post-processor ISNASPOST.
- Output is written to the file isnasexe.out containing information about the problem run as well as possible error messages and warnings. At the end of the run the tail of this file is echoed to the screen.

If in some way ISNASEXE is not adequate it is necessary to create your own main program. How this must be done is described in Chapter 6.

In case of a parallel environment, where the program ISNASEXE must run on several processors, the pre-processing and computational part are combined into one step. The command `isnasmpi` must be used to run both the preprocessor and ISNASEXE. The syntax is:

```
isnasmpi  input_file
```

where `input_file` is the file otherwise used by ISNASPRE.

3.4 Post-processing

Once the solution has been computed, it must be post-processed in order to print or plot the results. In the present version of Deft only the SEPRAN post-processor ISNASPOST is available.

The usage of ISNASPOST is described in Section 3.4.1

3.4.1 Usage of ISNASPOST

In the postprocessing part of SEPRAN, the mesh created by SEPMESH is read from the file finvol.new and from the files sepcomp.inf and sepcomp.out. These files have been created in the computational part. In this section the results are produced for the user in a more suitable form: prints, plots, integrals etc. The postprocessing part is performed by the program ISNASPOST. For a description of its possibilities the reader is referred to Chapter 7.

ISNASPOST is used in the same way as SEPMESH, i.e. the user creates a text input file and then runs ISNASPOST.
ISNASPOST is used as follows:

```
isnaspost inputfile >  outputfile
```

or

```
isnaspost inputfile
```

'inputfile is' the file created by the user. If no outputfile is specified all information (including error messages) is written directly to the screen.
ISNASPOST uses also the file created by SEPMESH (finvol.new) and those created by the Deft computational program (sepcomp.inf and sepcomp.out).
ISNASPOST does not produce plots directly but produces files named sepplot.001, sepplot.002, etc. containing plot information. Since this name is the same as for the plot files produced by SEPMESH these files will be destroyed. How the plot information is translated into a plot is described in Section 3.5.

Example: isnaspost pipe.pst > pipe.out

3.5 Display of SEPRAN plots

The SEPRAN mesh generation part or the postprocessing part may generate plot files named sepplot.001, sepplot.002, sepplot.003, etc.

In SEPRAN there are two ways of displaying these plots: you can make a picture at the screen, or you make a plot onto a laser printer or plotter.

To display the plot on the screen use the command:

```
sepdisplay
```

This interactive program tells you how many plots are available and asks you which one you want to see. sepdisplay is completely self explaining and should is by typing

```
sepdisplay     [RETURN] .
```

If your computer has several ways to display plot output, use the option *choose plotting device* to change the default plotting device into your own choice. This option gives you also the opportunity to choose the hard-copy output device. At present SEPRAN is able to produce both HPGL output (which can be used on many types of plotters and on laser printers that have an HPGL emulator build in), or Postscript output. Postscript can be used on Postscript printers only.
If you use the option *hard copy*, in fact SEPDISPLAY does not make a hard copy but produces a file sephpgl.xxx or sepposc.xxx containing HPGL or Postscript code respectively. xxx stands for 001, 002 etc. For each new hard copy command the sequence number is increased. As soon as sepdisplay has been started it removes files with names sephpgl.xxx or sepposc.xxx.
If you want to plot or print the hard copies, you have to send the files sephpgl.xxx or sepposc.xxx to the plotter or the printer. How this should be done depends on the local installation of your computer. Consult your system manager on this issue.

For a UNIX environment under X-Windows there is a windows based alternative for SEPDISPLAY, the program SEPVIEW. The command SEPVIEW is activated by typing:

```
sepview
```

or

```
sepview sepplot.xxx
```

where sepplot.xxx is the file to be plotted.
If sepview is used without file name, the file may be selected by the option file. Once a file is selected all files with the same basename and extension .001, .002, ... may be viewed. The first file is the file selected.
SEPVIEW has the following options:

Zooming in Press the left mouse button down and move the cursor upwards while pressing the button. Release the mouse button if the created rectangle is large enough. The picture within the rectangle will be drawn in the full window.

Zooming out Zooming out means displaying the previous window. Zooming out is done by moving the cursor downwards while creating a rectangle.

Panning Panning is done by pushing and releasing the left mouse button on the same place in the picture. The picture is panned towards the mouse position. How much the picture is panned depends on the distance between the mouse button and the middle of the picture.

Hardcopy Pressing the 'Hardcopy' button will show you a pull down menu with two possible choices. 'Postscript' produces an encapsulated postscript

file <name>_<nn>.eps from the current view. An HPGL file <name>_<nn>.hpgl is generated if you press the 'HPGL' button.
<name> is the name of the Sepran plot file and <nn> is a sequence number. It will be increased each time a new file is generated.

Play / Stop / Previous / Next At the lower right corner of the plot window, there are three buttons, a left arrow, a right arrow and a push button labelled 'Play' or 'Stop'.

The name of a SEPRAN plot file is of the form nnnplot.xxx, where nnn is an arbitrary name, usually sep and xxx is a number. This number can be used to select a previous/next plot file of the same set with a higher/lower number, using the right and left arrow. If there is no plot file with a higher/lower number, the right/left arrow is disabled.
To show a set of plot files as an animation, you can use the 'Play' button. As soon as SEPVIEW has started playing, the label on the button is changed to 'Stop' to stop the animation. As soon as the last file in the set is shown, the animation is reversed.

Defaults Sepview understands all of the OSF/Motif resource names and classes as well as the ones defined below. The class name for the SEPVIEW resources is "Sepview".

highlightThickness Specifies the thickness of the highlighting rectangle around the buttons and text areas.
Default: 0

background Specifies the default background colour for drawing.
Default: medium turquoise

drawArea*background Defines the drawing areas background colour.
Default: turquoise

An example resource for Sepview is shown below:

```
Sepview*background:          white
Sepview*drawArea*background: blue
```

3.6 An overview of simple Deft commands

In this section we give an overview of some of the available Deft and SEPRAN commands.

The following Deft/SEPRAN commands are available:

- sepmesh (creates a grid, see Section 3.1.1)
- isnaspre (reads and interprets the Deft input file, see Section 3.2)
- isnasexe (performs the computational part of Deft, see Section 3.3)

- isnaspost (performs the SEPRAN postprocessing, see Section 3.4.1)
- sepdisplay (displays SEPRAN plot files to the screen or produces files with hard copies, see Section 3.5)
- sepview (Plot SEPRAN files under X, see Section 3.5)

If you want to use the Deft/SEPRAN commands in a UNIX operating system, it is necessary to add the Deft and SEPRAN bin directory to your path. Consult your local system officer on this issue.

3.7 Syntax of input files

The ASCII input files that are used by Deft and also by SEPRAN have to satisfy syntax rules. In this section we shall explain these rules, we will use them in the following sections without explanation.
The Deft and SEPRAN input files provide the following features:

record A record consists of at most 80 characters. All characters behind column 80 are neglected. An input file consists of records.
In Deft the division into records does not have a special meaning, hence whether items are placed in one or more records does not alter the meaning. However, to increase readability it is recommended to put each command or data item in a new record. This also simplifies maintenance.
In SEPRAN it is usually necessary to start each command at a new line.

separator All characters except letters, digits and the underscore sign (_) will be regarded as separator between items. This includes also a space and end of line character.

keyword A keyword is defined as a set of characters consisting of letters and the underscore sign (_) only. The input is in case insensitive, except for strings used in output.
It is not always necessary to type the complete keyword. In most cases only a limited number of characters is significant. The significant characters are written in capitals in this manual. In the input file they may be in lower case. However, it is recommended not to restrict yourself to the significant characters, since this may reduce readability.

comment record Each record with a $*$ sign in the first column will be regarded as a comment record. It will be skipped when the input file is processed.

comment character It is also possible to provide a comment within a record. The hash sign(#) is then used as comment character. All information behind # is treated as comment.

number Numbers in records are represented in the same way as FORTRAN constants, for example: 1.0, 1.0D0, 1.0E-1, 1, .01 ; they may

not contain any spaces. The first character of a number must be a digit, minus sign or a point.

special characters In some cases the opening and closing brackets (and) have a special meaning. If this is the case, this is explicitly remarked in the description of the input file.

SET COMMANDS With the use of the so-called SET commands the user may give special information to the program reading the input file. These SET commands may be placed anywhere in the input file. They are active from the moment they are read.
For Deft the following SET commands may be useful:

SET OUTPUT OUT Once this set command is read all input read from the input file is not echoed anymore, until set output on is read.

SET OUTPUT ON Reactivates the echoing of the input file.

SET SKIP ON All input read after this command is skipped, which means that it is treated as comment that is not echoed. Reading is presumed in the standard way as soon as set skip off is read. This command may for example be used to prepare input files for a complete job without actually carrying out all commands.

SET SKIP OFF Reactivates standard reading of the input file.

Chapter 4

Grid generation

The first stage of an Deft job is to generate a grid. In that stage the user must decide whether he wants to use a single block approach or if multi block is necessary. Furthermore in the grid generation part it is also necessary to mark boundaries for example by a name or number in order to identify them in the pre-processing part. The reason is the prescription of boundary conditions at items that are known by some name.

Grid generation may be performed with any available package. However, Deft requires a special file format to be made by this grid generator and hence some "file translator" may be necessary.

The present version of the Deft incompressible pre-processor expects that the grid has been made by the SEPRAN grid generator SEPMESH, using the special option "isnas", see Section 4.1 or alternatively by the grid generator Liss.

4.1 Grid generator SEPMESH

4.1.1 General remarks

Before the grid may be created the user must keep in mind that an Deft grid consists of one or more blocks. Each block will be mapped homeomorphically onto a rectangle (2D) or a rectangular hexahedron (3D). This means that the mapping is continuous with continuous inverse. As a consequence a block in 2D has four sides and four vertices, although each side itself may contain several subsides. In R^3 the grid must be restricted to a single block, since multi block has not yet been implemented for R^3. A block can not contain any holes.

The sides of the 2D block or the surfaces of the 3D block may not degenerate to a quantity of lower dimension (point, side). Furthermore opposite sides in the "rectangle" must have different points although co-ordinates may coincide.
Consider for example the region in Figure 4.1.1 with four sides C1 to C4. It is

not allowed that curve C4 reduces to a single point. The curves C1 and C3 are identical in the sense that they have the same co-ordinates. However, with respect to the grid generation they are completely different. They will be treated as independent curves. Identification of these curves in the computational program is only possible by defining periodical boundary conditions at the curves C1 and C3.

There are no limitations in the ways blocks may be coupled. Hence one side of

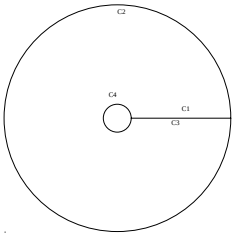


Figure 4.1.1: C-type region with four sides C1 to C4

a block may be coupled to (parts of) sides of two other blocks. Of course in that case it is necessary to divide such a side into subsides since, if tow different blocks have a common side or subside, they should have the same name in order to be able to identify them as common. At this moment it is not allowed that the number of blocks that coincide in one point is more than four.

The generation of the single block grids may be done by a standard SEPRAN sub grid generator, by a user written sub grid generator or by input from the standard input file. In this manual only the first possibility is considered. For the other cases see the SEPRAN Users Manual.
The only sub grid generators allowed for Deft are RECTANGLE for two-dimensional grids and BRICK for three-dimensional grids.

4.1.2 Definition of points, curves, surfaces and volumes

For the generation of grids we define the following quantities:

Points, Curves, Surfaces and Volumes

Points form the basis for all other components. The user must define the main points necessary for the generation of curves. These points must be numbered sequentially from 1 onwards. After the generation of the grid they are connected to nodal point numbers. The corresponding nodal point numbers are generally not equal to the point numbers defined by the user.

Curves form the one-dimensional quantities of the grids. For example lines and arcs are curves. The initial and end points of any curve must already have been defined as points. Curves have an orientation, defined by the initial and end

points, hence line C3 = (P3, P4) is different from line C4 = (P4, P3).

Surfaces form the two-dimensional quantities of the grid. The boundaries of the surfaces must already have been defined as curves. The boundary of a surface must be closed in itself. Whenever in a description of a surface a curve is needed in the opposite direction of which it was defined, then its number must be preceded by a minus sign. (See Figure 4.1.4).

Volumes form the three-dimensional quantities of the grid.

All points, curves, surfaces and volumes must be numbered sequentially, each starting with number one. The outer and inner boundaries as defined in 2.2 must consist of points (in R^1), points and curves (in R^2), and points, curves and surfaces (in R^3).

The sub grids as defined in 2 must coincide with curves (in R^1), surfaces and sometimes curves (in R^2), or with volumes and sometimes curves and surfaces (in R^3).

Anywhere in the manuals where curves, points and surfaces are mentioned, the curves, points and surfaces generated by the grid generator are meant. Nodal points of the grid must be coupled with these points, curves and surfaces.

Examples

Consider the regions in Figure 4.1.2 and 4.1.3. In Figure 4.1.4 the points, curves and surfaces for these regions are defined. Points are indicated by Pk (k=1 ,2 ,,,), curves by Cl (l=1 ,2 ,,,) and surfaces by Sm (m=1 ,2 ,,,). The corresponding commands are POINTS, CURVES and SURFACES.
The right upper region in FIGURE 4.1.2 is not allowed in Deft, because subblock II degenerates into a triangle.

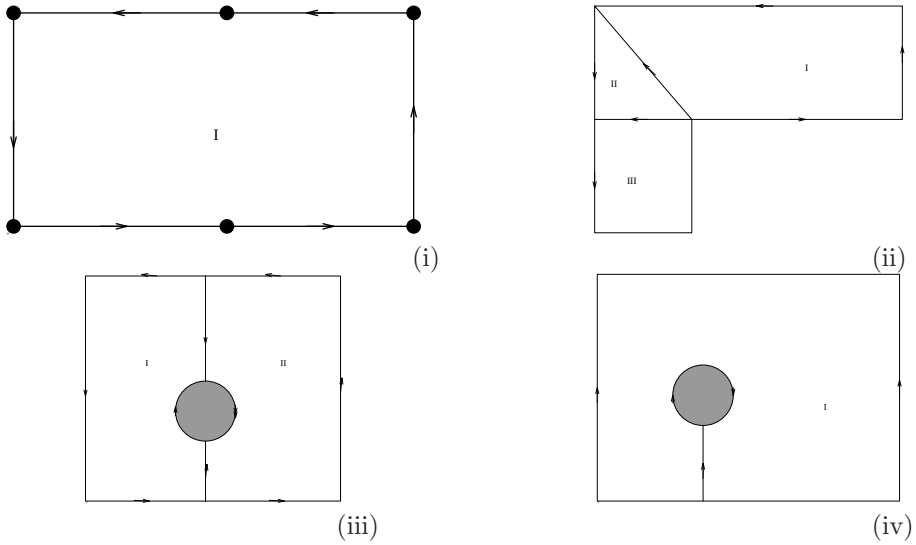


Figure 4.1.2: Examples of regions consisting of 1 (i),(iv) 3 (ii) and 2 (iii) subregions

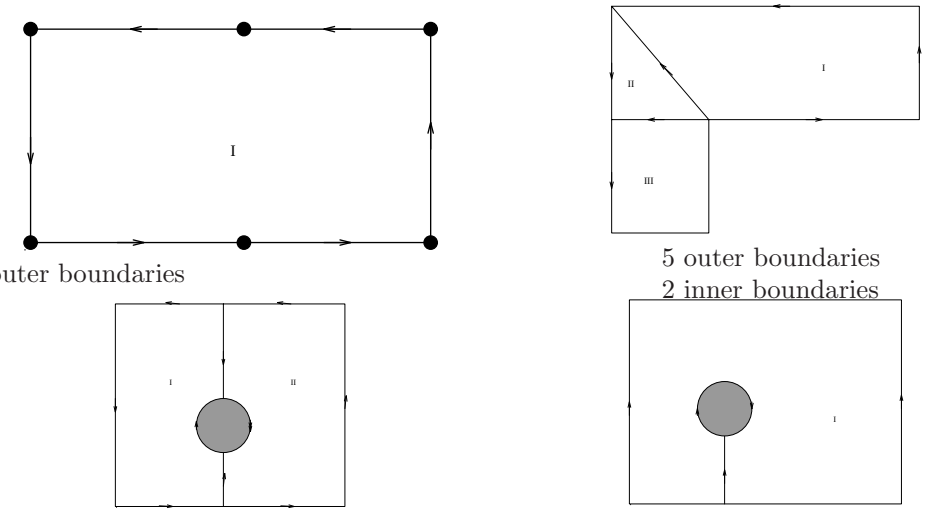
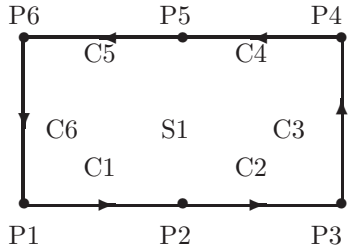
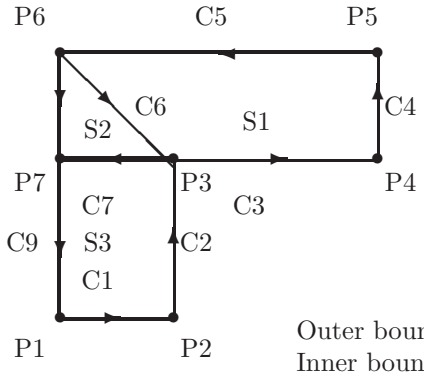


Figure 4.1.3: Examples of inner and outer boundaries each provided with a direction



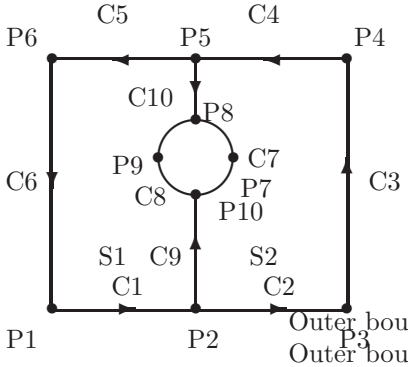
C1 = (P1,P2) C2 = (P2,P3)
C3 = (P3,P4) C4 = (P4,P5)
C5 = (P5,P6) C6 = (P6,P1)
S1:(C1,C2,C3,C4,C5,C6)

Outer boundaries: C1, C2, C3, C4, C5, C6



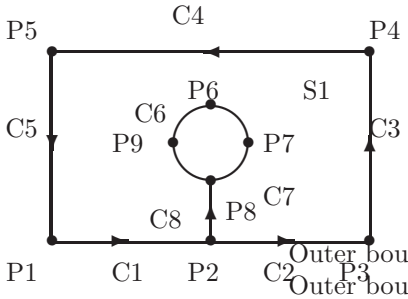
C1 = (P1,P2) C2 = (P2,P3)
C3 = (P3,P4) C4 = (P4,P5)
C5 = (P5,P6) C6 = (P6,P3)
C7 = (P3,P7) C8 = (P6,P7)
C9 = (P7,P1)
S1:(C3,C4,C5,C6)
S2:(-C7,-C6,C8)
S3:(C1,C2,C7,C9)

Outer boundaries: C1, C2, C3, C4, C5, C8, C9
Inner boundaries: C6, C7
Attention: This region is not allowed in Deft.



C1 = (P1,P2) C2 = (P2,P3)
C3 = (P3,P4) C4 = (P4,P5)
C5 = (P5,P6) C6 = (P6,P1)
C7 = (P8,P7,P10) C8 = (P10,P9,P8)
C9 = (P2,P10) C10 = (P5,P8)
S1:(C1,C9,C8,-C10,C5,C6)
S2:(C2,C3,C4,C10,C7,-C9)

Outer boundaries part 1: C1, C2, C3, C4, C5, C6
Outer boundaries part 2: C7,C8
Inner boundaries: C9, C10



C1 = (P1,P2) C2 = (P2,P3)
C3 = (P3,P4) C4 = (P4,P5)
C5 = (P5,P1) C6 = (P6,P9,P8)
C7 = (P8,P7,P6) C8 = (P2,P8)
S1:(C8,-C6,-C7,-C8,C2,C3,C4,C5,C1)

Outer boundaries part 1: C1, C2, C3, C4, C5
Outer boundaries part 2: -C6, -C7
Inner boundaries: C8

Figure 4.1.4: Points, Curves and Surfaces

4.1.3 Generation of the curves

First the user must define all points, secondly all curves and finally all surfaces.
For the definition of curves, the user may specify both the number of nodal points on a curve, and the distribution of these points.
For the definition of the curves the following FUNCTIONS are available:

LINE< *cell_type* >: generates a straight line from point Pi to Pj.
ARC< *cell_type* >: generates an arc from point Pi to Pj; the centroid Pc must be given.
USER< *cell_type* >: the user gives all coordinates of the nodal points on the line.
CURVES: generates a curve consisting of the subsequent curves Ck, Cl, Cm.

For other functions see Section 4.1.6.
< *cell_type* > is an integer which defines the type of cells along the curves to be created. In Deft only *cell_type* = 1 is permitted.

The FUNCTIONS LINE, ARC, USER and CURVES have the following shape:

```
c1 = line <cell_type> ( p1,p2,nelm=n,ratio=r,factor=f )
c2 = arc  <cell_type> ( p1,p2,pc,nelm=n,ratio=r,factor=f )
c3=user <cell_type> ( p1,p2,p3, . . . , pn )
c6 = curves ( ck, cl, cm, . . )
```

with n the number of cells in the curve.

The distribution of the nodal points is given by the parameters RATIO and FACTOR:
- r=0: equidistant grid size (default)
- r=1: the last cell is f times the first cell
- r=2: each consecutive cell is f times the preceding cell

4.1.4 Generation of surfaces

Each surface must coincide with a subgrid (in two-dimensional problems). For the generation of nodal points and cells in the surface, a number of so-called surface generators are available. Of these surface generators only one treated in this manual. For the other ones the user is referred to the SEPRAN users manual.

The surface generator described in this manual is RECTANGLE.

RECTANGLE has the following characteristics:

The function RECTANGLE has the following shape:

```
S1 = RECTANGLE <cell_type> ( C1, C2, C3, C4)
```

< *cell_type* > is an integer which defines the type of cells in the surfaces to be created. In Deft only *cell_type* = 5 is permitted, indicating that the grids consists of four-point quadrilaterals.

4.1.5 Input for program SEPMESH from standard input

The input for SEPMESH must be opened by the COMMAND mesh1D, mesh2D or mesh3D, depending on whether the problem is one-, two- or three-dimensional, and must be closed by the COMMAND END.

COMMAND and DATA records.

The records must be given in the order as specified.
An option is indicated like this [option].

ISNAS (mandatory)
COMMAND record: indicates that an Deft output file finvol.new must be created. If omitted only the SEPRAN output file meshoutput will be generated.

MESHnD (mandatory)
COMMAND record: opens the input for SEPMESH, and defines the dimension of the space NDIM. (NDIM = n).
After the command MESHnD a number of optional commands may be given. These commands must be given between MESHnD and the mandatory command POINTS. Their mutual sequence is arbitrary.

MAXPOINTS = *mp* (optional)
mp defines the maximum number of user points that are allowed in the grid. The default value is 1000. If a smaller value is used, some arrays may be smaller, but in general this has no effect on the total space. In fact, this option is meant for those cases that 1000 user points do not suffice.

MAXCURVES = *mc* (optional)
mc defines the maximum number of curves that are allowed in the grid. The default value is 1000. Compare with MAXPOINTS.

MAXSURFACES = *ms* (optional)
ms defines the maximum number of surfaces that are allowed in the grid. The default value is 1000. Compare with MAXPOINTS.

MAXVOLUMES = *mv* (optional)
mv defines the maximum number of volumes that are allowed in the grid. The default value is 500. Compare with MAXPOINTS.

POINTS (mandatory)
COMMAND record: defines the points. Must be followed by data records of the type:

```
P1 = ( x_1 , y_1 , z_1 )
P2 = ( x_2 , y_2 , z_2 )
```

```
                .
                .
                .
    Pi = ( x_i , y_i , z_i )
```

with i the point number and x_i, y_i and z_i the co-ordinates of point i. For one-dimensional problems only x_i is required, etc. Default values for the co-ordinates: 0.

Remark: The sequence in which the points are given is arbitrary. If points are skipped, they get the co-ordinates (0,0,0) automatically. The largest number i used in $P_i = \ldots$ defines the maximal number of user points.
If the user wants, he may also give the co-ordinates in polar co-ordinates instead of Cartesian co-ordinates. In that case the input is

PDi $= (r_i, \phi_i, z_i)$, with ϕ in degrees or

PRi $= (r_i, \phi_i, z_i)$, with ϕ in radians

instead of Pi $= (x_i, y_i, z_i)$.

These co-ordinates are automatically transformed into Cartesian co-ordinates.

CURVES (mandatory)
COMMAND record: defines the curve. Must be followed by data records of the type:

```
Ci = LINE  <cell_type> ( P1, P2, NELM=n [, RATIO=r, FACTOR=f ] )
Ci = ARC   <cell_type> ( P1, P2, P3, NELM=n [, RATIO=r, FACTOR=f ])
Ci = USER  <cell_type> ( P1, P2, P3, . . . , Pn )
Ci = PARAM <cell_type> ( P1, P2, NELM=n [,INIT=t_0] [,END=t_1]
                         [, RATIO=r, FACTOR=f ] )
Ci = SPLINE<cell_type> ( P1, P2, ... ,Pm, NELM=n [, RATIO=r, FACTOR=f ]
                         [,TYPE=t [,tang=Pk, tang=Pl ] ] )
Ci = CURVES ( Ck, Cl, Cm, . . )
Ci = TRANSLATE Cj ( P1 [,P2, P3, . . . ] )
Ci = ROTATE Cj ( P1, P2, P3 [,P4, P5, . . . ] )
Ci = REFLECT Cj ( AXIS = P1, P2; P3 [,P4, P5, . . . ] )
```

Curves that have not been defined explicitly, will be treated as non-existing curves. These curves are not available in the SEPRAN programs.
For an explanation of the various possibilities, see Section 4.1.6.

SURFACES (mandatory)
COMMAND record: defines the surfaces. Must be followed by data records of the type:

```
Si = RECTANGLE<cell_type> (C1, C2, C3, C4 [, SMOOTH = i ] )
```

with Si the surface number.
Surfaces that have not been defined explicitly, will be treated as non-existing surfaces. These surfaces are not available in the SEPRAN programs.
For an explanation of RECTANGLE see section 4.1.7.

VOLUMES (optional)
COMMAND record: defines the volumes. Must be followed by data records of the type:

```
Vi = BRICK<cell_type> ( S1, S2, S3, S4, S5, S6 )
```

with Vi the volume number.
$< cell\_type >$ is an integer which defines the type of cells in the volumes to be created. In Deft only $cell\_type = 13$ is permitted, indicating that 8-point hexahedra must be created. Volumes that have not been defined explicitly, will be treated as non-existing volumes. These volumes are not available in the SEPRAN programs.
For an explanation of BRICK see section 4.1.8.

PLOT (optional) COMMAND record: indicates that the points, curves, the surfaces and the grid must be plotted, each on a new picture. This command record may contain data. In that case it has the following shape:

```
PLOT ( PLOTFM = l, YFACT = y, JMARK = j, NUMSUB = n, CURVE = c,
       NODES = no, USERP = u, COLOUR = cl,
       SUPPRESS = su, ROTATE = r, EYEPOINT = (x_e,y_e,z_e) )
```

with PLOTFM $= l$ the length of the plot in centimeters.
Default value: depending on the computer installation, usually 15 or 20.
Instead of PLOTFM $= l$, the user may set SCALE $= s$. In that case the size of the plot of the grid and sub grids is not fixed, but determined by the co-ordinates of the grid and sub grids.
Hence the length in the x-direction is given by s dx and the length in the y-direction by s dy, where dx is the maximal difference of the x-co-ordinates in the grid or sub grid, and dy the same for the y-co-ordinates.

YFACT $= y$: Scale factor; all y-co-ordinates are multiplied by y before plotting the grid. $y \neq 1$ should be used when the co-ordinates in x and y direction are of different scales, and hence the picture becomes too small.
Default value: 1.

JMARK $= j$: Indication of how the plot of the grid must be made. Possibilities:

0,3 Each nodal point will be marked with a star and its nodal point number.

1,4 Each nodal point will be marked with a star. Nodal point numbers will **not** be plotted.

2,5 Nodal points will not be marked and nodal point numbers will not be plotted.

When JMARK < 3 all cell numbers will be plotted in the centroid of the cells, when JMARK ≥ 3 no cell numbers will be plotted.

Default value: 5

NUMSUB $= n$: The sub grids with numbers $\leq$ NUMSUB are not plotted.
Default value: 0.

CURVE $= c$: This parameter indicates if the curves must be plotted in a separate picture. Possible values:

0 Curves are not plotted.

1 Curves are plotted without curve number.

2 Curves are plotted provided with curve number.

Default value: 2.

NODES $= no$: This parameter indicates if nodes along the curves must be plotted in the picture containing the curves. So this parameter makes only sense for $c > 0$. Possible values:

0 Nodes are not plotted.

1 Each node is indicated with a star-symbol ($\times$).

> 1 Each node is indicated with a symbol from the symbol table. The sequence number on the symbol table is equal to $no - 1$.
Which symbols are stored in the symbol table depends on your plotting package.

Default value: 0.

SUPRESS $= su$: This parameter indicates if pictures must be provided with texts ($su = 1$) or not ($su = 0$).
Default value: 1.

ROTATE $= r$: This parameter indicates whether plots must be rotated over 90 degrees or not. Possibilities:

0 The plots are made such that the plotting paper used is minimal.

1 The plot is not rotated.

2 The plot is always rotated over 90 degrees.

Default value: 0.

EYEPOINT = (x_e, y_e, z_e): This command makes only sense in case of a 3D region. The use of EYEPOINT indicates that a final 3D grid is plotted with hidden lines. In the case that there are many cells this plot may take much time. (x_e, y_e, z_e) defines the point where the observer is positioned. *Remark:* EYEPOINT must be written as one word.

In case of a 3D grid only the sub grids are plotted, without the removal of hidden lines, except when EYEPOINT is given. For a final plot of the complete region with hidden lines removed, one may use PLOTMESH.

END (mandatory)
End of the input for SEPMESH.

Remark:

The input must be given in the sequence:
ISNAS
MESH record
optional commands
POINTS
CURVES
SURFACES
VOLUMES
PLOT
END

4.1.6 Curve generators

In this section the various curve generators will be treated. These curve generators are activated by the command CURVES in the input for the program SEPMESH. The following types of curve generators are available:

LINE
ARC
USER
PARAM
SPLINE
CURVES
TRANSLATE
ROTATE
REFLECT

These curve generators have the following global functions:

LINE generates a straight line between two end points.

ARC generates an arc from begin point to end point; the centroid must be given.

USERi the user gives all coordinates of the nodal points on the line.

SPLINE A curve is defined by a spline through a number of points.

PARAM The user defines a curve by a function subroutine FUNCCV using a parameter representation.

TRANSLATE Copy a curve and translate it over a fixed distance.

ROTATE Copy a curve and translate and rotate this new curve.

REFLECT Make a reflection of a curve with respect to a given line.

CURVES Create a new curve by combining old curves.

The following options have a global meaning for each of the curves, where they may be used:

NELM=n gives the number of cells that must be created along the curve (linear or quadratic depending on the value of j).

RATIO=r indicates the options for distribution of the nodal points. Possibilities:

r=0: equidistant grid size (default)

r=1: the last cell is f times the first one.

r=2: each next cell is f times the preceding one.

r=3: the last cell is $1/f$ times the first one.

r=4: each next cell is $1/f$ times the preceding one.

FACTOR=f the factor to be used when r >1. Default: f=1.

INIT=t_0 gives the starting value of the parameter t along the curve. This parameter t is used in the call of subroutine FUNCCV (See the SEPRAN Users Manual 2.3.1).
Default value: $t_0 = 0$.

END=t_1 gives the end value of the parameter t along the curve.
Default value: $t_1 = 1$.

Extended description of the various curve generators

LINE The input for LINE must be given in the following way:

```
Ci = LINE 1 ( P1, P2, NELM=n [, RATIO=r, FACTOR=f ] )
```

This means that a straight line is generated from point P1 to point P2, with a division of cells as indicated by the options.

ARC The input for ARC must be given in the following way:

```
Ci = ARC 1 ( P1, P2, P3, NELM=n [, RATIO=r, FACTOR=f ])
```

When ARC is used an arc is generated from point P1 to P2 with centre P3.
In R^2 the sign of P3 indicates the direction of the arc. When P3 is given the arc is created counter clockwise, when -P3 is given it is created clockwise. In R^3 the smallest arc from point P1 to point P2 is chosen. If the angle is exactly 180°, that is if the points P1, P2 and P3 are positioned on a straight line, then the direction of the arc is undefined. The arc is positioned in the plane through P1, P2 and P3.

Remark: The user may give the centroid of an arc in an inaccurate way. The centroid is computed as the projection of the centroid given by the user on the line orthogonal to the line through the two end points of the arc and going through the midpoint of these two points. See Figure 4.1.5. Of course this is only possible when initial point and end point of the arc are essentially different points.

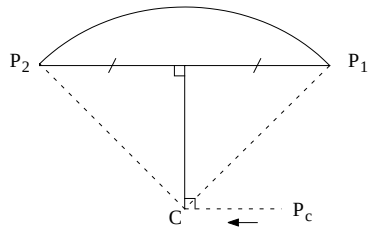


Figure 4.1.5: Computation of the centroid of an arc

USER The input for USER must be given in the following way

```
Ci = USER 1 ( P1, P2, P3, . . . , Pn )
```

The curve is defined by the points P1, P2, P3, . . . , Pn in that sequence.

SPLINE: The input for SPLINE must be given in the following way:

```
Ci = SPLINE 1 ( P1, P2, ... ,Pm, NELM=n [, RATIO=r, FACTOR=f ]
                [,TYPE=t [,tang=Pk, tang=Pl ] ] )
```

When SPLINE is used, the curve is defined by a cubic spline through the points P1, P2, P3, . . . , Pm. At least 3 points are required. The curve passes through all points P1, P2, ... Pm and has continuous derivative and curvature. None of the internal points P2, P3, ... Pm-1 is necessarily a nodal point. These points are not connected to nodal points either, so they can not be used in later stages of SEPRAN programs. In each sub interval [Pi, P$i+1$] the curve is a polynomial of the third degree. In SEPRAN the following SPLINE types are accessible by the option TYPE=t:

t=1 The tangent of the curve is zero in the end points P1 and Pm.

t=2 In [P1,P2] and [P$m-1$,Pm] the curve is a polynomial of degree 2.

t=3 The spline is a closed curve, i.e. there is no begin or end point: P1 and Pm must be the same point!

t=4 The spline is defined by the points P1, P2, . . . , Pn with derivatives prescribed in both begin and end point of the curve. The user must give the direction and magnitude of these derivatives by the phrase tang = Pk, tang = Pl. It is assumed that the vector Pk - P1 is the derivative in the initial point P1, and the vector Pl - Pm in the end point Pm. Hence the points Pk and Pl must have been defined already in the section points. Note that Pk is connected with the starting point and Pl with the end point.

If TYPE = t is omitted, t=1 is assumed.

The division of cells on the curve is defined by the parameter i, NELM=n, and (optional) RATIO=r, FACTOR=f.

PARAM The input for PARAM must be given in the following way:

```
Ci = PARAM 1 ( P1, P2, NELM=n [,INIT=t_0][,END=t_1]
     [, RATIO=r, FACTOR=f ] )
```

PARAM generates a user defined curve. The user must give the coordinates x, y and z as function of a parameter t with the aid of a user written subroutine *FUNCCV*. The parameter t goes from t_0 to t_1. The initial point is given by P1 and the end point by P2.
In this case, the length of the cells is created according to the rules defined by the parameters NELM, RATIO and FACTOR. As a consequence, the parameter t does not have to be distributed according to these same rules. Therefore, during the generation of the curves it is necessary for the program to compute the length of the curve and hence the function FUNCCV is called far more times then may be expected beforehand.

It is also permitted to give the distribution of the t-values over the interval. To that end 5 negative values of RATIO = r are permitted, with the following meaning:

r=-1: equidistant distribution of t, compare with r=0.

r=-2: the last t-value is f times the first one, compare with r=1.

r=-3: each next t-value is f times the preceding one, compare with r=2.

r=-4: the last t-value is $1/f$ times the first one, compare with r=3.

r=-5: each next t-value is $1/f$ times the preceding one, compare with r=4.

TRANSLATE The input for TRANSLATE must be given in the following way

```
Ci = TRANSLATE Cj ( P1 [,P2, P3, . . . ] )
```

When TRANSLATE is used, the curve Ci is a copy of curve Cj translated over a distance $\boldsymbol{\Delta x} = ((P1_i - P1_j)_x, (P1_i - P1_j)_y, (P1_i - P1_j)_z)$ with $P1_i$ the first point on Ci and $P1_j$ the first point on Cj. j must be smaller than i.
If the points $P2, P3, P4, ...$ are given, these points correspond to the second, third etc. user points on Cj in that sequence. When these user points have co-ordinates (0,0,0), they get the new co-ordinates as computed by the translation, otherwise it is checked whether these points have the correct co-ordinates, that is if these points are indeed positioned on Ci. The point numbers i of Pi may not exceed the maximal number of user points.
For most applications it is necessary that both the initial and end point of a curve are identified with user points. However, if the curve to be copied consists of many user points, defining the end point of the new curve requires a large number of (possibly unnecessary) user points on this new curve. For that reason the user may identify the last user point at the new curve by preceding the point number by a minus sign.
So

```
TRANSLATE Cj ( P1, -P5 )
```

indicates that the begin point on curve Cj is the user point $P1$ and the end point is user point $P5$. If more user points are defined on the new curve, then the negative point must always be the last one in the row.

ROTATE The input for ROTATE must be given in the following way:

```
Ci = ROTATE Cj ( P1, P2, P3 [,P4, P5, . . . ] )
```

When ROTATE is used, the curve Ci is a copy of curve Cj translated and rotated, such that the first three user points at Ci (P1, P2 and P3) are the

copies of the corresponding user points at Cj. For two-dimensional grids it suffices to give two points only. If a straight line has to be translated and rotated in 3D it also suffices to give two user points on the curve Ci. These user points define the translation as well as the rotation. ROTATE may only be used for curves in a plane. j must be smaller than i.
If the points $P4, P5, P6, ...$ are given, these points correspond to the fourth, fifth etc. user points on Cj in that sequence. When these user points have co-ordinates (0,0,0), they get the new co-ordinates as computed by the rotation, otherwise it will be checked whether these points have the correct co-ordinates, that is if these points are in fact positioned on Ci. The point numbers i of Pi may not exceed the maximal number of user points.
In the same way as for TRANSLATE the last user point in the case of ROTATE may be identified by a minus sign.

REFLECT The input for REFLECT must be given in the following way:

```
Ci = REFLECT Cj ( AXIS = P1, P2; P3, P4[, P5, . . . ] )
```

When REFLECT is used, curve Ci is a reflection of Cj with respect to the reflection line $P1$ - $P2$. At least two user points $P3$ and $P4$ have to be given. If the points $P5, P6, ...$ are given, these points correspond to the third, fourth etcetera user points on Cj in that sequence. When these user points have co-ordinates (0,0,0), they get the new co-ordinates as computed by the reflection, otherwise it is checked whether these points have the correct co-ordinates, that is if these points are indeed positioned on Ci. The point numbers i of Pi may not exceed the maximal number of user points.
In the case that a curve has to be reflected in R^3 instead of R^2 AXIS = $P1, P2$; should be replaced by RPLANE = $P1, P2, P3$; since in the three-dimensional space a reflection plane is required.
In the same way as for TRANSLATE the last user point in the case of REFLECT may be identified by a negative sign.

CURVES The input for CURVES must be given in the following way:

```
Ci = CURVES ( Ck, Cl, Cm, . . )
```

When CURVES is used a curve is defined by the subsequent curves Ck, $Cl, Cm, ...$ When the sign of the curve number is positive, the positive direction will be used, otherwise (negative sign), the reversed direction of the curve will be used. The curve numbers Ci must be larger than Ck, Cl, and Cm.

4.1.7 Surface generator RECTANGLE

The surface generator RECTANGLE is called by the program SEPMESH. The user may activate RECTANGLE by data records of the type:

```
Si = RECTANGLE 5 ( C1, C2, C3, C4 [, SMOOTH = i] )
```

with Si the surface number, 5 the shape number of the cells created in this surface, and C1, C2, C3 and C4 the curves enclosing Si.

Characteristics of RECTANGLE:

Generates a subgrid that can be homeomorphically mapped onto a rectangular grid. The number of curves along the boundary must be exactly equal to four and it is assumed that N is equal to the number of cells at the first curve and M equal to the number of cells at the second one. Of course it is necessary that the number of points at the third curve is equal to the number of points at the first curve and the number of cells at the fourth curve is also equal to M.
If sub curves are used, the curves along the boundary must be packed by the curve generator CURVES, which creates curves of curves.

With the parameter SMOOTH it is possible to define a kind of smoothing in the grid. First the grid is generated by a algebraic method and then, if $i > 0$, the grid is smoothed by a so-called potential smoother. The smoothing is stopped if the relative difference between two steps in the smoothing process is less than 10^{-i}. If SMOOTH is not given $i = 0$ is assumed and no smoothing takes place. Smoothing may be especially useful if the grid is used for a boundary fitted finite volume or finite difference program. Figure 4.1.6 shows the grid in an l-shaped region using the non-smooth grid generated by the following input:

```
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(1,0)
      p3=(1,3)
      p4=(4,3)
      p5=(4,4)
      p6=(0,4)
   curves
      c1 = line1(p1,p2,nelm=16)
      c2 = line1(p2,p3,nelm=16)
      c3 = line1(p3,p4,nelm=16)
      c4 = line1(p4,p5,nelm=16)
      c5 = line1(p5,p6,nelm=16)
      c6 = line1(p6,p1,nelm=16)
      c7 = curves(c2,c3)
      c8 = curves(c5,c6)
   surfaces
      s1 = rectangle5(c1,c7,c4,c8)
   plot
end
```

Also in Figure 4.1.6 the result is shown once the record with RECTANGLE is replaced by:

```
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(1,0)
      p3=(1,3)
      p4=(4,3)
      p5=(4,4)
      p6=(0,4)
   curves
      c1 = line1(p1,p2,nelm=16)
      c2 = line1(p2,p3,nelm=16)
      c3 = line1(p3,p4,nelm=16)
      c4 = line1(p4,p5,nelm=16)
      c5 = line1(p5,p6,nelm=16)
      c6 = line1(p6,p1,nelm=16)
      c7 = curves(c2,c3)
      c8 = curves(c5,c6)
   surfaces
      s1 = rectangle5(c1,c7,c4,c8,smooth=2)
   plot
end
```

Remark

In R^3 subgrid generator RECTANGLE may only be applied in a plane.

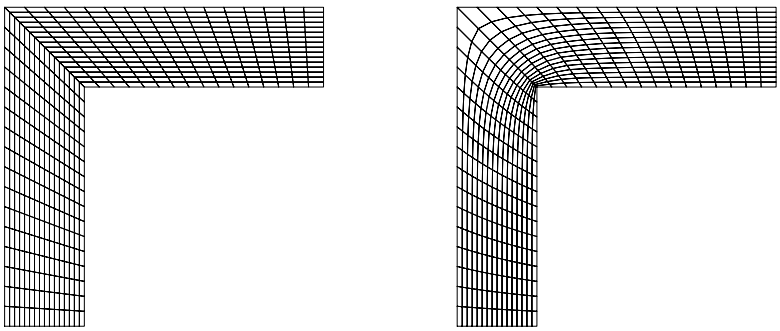


Figure 4.1.6: grid in L-shaped region without and with smoothing.

Examples of regions that may be subdivided by RECTANGLE

Actual grids

4.1.8 Volume generator BRICK

The volume generator BRICK is called by program SEPMESH. The user may activate BRICK by data records of the type:

```
Vi = BRICK 13 ( S1, S2, S3, S4, S5, S6 )
```

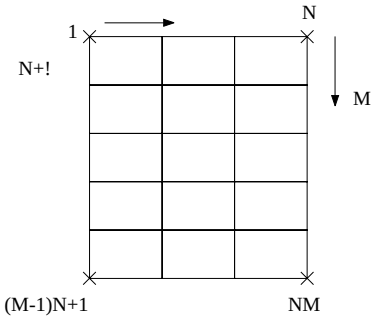
with Vi the volume number and S1, S2, . . . the surfaces enclosing Vi. The volume must be enclosed by exactly 6 surfaces. If sub surfaces are required the user must define surfaces of surfaces. See the SEPRAN Users Manual for a description.

Characteristics of BRICK:

Generates a sub mesh that can be mapped onto a rectangular (three-dimensional) grid. This rectangular region is plotted in Figure 4.1.7.
The region is defined by the 6 surfaces. These surfaces must each be triangulated by the surface generator RECTANGLE. The surfaces must be given in the sequence S1, S2, . . . , S6, where

S1 is defined by the face 1,2,3,4,

S2 is defined by the face 1,2,6,5,



Computational grid

N = 3, M = 5

Number of cells along the boundary:

2 (N + M)

S3 is defined by the face 2,3,7,6,

S4 is defined by the face 4,3,7,8,

S5 is defined by the face 1,4,8,5,

S6 is defined by the face 5,6,7,8.

The numbers refer to the points in Figure 4.1.7. These surfaces must each be generated in the way as indicated above, hence S1 must start with point 1, then point 2, point 3 and point 4, etc.
The parameters N, M and L correspond to the number of elements to be created along the surfaces in the following way:

Curves (1,2), (5,6), (4,3), (8,7): n elements.

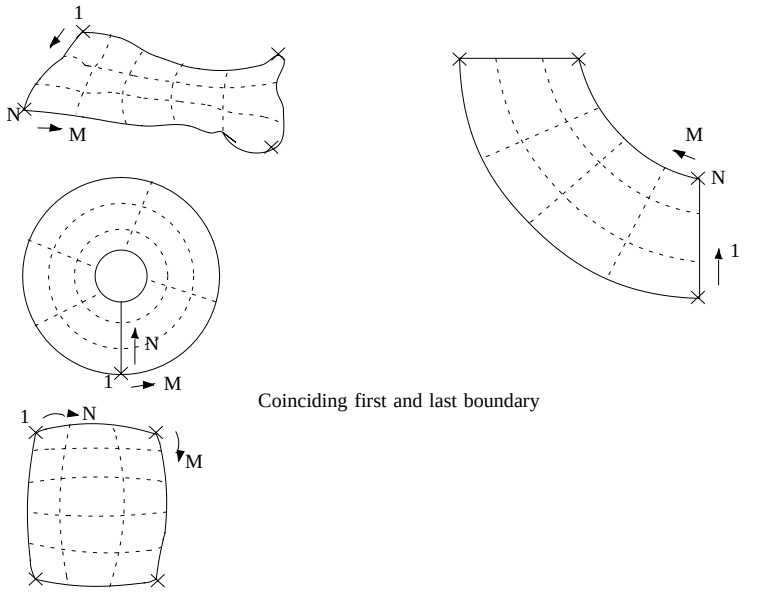
Curves (1,4), (2,3), (5,8), (6,7): m elements.

Curves (1,5), (2,6), (3,7), (4,8): l elements.

The surfaces may be curved and do not have to be part of a plane. The number of elements to be created is equal to αnml where α=1 for hexahedral elements and α=6 for tetrahedral elements.

Remark

Instead of the surface generator RECTANGLE also the surface generators COONS and PARSURF may be used to generate the surfaces, provided the number of nodes is the same at opposite curves. In fact in these cases the underlying sub mesh generator is RECTANGLE. See the SEPRAN Users manual for details.



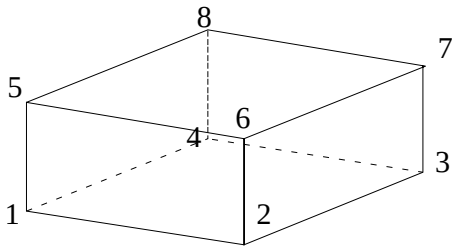


Figure 4.1.7: Rectangular region with 6 sides

Chapter 5

Input for the computational part

In this chapter we shall give a complete description of the Deft input file to be read by program ISNASPRE. This input file is a simple ASCII text file satisfying the rules described in Section 3.7. In contrast to SEPRAN files, newline characters have no special meaning except that they act as separator. Nevertheless the use of indents and newlines improves the readability and is therefore strongly recommended.
Keywords in the Deft input file may be abbreviated. It is advised, however, to use full names. The significant characters are set in capitals in this manual. The input file itself is case insensitive which means that there is no difference between capitals and lower case letters.

All keywords between the square brackets [and] may be considered as optional and hence may be neglected. In that case default values are used.

In Section 5.1 the general structure of the input file is described. The description of the sub blocks is postponed to subsequent sections.

5.1 Global description of the Deft input file

The Deft input file contains a number of so-called main keywords which control the global flow of the program. Some of these main keywords define parameters, others denote the beginning of a sub block. These sub blocks define a special sort of parameters, for example all parameters associated with the linear solver or all parameters corresponding to the coefficients.

Some of the main keywords are mandatory others are optional. If optional keywords are neglected, default values are used instead.

The main keywords are given in the following list:

Keyword	Default value	mandatory
NUMBER_OF_TRANsport_equations = n	0	no
NUMBER_OF_COMPuters = n	1	no
TIMEON / TIMEOFF	off	no
OUTPut_level = n	0	no
POSTTYPe = n	0	no
STATionary	time-dependent	no
DISCRETization		no
TIME_integration		yes
BOUNdary_conditions		yes
COEFficients		yes
LINEar_solver		no
INITial_conditions		yes
TURBulence	none	no
MULTI_BLOCK		no
COMPRESSIBLE		no
FULLY_COMPRESSIBLE		no
CAVITY		no
COLLOcated_grid	staggered_grid	no
STAGGered_grid	staggered_grid	no
MULTI_PHase_gas_flow	standard flow	no
FREE_SURFACE_FLOW	none	no
NO_TIME_LOOP	time-dependent	no
MAIN_STRUCTURE	none	no
PROFILE_INPUT	none	no
FREQUENT_OUTPUT	none	no
END_input		no

Meaning of these keywords:

NUMBER_OF_TRANSPORT_EQUATIONS = n defines the number of transport equations that must be solved simultaneously with the momentum equations. Turbulence equations like the k and ε equations should not be included in this number since their presence is dealt with in the part treated by TURBULENCE. Transport equations are solved taking **all** dependent variables at the old time level.
The default value for n is 0, which means that only the momentum equations, including the pressure and possibly the turbulence equations are solved.

NUMBER_OF_COMPuters = n defines the number of processors that may be used in parallel. If this option is used, it is supposed that you have the

possibility to use several computers or processors in parallel and that the MPI message passing system has been installed on your computer.
If n = 1, only one computer is used and the standard serial algorithm is applied.
For n > 1, parallel computing is applied at the n processors available.
The default value for n is 1.

TIMEON / TIMEOFF These keywords indicate whether the CPU time must be printed after each main subroutine (on) or not (off).

OUTPUT_LEVEL = n Defines the amount of output to be produced.
The following values of n may be used:

n = -1: almost all output is suppressed,

n = 0: standard amount of output,

n > 0: extra information, depending on the value of n. At this moment n < 3 is allowed.

The default value is n = 0.

POSTTYPE = n Defines how the unknowns in the centroid are translated to the vertices. This parameter makes only sense for post processing purposes, since it is applied before writing the results to the output file(s).

n = 0: Interpolation is performed in physical space. A Newton process is applied to detect the position of a vertex with respect to its four surrounding centroids. This approach is accurate but more expensive than the interpolation in computational space.

n = 1: Interpolation is performed in computational space. In case of non-smooth grids this approach is inaccurate.

The default value is n = 0.

STATIONARY means that the solution to be computed is stationary. If omitted it is assumed that the solution is time-dependent.
If this keyword is given it is checked if the stationary stop criterion is satisfied and if so, the computation is stopped.
However, the computation performed is instationary, hence the stationary solution is reached by a time-stepping process.

DISCRETIZATION This keyword indicates that the user wants to give some extra information about the space-discretization. This keyword must be followed by subkeywords containing this extra information. If omitted the standard discretization is used.
See Section 5.2

TIME_INTEGRATION This keyword must be followed by subkeywords containing information about the time-integration to be applied. Also

information as initial time, end time and time-step should be given in this part. For that reason the keyword time_integration is mandatory.
See Section 5.3

BOUNDARY_CONDITIONS This keyword must be followed by subkeywords containing information about the boundary conditions at the external boundaries. This keyword is mandatory.
See Section 5.4

COEFFICIENTS This keyword must be followed by subkeywords containing information about the coefficients of the various differential equations (momentum and transport equations) but not of the turbulence equations. This keyword is mandatory.
See Section 5.5

LINEAR_SOLVER This keyword must be followed by subkeywords containing information about the linear solver for the various differential equations (momentum, pressure, turbulence and transport equations). It concerns questions like which linear solver to use, which accuracy is required, what type of pre-conditioner and so-on. If omitted the default values are used. See Section 5.6

INITIAL_CONDITIONS This keyword must be followed by subkeywords containing information about the initial conditions for the various equations. If omitted the default values are used, which means that all degrees of freedom are initialized to zero, except the turbulence quantities, which are set to 10^{-4} See Section 5.7

TURBULENCE This keyword must be followed by subkeywords containing information about the type of turbulence modeling and if necessary about the coefficients to be used. If omitted a laminar flow is assumed. See Section 5.8

MULTI_BLOCK This keyword must be followed by subkeywords containing information about the multi block process for the various differential equations (momentum, pressure, turbulence and transport equations). It concerns questions like which type of algorithm to use, which accuracy is required and so-on. If omitted the default values are used. See Section 5.9

COLLOCATED_GRID Indicates that the momentum equations must be solved on a collocated grid instead of a staggered grid.

STAGGERED_GRID Is in fact superfluous, but has been added as opposed to COLLOCATED_GRID. It indicates that the momentum equations are solved on a staggered grid, which is in fact the default.

COMPRESSIBLE This keyword must be followed by subkeywords containing information about the compressible flow computation. If omitted the default values are used. See Section 5.10

FULLY_COMPRESSIBLE This keyword must be followed by subkeywords containing information about the compressible flow computation. If omitted the default values are used. See Section 5.10
The only difference with compressible is that not the pressure correction method will be used but that the continuity equation, the momentum equation and the energy equation are solved in a time-dependent semi implicit way. This option has not yet been implemented in Deft.
The keywords COMPRESSIBLE and FULLY_COMPRESSIBLE are mutually exclusive.

CAVITY This keyword must be followed by subkeywords containing information about the cavity model. If omitted the default values are used. See Section 5.11

MULTI_PHASE_GAS_FLOW means that the multi phase gas flow equation is solved instead of the standard equation.

FREE_SURFACE_FLOW When this keyword is found it is assumed that at least one of the boundaries is a free-surface boundary with adapted boundary conditions. The coordinates of this boundary may change in time.
The keyword may be followed by subkeywords defining information about the way the boundary must be changed in time. See Section 5.12

NO_TIME_LOOP If this keyword is found the solution is not only assumed to be stationary, but also a stationary solver is used. This means that no time-stepping algorithm is applied.
The keywords `no_time_loop` and `stationary` are mutually exclusive.

MAIN_STRUCTURE This keyword is meant to have some influence on the structure of the main time-stepping subroutine. This keyword is meant for specialists only.
The keyword may be followed by subkeywords defining information about the structure of the main program. See Section 5.13

PROFILE_INPUT This keyword is meant to define some information with respect to a flow around a (two-dimensional) profile.
At this moment it is only implemented in the unstructured finite volume program, not yet in Deft.
The keyword may be followed by subkeywords defining information about the profile. See Section 5.14

FREQUENT_OUTPUT This keyword is meant to define which quantities must be written in each time step to a special file.
This is especially useful if some quantities must be followed in time. It concerns a limited number of quantities, complete fields are only written at the time-steps indicated by tout.
At this moment it is only implemented in the unstructured finite volume

program, not yet in Deft.
The keyword may be followed by subkeywords defining information about which quantities must be written. See Section 5.15

END_INPUT defines that the end of the input has been reached. If this keyword is not available all information until the end of the file is read.

Input with respect to the restart file must be given in the part INITIAL_CONDITIONS (reading from the restart file) and TIME_INTEGRATION (writing to the restart file).

5.2 The keyword DISCRETIZATION

The keyword DISCRETIZATION indicates that the user wants to give some extra information about the space discretization. This keyword must be followed by subkeywords containing this extra information. If omitted the standard discretization is used.
The keyword may be followed by the following subkeywords:

```
MOMentum_equations
TRANSport_equation iseq
TURBulence_equation iseq
```

These subkeywords indicate to which equations the next subsubkeywords refer. In case of a transport equation or turbulence equation, the keyword must be followed by *iseq*.
iseq denotes either a number i or the keyword ALL. If a number is given this means that the information is restricted to the corresponding equation, if ALL is given it refers to all transport or turbulence equations.
These subkeywords itself may be followed by subsubkeywords that indicate whether these equations or part of it are skipped and which type of discretization is used. The following subsubkeywords are recognized:

Keyword	Default value	mandatory
SKIP/NOSKIP	noskip	no
SKIP_CONTINUITY_EQUATION	noskip	no
COUPLED/DECOUPLED	depends on grid type	no
CONVection/NOCONVection	convection	no
LIN_CONVection = type	Newton	no
DISCR_METhod = type	classical	no
UPWind = type	no	no
DIFFusion = type	standard	no
PRINT_MATrix	no	no
PRINT_GMATrix	no	no
PRINT_PMATrix	no	no
PRINT_VECtor	no	no

```
PRINT_PVECtor                          no              no
PRINT_STeps = (itime1,itime2,itstep)   (1,1,1)         no
CONSERVATIVE                           no              no
AXIsymmetric                           no              no
PRESSURE_Grad = type                   path_six        no
CONTR_VOL = type                       two_half_tr     no
NO_TIME_DERIV                          no              no
NO_PRES_GRAD                           no              no
CONSISTMOM                             no              no
```

SKIP/NOSKIP If SKIP is used the complete equation is skipped. NOSKIP is the opposite of SKIP.

SKIP_CONTINUITY_EQUATION This keyword may only be used for the momentum equations. If SKIP_CONTINUITY_EQUATION is used the continuity equation is skipped and the pressure and density do not change in time.
This keyword is for example useful if only the momentum equations must be tested. See for an example the Burgers Equation in Section 9.10.

COUPLED/DECOUPLED If COUPLED is used the momentum equations are solved as coupled system of equations. If decoupled is used the momentum equations are solved one at a time. At this moment only the combinations STAGGERED_GRID and COUPLED, or COLLOCATED_GRID and DECOUPLED are allowed.
If a staggered grid is used the default value is COUPLED, in case of a collocated grid the default is DECOUPLED.

CONVECTION/NOCONVECTION If NOCONVECTION is used, the convective terms in the momentum equations are neglected.

LIN_CONVECTION defines the type of linearization to be applied with respect to the convective terms. The following two values for type are available:

```
NEWton
PICard
```

In the case of upwinding only Picard linearization is allowed except in combination with cavity.

AXiSYMMETRIC defines that axi-symmetric coordinates (r,z) are used instead of Cartesian coordinates.

DISCR_METHOD defines the type of discretization. The following values of type are available:

```
CLAssical
WESBeek
REDUCed
BILInear_interpolation
```

The keyword CLASSICAL indicates that the classical Deft discretization as described in report 91-09 [51] for staggered grids is used. WESBEEK refers to the improved Wesseling and van Beek scheme either for staggered grids as explained in [48], or for collocated grids. In the latter case, a lack of accuracy may appear due to the too simple expression of the pressure gradient on non-smooth grids.
The keyword REDUCED implies that the cross derivatives in the stress term are eliminated using the incompressibility condition. This is only allowed if the viscosity is constant, no turbulence model is used and the flow is incompressible. This option makes it possible to compare the results with a Cartesian code and is available for staggered grids.
The keyword BILInear_interpolation indicates that bilinear interpolation is used to get quantities at the cell face center of the control volumes. At this moment, it is used for collocated grids only, to evaluate accurately the gradients and the divergences, in combination with the Wesseling and VanBeek scheme which allows to calculate the stress term and the Laplacian in the pressure-correction equation. The method is explained in [27].

UPWIND defines the type of upwinding applied. The following values of type are available:

```
NONe
FIRst_order
HYBrid
HIGher_order, KAPpa = kappa
TVD
LUDs
FROmm
CUI
QUIck
MINmod
SOUcup
SUPerbee
VAN_Leer
HARmonic
HLPa
ISNas
NOTable
VAN_Albada
OSPre
DAVis
```

```
BSOu
MUScl
KORen
SMArt
UMIst
NFIRst_order
STREAM_FIRst, method = g
OLD_NONe
OLD_FIRst_o
```

Mark that if upwind is applied only Picard linearization of the convective terms may be utilized, except in combination with cavity.

The keyword NONE indicates that no upwinding is applied, hence the standard central difference scheme is used.
The keyword FIRST_ORDER indicates that the standard first order upwind scheme is used.
The keyword HYBRID indicates that the standard hybrid central/upwind scheme is used.
With the keyword HIGHER_ORDER a higher order upwind scheme is activated. The keyword KAPPA defines the parameter κ which must be in the range [-1,1] and defines the type of scheme used. For example $\kappa = \frac{1}{2}$ gives the QUICK scheme and $\kappa = 0$ the Fromm's scheme. If omitted the default value $\kappa = \frac{1}{2}$ is used.
In order to get a higher order upwind scheme which preserves monotonicity of the solution, the keyword TVD must be chosen. This keyword must be followed by a subkeyword which specifies a flux limiter:

```
LIMiter = limtype
```

where limtype may take one of the following values:

```
sweby_phi_limiter [,phi=phi]
r_kappa_limiter [,kappa=k]
mr_kappa_limiter [,kappa=k]
symm_ratio_limiter [,mbound=m]
pl_kappa_limiter [,kappa=k, mbound=m, alpha=a]
mplone_kappa_limiter [,kappa=k, mbound=m, alpha=a]
mpltwo_kappa_limiter [,kappa=k, mbound=m, alpha=a]
symm_pl_kappa_limiter [,kappa=k, mbound=m]
```

The keyword SWEBY_PHI_LIMITER indicates that one of the limiters of this type, which is specified by the parameter PHI, is used. For example $\Phi = 1$ defines the Minmod limiter.
If omitted the default value $\Phi = 1$ is used.

The keyword R_KAPPA_LIMITER indicates that one of the limiters of

this type, which is specified by the parameter KAPPA, is used. For example $\kappa = \frac{1}{2}$ defines the ISNAS limiter.
If omitted the default value $\kappa = \frac{1}{2}$ is used.

The keyword MR_KAPPA_LIMITER indicates that one of the limiters of this type, which is specified by the parameter KAPPA, is used. With this class a more accurate solution may be obtained.
If omitted the default value $\kappa = \frac{1}{2}$ is used.

The keyword SYMM_RATIO_LIMITER indicates that one of the limiters of this type, which is specified by the parameter MBOUND, is used. For example $M = 1$ defines the Van Albada limiter.
If omitted the default value $M = 1$ is used.

The keyword PL_KAPPA_LIMITER indicates that one of the limiters of this type, which is specified by the parameters KAPPA, MBOUND and ALPHA, is used. For example $\kappa = \frac{1}{2}, M = 4, \alpha = 0$ gives the SMART scheme.
If omitted the default values $\kappa = \frac{1}{2}$, $M = 2$ and $\alpha = 0$ are used.

The keywords MPLONE_KAPPA_LIMITER and MPLTWO_KAPPA_LIMITER indicate that one of the limiters of these types, which is specified by the parameters KAPPA, MBOUND and ALPHA, is used. With these classes a more accurate solution may be obtained.
If omitted the default values $\kappa = \frac{1}{2}$, $M = 2$ and $\alpha = 0$ are used.

The keyword SYMM_PL_KAPPA_LIMITER indicates that one of the limiters of this type, which is specified by the parameters KAPPA and MBOUND, is used. For example $\kappa = \frac{1}{2}, M = 2$ gives the UMIST limiter.
If omitted the default values $\kappa = \frac{1}{2}$ and $M = 2$ are used.

The keywords LUDS, FROMM, CUI, QUICK, MINMOD, SOUCUP, SUPERBEE, VAN_LEER, HARMONIC, HLPA, ISNAS, NOTABLE, VAN_ALBADA, OSPRE, DAVIS, BSOU, MUSCL, KOREN, SMART and UMIST are the well-known and frequently used schemes or limiters in the literature. For details and further references, see Section 2.2.2.

The keyword NFIRST_ORDER stands for a first order upwind approach for tudfinvol (unstructured finite volume solver). The keyword STREAM_FIRST is obsolete.
The keywords OLD_NONE and OLD_FIRST_O are are only available for tudfinvol (unstructured finite volume solver). They stand for respectively central interpolation and first order upwind using an old approach to these interpolation schemes. For more information, see the manuals for tudfinvol.

DIFFUSION defines whether the diffusion terms in the transport and tur-

bulence equations are discretized in the standard way or by a special monotonous scheme. The following values of type are available:

```
STandard
HALF_Monotonous
MOnotonous
```

The keyword STANDARD indicates that the standard central difference scheme is applied, MONOTONOUS that an adapted scheme is used to get a monotonous scheme even if the cells are skewed, see [67]. However, this scheme is one-sided and thus first-order accurate. The keyword HALF_Monotonous gives second-order accurate scheme which is under certain circumstances monotone, see the thesis of Demirdzic [11].

Remarks:

- At this moment all the upwind schemes mentioned above, except the hybrid upwind scheme, can be used in the case of momentum equations.
- In order to employ the upwind schemes for the momentum equations, Picard linearization should be used (see the keyword LIN_CONVECTION).
- At this moment monotonous schemes with respect to diffusion are only possible for transport and turbulence equations.
- The default discretization for the convective terms in the momentum equations is the central difference scheme and in the turbulence equations is the hybrid upwind scheme.

PRINT_MATRIX indicates that the standard matrix must be printed. The matrix is printed for all steps indicated by PRINT_STEPS. Mark that in general the matrix is large and hence printing of the matrix produces a large amount of output.
This option is only meant for debug purposes. If a row of the matrix is completely zero this row will not be printed.
The layout of the print may be influenced by the isnas.dbg file.

PRINT_GMATRIX indicates that the gradient matrix must be printed. This option makes only sense for the momentum equations.

PRINT_PMATRIX indicates that the pressure matrix must be printed. This option makes only sense for the momentum equations.

PRINT_VECTOR indicates that the standard right-hand side must be printed. The right-hand side is printed for all steps indicated by PRINT_STEPS.

PRINT_PVECTOR indicates that the pressure right-hand side must be printed. This option makes only sense for the momentum equations. The right-hand side is printed for all steps indicated by PRINT_STEPS.

PRINT_STEPS indicates that the printing defined by the options PRINT (P)VECTOR or (G/P)MATRIX must be carried for the time steps ITIME1, ITIME1+ITSTEP, ITIME1+2×ITSTEP, ... , ITIME2

CONSERVATIVE indicates that a conservative discretization of the convective terms must be used. This option is only available in 2D for the classical discretization.
At this moment a conservative discretization usually does not improve the computations except in the combination of upwind and discontinuous coefficients.

PRESSURE_GRAD gives the user the opportunity to compute the pressure gradient using distinct methods (only for tudfinvol). The following values of type are available:

```
PATH_Six
PATH_Three
AUXLine
FOURPoint
CONTINt
```

Keyword PATH_SIX indicates that the ordinary path-integral method using six surrounding pressure points is used. Keyword PATH_Three indicates that the path-integral method using a three point stencil is used. Keyword AUXLINE indicates that auxiliary points, between the stencil points, are used. Keyword FOURPOINT indicates that the four quadrant method is used. Keyword CONTINT indicates that the pressure gradient is computed using the contour integral approach.

CONTR_VOL gives the user the opportunity to use different control volume for the momentum equation (only for tudfinvol). The following values are available:

```
TWO_WHOLE_TR
TWO_HALF_TR
```

Keyword TWO_WHOLE_TR indicates that the control volume for a certain face consists of the two adjacent triangles. Keyword TWO_HALF_TR indicates that the control volume for a certain face consists of the half of the two adjacent triangles.

NO_TIME_DERIV indicates that the time derivative is omitted.

NO_PRES_GRAD indicates that the pressure gradient in the momentum equation is omitted.

CONSISTMOM indicates that the consistency of a term in the momentum equation is investigated.

5.3 The keyword TIME_INTEGRATION

The keyword TIME_INTEGRATION indicates that the user wants to define information about the time-integration process. This keyword must be followed by subkeywords containing this information.
The following subsubkeywords are recognized:

Keyword	Default value	mandatory
METHOD = n	THETA	no
TINIT = t0	0	no
TEND = (t1,t2,t3,...,tl)	1	no
THETA = (theta1, theta2,...)	1	no
TSTEP = (dt1,dt2, ...)	0.1	no
TOUTInit = t	t1	no
TOUTEnd = t	t1	no
TOUTStep = DT	dt	no
TOUTStep = DT	dt	no
ABS_STATIONARY_ACCURACY = eps	0	no
REL_STATIONARY_ACCURACY = eps	0	no
OUTSESSION = sessionname	1	no
RINIT = t0	TOUTEND	no
REND = t1	TOUTEND	no
RSTEP = tstep	TOUTSTEP	no
FORCE_DELETION = n	NO	no
RESTART = n	NONE	no
OUTPUT = n	DUMP	no
NORM = type	LTWO	no
NSUBSTEPS_TURBULENCE = n	1	no
PRESS_CORR_TIME_ITERATION	no	no
ABS_PRESS_CORR_ACCURACY = eps	1d-4	no
RELAXATION_PRESS_CORR = r	0	no

METHOD = n defines the type of time-integration method to be used. The following values of n are available:

```
THETA
FRACTIONAL_STEP
GENERALIZED_THETA
```

THETA The classical θ-method with exactly one value of θ is used. For $\theta = 1$, this is the classical Euler implicit method and for $\theta = \frac{1}{2}$ the Crank-Nicolson scheme. Only values of θ in the range $[0.5, 1]$ are allowed. In this case the default value of θ is 1.

FRACTIONAL_STEP defines the fractional step method defined in Section 2.3. The fractional step method uses three fractional steps

consisting of six values of θ. The default values for θ are:

$$\theta_1 = \theta_5 = \beta\theta, \quad \theta_3 = \alpha(1-2\theta), \quad \theta_2 = \theta_6 = \alpha\theta, \quad \theta_4 = \beta(1-2\theta) \tag{5.1}$$

with

$$\alpha = \frac{1-2\theta}{1-\theta}, \quad \beta = \frac{\theta}{1-\theta}, \quad \theta = 1 - \frac{\sqrt{2}}{2} \tag{5.2}$$

GENERALIZED_THETA defines the generalized θ method defined in Section 2.3. The number of steps used in this method is implicitly defined by the input after $THETA$. The number of θ-values given must be equal to two times the number of steps. If no θ-values are given the default number of three steps with the following θ-values are used.

$$\theta_1 = \theta_5 = \frac{\alpha}{2}, \theta_3 = 0, \theta_2 = \theta_6 = \alpha\frac{\sqrt{3}}{6}, \theta_4 = \alpha\frac{\sqrt{3}}{3} \tag{5.3}$$

with

$$\alpha = \left(1 + \frac{2}{\sqrt{3}}\right)^{-1}. \tag{5.4}$$

TINIT $= t_0$ defines the initial time.

TEND $= t_1$ defines the end time of the integration.
If the user wants to use various time-steps Δt, for each new time-step a separate end time must be given. The number of time-steps and the number of end times must be equal.
Of course it is necessary that $t_1 < t_2 < t_3 ...$

TSTEP $= \Delta t$ defines the time step of the integration.
If the user wants to utilize different time steps for different time intervals he may give a number of time steps and a number of end times provided these numbers are equal.
For example TEND $= t_1, t_2, t_3$; TSTEP $= \Delta t_1, \Delta t_2, \Delta t_3$ means that in the interval $[t_0, t_1]$ time step Δt_1 is used, in the interval $[t_1, t_2]$ time step Δt_2 and in the interval $[t_2, t_3]$ time step Δt_3.

THETA $= \theta$ defines the parameter in the θ method.
In case of the fractional θ method the user must give exactly six θ-values, unless the default values are used.
In case of the generalized θ-method the user must give $2 \times NFRAC$ θ-values, where $NFRAC$ is the number of fractional steps, unless the default values are used.

TOUTINIT $= t$ defines the first time at which output of all solutions to the output file is written. If this parameter is not defined only the last time-step is written.

TOUTEND = t defines the last time at which output of all solutions to the output file is written. The default value is TEND.

TOUTSTEP = DT defines the frequency with which output of all solutions to the output file is written. The default value is Δt_1, which means that all time-steps from TOUTINIT to TOUTEND are written.

ABS_STATIONARY_ACCURACY = ϵ_1 indicates that the solution is assumed to be stationary and that the process stops as soon as steady state has been reached. This is the case when

$$\|u^{k+1} - u^k\| < \frac{1-\lambda}{\lambda}(\epsilon_1 + \|u^k\|\epsilon_2), \tag{5.5}$$

where λ is the computed speed of convergence,
ϵ_1 is the $ABS\_STATIONARY\_ACCURACY$ given and
ϵ_2 the $REL\_STATIONARY\_ACCURACY$.
u^k is the vector of all unknowns at the k^{th} time-step.
In any case the process stops if t reaches TEND.

REL_STATIONARY_ACCURACY = ϵ_2 defines the relative accuracy part of the stationary stopping criterion. If neither the absolute nor the relative stationary accuracy are given, the solution is assumed to be instationary.

OUTSESSION = *sessionname* sets the name of the session to be written to the restart file. If *sessionname* is a new name of a session in the restart file, then if 'RESTART = overwrite' the last session in the restart file will be overwritten. If 'RESTART = append' the session will be appended to the restart file.
If *sessionname* is an existing name of a session in the restart file, then if 'RESTART = overwrite' the session in the restart file will be overwritten. If 'RESTART = append' the session will be appended to the restart file from the time given by RINIT.
At this moment sessionname is restricted to numbers.

RINIT = t_0. The first solution will be written to the restart file at $t = t_0$.

REND = t_1. The last solution will be written to the restart file at $t = t_1$.

RSTEP = *tstep*. Solutions will be written at times $t_k = t0 + k \times tstep$.

FORCE_DELETION = n. When inserting a new session in the restart file, all sessions following that session will be deleted. $n = yes$ indicates that this is allowed, $n = no$ means not allowed. With $n = no$, the Deft program will print an error message and stop execution.

RESTART = n. Indicates if and how the solution is written to the restart file (isnasback). The following values for n are available:

```
append
overwrite
none
```

append means that the solution must be appended to the specified session. Append can only be used if the current job is restarted from the same session that we want to append to. Also, the numbers of degrees of freedom must be the same. Specifically, if the input job (INSESSION) is laminar, the output job cannot be turbulent.

overwrite means that the indicated session must be overwritten if it already exists. Otherwise, it is appended to the restart file.

none means that no restart file will be written.

The default value is `none`

If there are any other sessions in the restart file after the indicated session, these will be deleted if the FORCE_DELETION option is present. Otherwise the Deft program will print an error message and stop execution.

OUTPUT $= n$ indicates in which form the solution is written to the restart file.
The following values for n are available:

```
dump
Cartesian
```

dump means that the computed solution is written without applying any transformation. This option is only useful if the solution is reused with exactly the same grid. In that case it is also the most accurate one.

Cartesian implies that the velocity components are transformed from contravariant (is computational) ones into Cartesian (is physical) components. This option is less accurate than the option dump and requires an extra transformation. However, if the solution must be interpolated to a different grid (for example a refined mesh), it is necessary to make this transformation since the contravariant solution is grid dependent.

NORM $=$ *type* indicates what type of norm is used to compute the stopping criterion. Possible values for *type* are:

```
ltwo
max
```

ltwo The L_2 norm is used.

max The max norm is used.

Default value: L_2 norm.

NSUBSTEPS_TURBULENCE $= n$ indicates the number of sub-steps the time integration for the turbulence equations is subdivided into. This means that in each time step, the turbulence equations are solved with a time-step equal to $\frac{\Delta t}{n}$.
The reason to use sub-steps is that the time scale of the turbulence equations may be much smaller than that of the momentum equations. Hence for stability reasons it may be necessary to use a smaller time step. If an overall smaller time step is used, more work per time step must be carried out.
Default value: 1

PRESS_CORR_TIME_ITERATION indicates that an iteration per time step is performed in order to make the pressure correction method implicit. Hence in each time step several pressure correction steps are carried out. In this way the continuity equation could be satisfied more accurately.

ABS_PRESS_CORR_ACCURACY $= \epsilon$ defines to which accuracy the pressure correction iteration must be carried out (infinite norm).

RELAXATION_PRESS_CORR $= \alpha$ defines a relaxation parameter for the update of the pressure during the iteration. The pressure is updated in the following way:

$$p^{new} = p^{old} + (1 - \alpha)\delta p \tag{5.6}$$

Default value α=0; $(-0.5 \leq \alpha \leq 0.5)$

5.4 The keyword BOUNDARY_CONDITIONS

The keyword BOUNDARY_CONDITIONS must be followed by a description of the boundary conditions. This means that both the types and values of the boundary conditions must be prescribed and the sub-faces where the boundary condition is imposed. This description in general looks like:

[subface description] [boundary conditions for velocity] [boundary conditions for each transport equation] [boundary conditions for turbulence quantities]

All items in this sequence have to be in this order!
The description of the the set of subfaces where the boundary condition must be imposed is different depending on the type of grid generation used.

If the SEPRAN grid generator is used, the concept of curves and surfaces is applied. In this case the keyword `curves` or `surfaces` is used to describe subfaces. See Section 5.4.1 for a description.

Besides SEPRAN, Deft also supports the LiSS grid generator. In this case it is necessary to describe the set of subfaces using the keywords `BLOCK, FACE` and `SUBFace` keywords as described in Section 5.4.2.

5.4.1 Using CURVE to describe subfaces

The following types of curve description are recognized when SEPRAN grid generation is used:

```
CURVE i TO j
CURVE i
```

CURVE i TO j means that the boundary conditions refer to all SEPRAN curves i, i+1, i+2, ... ,j.
CURVE i means of course that the boundary conditions is restricted to curve i only.

5.4.2 Using BLOCK, FACE and SUBFACE to describe subfaces

The BLOCK keyword describes the blocks at which the boundary condition must be imposed. Blocks may be described as follows:

```
BLOCK i TO j
BLOCK i
```

The first means blocks i to j and the second means only block i. The BLOCK keyword is optional for single block context. After describing the blocks, the faces **must** be described. Not doing so will result in an error from the preprocessor. Faces are described as follows:

```
FACE i TO j
FACE i
```

After describing the face number, the SUBFACE numbers may be specified as follows:

```
SUBFace i TO j
SUBFace i
```

If the subface numbers are not specified, the entire face is assumed. A subface may only be prescribed once the face number has been prescribed.

Examples:

- A single block problem, the block keyword is optional:

```
face 1: inflow 1.0
face 2: outflow
face 3 to 4: noslip
```

- Boundary conditions may be specified in any order so

```
block 1:
  face 1: noslip
  face 2: outflow

block 2:
  face 3: noslip
```

is equivalent to

```
block 1:
  face 1: noslip

block 2:
  face 3: noslip

block 1 face 2 : outflow
```

- A subface may only be specified after the face has been specified, so

```
block 1 face 2 subface 3: noslip
block 2        subface 2: outflow
```

gives an error because a face for block 2 has not been specified.

5.4.3 Boundary condition types and values

Boundary conditions for the velocity

In case of staggered grid, for the velocity the following types of boundary conditions may be given:

```
NOSLip
INFlow umax
OUTFlow
PARALlel_outflow
FREESlip
UN = g
UT = g
UX = g
UY = g
UZ = g
SIGMANN = g
SIGMANT = g
WALL_Functions = s [, ROUGHness = h]
```

```
PERIODIC i
U_LEN = g
ANGLE = g
SUPEROUTFLOW
```

Meaning of the various boundary conditions:

NOSLIP The boundary condition NOSLIP effectuates the noslip boundary condition $u_n = 0$, $u_t = 0$.

INFLOW The boundary condition INFLOW prescribes a parabolic velocity profile in the normal direction and a zero tangential velocity. The parameter UMAX defines the maximal value of the inward normal component.

OUTFLOW The boundary condition OUTFLOW prescribes the least restrictive outflow boundary condition, viz. stress equals zero at the boundary ($\sigma^{nn} = 0$, $\sigma^{nt} = 0$). In most applications this boundary condition may be interpreted as pressure zero and no restriction to the tangential velocity component.

PARALLEL_OUTFLOW The boundary condition PARALLEL_OUTFLOW prescribes an alternative outflow boundary condition, tangential component of the velocity zero and normal component of the stress zero ($u_t = 0$, $\sigma^{nn} = 0$). In most applications this boundary condition may be interpreted as a parallel outflow with zero pressure.

FREESLIP The boundary condition FREESLIP prescribes a boundary condition that may be used for example for free slip boundaries. In fact the actual boundary condition is normal component of the velocity is zero and the shear stress is zero ($u_n = 0$, $\sigma^{nt} = 0$)

UN, UT The boundary condition UN = g prescribes the normal component of the velocity. With normal we mean the outward directed normal. This boundary condition may only be used in combination with the boundary condition UT = g.

Here and in the rest of this section the parameter g may take one of the forms:

```
number
FUNC = i
TIME_FUNC = i
```

where number indicates the value of the component and FUNC=i as well as TIME_FUNC=i refers to a user function subroutine usfunb (6.3), which is called by the ISNAS program in the following way:

```
value = USFUNB ( i, x, y, z, t )
```

If TIME_FUNC is used it is assumed that the boundary condition is time-dependent, which means that the boundary condition is computed in each time-step again. All other boundary conditions are assumed to be time-independent and are computed only once.

The boundary condition UT $= g$ prescribes the tangential component of the velocity. The tangential direction in R^2 is defined as the direction perpendicular to the normal direction in the counter clockwise sense. This boundary condition may only be used in combination with the boundary condition UN $= g$.

UX, UY, UZ The boundary conditions UX $= g$, UY $= g$ and UZ $= g$ prescribe the Cartesian component of the velocity in the indicated direction. If one of them is given, the other ones should be given also, except in R^2 where there is no reason to prescribe UZ.

SIGMANN, SIGMANT The boundary conditions SIGMANN $= g$ and SIGMANT $= g$ prescribe the normal stress and the shear stress at the boundary respectively. The definition of normal and tangential vector is the same as for the velocity. If one of these boundary conditions is used at a boundary, the other one should be used also.

PERIODIC The keyword PERIODIC is used to indicate that a periodical boundary condition must be satisfied. This boundary condition must be given in the form:

```
CURVE i = PERIODIC j
```

meaning that the curves i and j are coupled through periodical boundary conditions and hence are actually the same boundary, or

```
SURFACE i = PERIODIC j
```

In this case the surfaces i and j are the same and have periodical boundary conditions.
Mark that `CURVE i = PERIODIC j` also implies that the boundary conditions `CURVE j = PERIODIC i` must be given. The same is true for surfaces. The reason is that Deft requires boundary conditions on each side.

If periodical boundary conditions are prescribed for the velocity, they are also automatically prescribed for the turbulence quantities, but not for the transport equations.
Periodical boundary conditions have not yet been implemented in combination with faces.

WALL_FUNCTIONS The boundary condition WALL_FUNCTIONS = s defines a law of the wall boundary condition for the momentum equations in case of turbulent flows. The parameter s in WALL_FUNCTIONS may take one of the forms:

```
SMOOTH
ROUGH
```

In the last case the roughness must be given by

```
ROUGHNESS = h
```

where h is the average roughness height of a rough wall.
In this case the boundary conditions for the velocities at the wall are given as follows:

$u_n = 0$ and $\sigma_{nt} = \tau_w$, where τ_w is computed with a log-law based wall condition depending on smoothness or roughness of the boundary. The user defines only the roughness or smoothness.

U_LEN,ANGLE The boundary condition U_LEN = g, ANGLE = g prescribes the the velocity vector. With U_LEN we intend **u**, and with ANGLE we intend the angle, in degrees, between the x-axis and the direction of the flow, the angle being positive in counterclockwise direction. For profile flow, ANGLE is usually called angle of attack.

SUPEROUTFLOW At supersonic outflow boundary nothing with respect to the momentum equation is prescribed; usually only a Neumann condition for the transport equations is given. In order to identify supersonic outflow boundaries the keyword SUPEROUTFLOW must be used.

In case of a collocated grid, the momentum equation is written in a decoupled way at this moment. The primitive variables are used. Only Dirichlet boundary conditions are available, for the time being. Boundary conditions are given by:

```
U_MOMentum = DIrichlet = g
V_MOMentum = DIrichlet = g
```

The parameter g can take one of the forms previously described.

Restriction:
The velocity requires exactly one boundary condition for the normal and one for the tangential direction (2D) or two for the tangential direction in 3D.

Boundary conditions for the transport equations

For the transport equation the following types of boundary conditions may be given:

```
TRANSport a = description
```

with description:

```
DIrichlet = g
NEumann = g
ROBbins: ALPha=g, H=g
MIxed: ALPha=g, H=g
WALL_Temperature = g
PERIODIC i
```

where g may take one of the forms $< number >$ or FUNC=i as described for the velocity boundary conditions and a is the sequence number of the transport equation.
These boundary conditions have the following meaning:

DIRICHLET The Dirichlet boundary condition prescribes the transport quantity T at the corresponding part of the boundary by $T = g$.

NEUMANN The Neumann boundary condition prescribes the flux of the transport quantity T at the corresponding part of the boundary by $\kappa_{ij} n_i \frac{\partial T}{\partial x_j} = g$

ROBBINS, MIXED The Robbins or mixed boundary condition prescribes a linear combination of the flux of the transport quantity T and T itself at the corresponding part of the boundary by $\alpha T + \kappa_{ij} n_i \frac{\partial T}{\partial x_j} = h$

WALL_TEMPERATURE prescribes the Dirichlet boundary condition for the temperature T at the corresponding part of the boundary by $T = g$. Only meant for turbulent flows with heat transfer in which the wall temperature must be provided in order to compute the heat flux at the wall using wall functions.

PERIODIC indicates that a boundary has periodical boundary conditions in exactly the same way as for the velocity.

Boundary conditions for the turbulence quantities

For the turbulence quantities the following types of boundary conditions may be given:

```
K_DIrichlet = g
K_NEumann = g
EPS_DIrichlet = g
EPS_NEumann = g
EPS_ASYmptote
OMEGA_DIrichlet = g
OMEGA_NEumann = g
OMEGA_ASYmptote
```

K_DIRICHLET prescribes a Dirichlet boundary condition for k, which means k given at the corresponding part of the boundary.

K_NEUMANN prescribes a Neumann boundary condition for k, which means $\frac{\partial k}{\partial n}$ given at the corresponding part of the boundary.

EPS_DIRICHLET prescribes a Dirichlet boundary condition for ε, which means ε given at the corresponding part of the boundary.

EPS_NEUMANN prescribes a Neumann boundary condition for ε, which means $\frac{\partial \varepsilon}{\partial n}$ given at the corresponding part of the boundary.

EPS_ASYMPTOTE prescribes the asymptotic behaviour of ε near the wall. Only meant for low-Reynolds-number modeling, in which ε must asymptote to the nonzero value at the wall in order to keep the equation of turbulent energy in balance.

OMEGA_DIRICHLET prescribes a Dirichlet boundary condition for ω, which means ω given at the corresponding part of the boundary.

OMEGA_NEUMANN prescribes a Neumann boundary condition for ω, which means $\frac{\partial \omega}{\partial n}$ given at the corresponding part of the boundary.

OMEGA_ASYMPTOTE prescribes the asymptotic behaviour of ω near the wall, which is given by

$$\omega = \frac{N_\omega \nu}{Y^2}, \qquad Y^+ < 5.0 \tag{5.7}$$

where

$$N_\omega = \begin{cases} 6/\beta, & \text{without viscous corrections} \\ 2/\beta^*, & \text{with viscous corrections} \end{cases} \tag{5.8}$$

The correction can be made by the subkeyword VISCOUS_CORRECTIONS as prescribed in the keyword TURBULENCE. It should be noted that grid refinement near the wall must be such that the wall-coordinate Y^+, for the point nearest to the wall, must not exceed 5.0. If this ever happens, an error will occur and the run will be terminated.

If for the velocity a law of the wall has been used then the boundary conditions for k and ε, are respectively

$$\frac{\partial k}{\partial n} = 0 \tag{5.9}$$

$$\varepsilon = \frac{c_\mu^{3/4} k^{3/2}}{\kappa Y} \tag{5.10}$$

and no explicit boundary conditions should be given.

Remark: it is necessary to give boundary conditions for the external subfaces only. Internal boundaries are treated by the multi block process.

5.5 The keyword COEFFICIENTS

The keyword COEFFICIENTS starts the block with information about the coefficients. This block is mandatory.
The keyword may be followed by the following subkeywords:

```
MOMentum_equations
TRANSport_equation i
```

These subkeywords indicate to which equation the next subsubkeywords refer. In case of a transport equation the keyword must be followed by a number indicating the sequence number of the transport equation.
These subkeywords itself may be followed by subsubkeywords that define the coefficients.
The following subsubkeywords are recognized after the keyword MOMENTUM_EQUATIONS:

Keyword	Default value	mandatory
MU = g	1	no
RHO = g	1	no
FORCE1 = g	0	no
FORCE2 = g	0	no
FORCE3 = g	0	no
MASS_FRaction = g	0	no
INTERFAce_drag = g	0	no
C_1 = g	0	no
C_2 = g	0	no
C_3 = g	0	no

These coefficients have the following meaning: g may take one of the forms $< number >$ or FUNC=i as described for the velocity boundary conditions.
If FUNC $= i$ is used a user written function subroutine is called depending on the parameter i, in the following way:

$0 < i < 100$ the function subroutine usfunc (6.4) is called:

```
value = USFUNC ( i, x, y, z, t ).
```

$100 < i < 200$ the function subroutine usfunc1 (6.5) is called:

```
value = USFUNC1 ( i-100, x, y, z, t, soluts, ndegfd ).
```

$1000 < i < 10000$ the subroutine usfilc (6.6) is called:

```
call usfilc ( i-1000, coefs, ncoefs, icoef, ni, nj, nk, ndim,
              nvirtual, coor, solut, ndegfd, t )
```

i > 10000 corresponds to special values.

i = 10000 The user may fill a series of time and space dependent coefficients in one call of subroutine usfilcsp (6.7). Internally all coefficients have a sequence number. In case of the momentum equations the sequence numbers are:

1. μ
2. ρ
3. f_1
4. f_2
5. f_3
6. ϵ
7. β
8. C_1
9. C_2
10. C_3

The coefficients are filled according to this sequence. If the user uses for one of the coefficients the value $g = 10000$, he may fill a series of coefficients himself by subroutine USFILCSP. However, if for these coefficients also another input is defined (except 0), the sequence of the coefficients is important, with respect to overwriting. The best is way is to define only one coefficient with $g = 10000$ and to skip all coefficients that are filled by subroutine USFILCSP.
The user is supposed to fill the coefficients in all cell centers in one call. The input consists of the number of cells in the various directions, the co-ordinates, the Cartesian velocity components in the vertices at the previous time level, as well as all solution vectors at the previous time level. The call is:

```
call USFILCSP ( coefs, ncoefs, ni, nj, nk, ndim, nvirtual,
                coor, solut, ndegfd, t, veloc )
```

i = 10001 This possibility is especially meant for the construction of the right-hand side of the energy equation in case of compressible flow.
A user written subroutine USFILSRC is required.
See (6.12) for a description.
The user is supposed to fill the coefficient in all cell centers in one call.
The call is:

```
      call usfilsrc ( coefs, ni, nj, nk, ndim, nvirtual,
     +                coor, solut, ndegfd, time, eddy, axisym )
```

i = 10002 This possibility is especially meant to compute the viscosity as function of other parameters.
A user written subroutine USCOMPVISC is required.
See (6.13) for a description.
The user is supposed to fill the coefficient in all cell centers in one call.
The call is:

```
      call uscompvisc ( coefs, eddy, ni, nj, nk, nvirtual,
     +                  ndim )
```

MU defines the dynamical viscosity μ of the fluid. If omitted the default value 1 is used.

RHO defines the density ρ of the fluid. If omitted the default value 1 is used. In case of compressible ρ is an unknown and for that reason it is necessary to give the coefficient RHO the value 1 (the default value), or no value at all.

FORCE1, FORCE2, FORCE3 define the external body forces for the fluid in the Cartesian directions. For each one omitted the default values 0 is used.

MASS_FRAC is only used in combination with multi phase gas flow.
In that case it defines the mass fraction ϵ.

INTERFACE_DRAG is only used in combination with multi phase gas flow.
In that case it defines the interface drag coefficient β.

C_1, C_2, C_3 are at this moment only used in combination with multi phase gas flow.
These coefficients define the zero-th order term in the equations, i.e. the u_i equation gets the extra term $+C_i u_i$ in the equation. This option is only implemented for Cartesian grids, where the contravariant direction is identical to the Cartesian direction.

The keyword TRANSPORT_EQUATION a may be followed by the following subkeywords:

Keyword	Default value	mandatory
CAPacity = g	1	no
DIFFusion = g	1	no
DIFXX = g	1	no
DIFXY = g	0	no
DIFYY = g	1	no
DIFXZ = g	0	no
DIFYZ = g	0	no
DIFZZ = g	1	no
SOURCE = g	0	no
CONStant = g	0	no

The meaning of these coefficients is implicitly defined by the differential equation:

$$c^* \frac{DT}{Dt} + \operatorname{div} k \operatorname{grad} T + CT = F, \tag{5.11}$$

CAPACITY defines the capacity c^*.

DIFFUSION defines the diffusion k, assuming it is a scalar.

DIFFXX, DIFFXY, DIFFXZ, DIFFYY, DIFFYZ, DIFFZZ define the diffusion, assuming it is a tensor quantity.

SOURCE defines the source F.

CONSTANT defines the constant C.

5.6 The keyword LINEAR_SOLVER

The keyword LINEAR_SOLVER indicates that the user wants to give some extra information about the solution of the linear systems. One may for example think about termination criteria, type of linear solver, type of preconditioner and so on.
This keyword must be followed by subkeywords containing this extra information. If omitted the standard discretization is used.
The keyword may be followed by the following subkeywords:

```
MOMentum_equations
TRANSport_equation iseq
PRESsure_equation
TURBulence_equation iseq
```

These subkeywords indicate to which equations the next subsubkeywords refer. In case of a transport equation or turbulence equation, the keyword must be followed by either a number or the keyword ALL. If a number is given this means that the information is restricted to the corresponding equation, if ALL is given it refers to all transport or turbulence equations.
These subkeywords itself may be followed by subsubkeywords that contain information about the linear solvers. The following subsubkeywords are recognized:

Keyword	Default value	mandatory
SOLVER = s	GMRES	no
MAXITer = n	200	no
ABSAccuracy = abs	0	no
RELAccuracy = rel	dependent	no
CONDAccuracy = con	0	no
DIVAccuracy = div	1e-4	no
PREConditioner = pre	dependent	no

```
POSTConditioner = post          dependent       no
POLYPREConditioner = n            0             no
AMOUnt_of_output = out            0             no
ERROroccurance = err            STOP            no
GMREStart = n                    40             no
ORTHogonal = n                  dependent       no
MODIFY = alpha                  dependent       no
STARTVector = start             dependent       no
RITZvalues = n                    0             no
PRINT_SOLution                    no            no
PRINT_STeps                     (1,1,1)         no
CG_RELax = omega                 0.7            no
CG_INNer = n                      1             no
NEUMayer                        neumayer        no
NO_NEUMayer                     neumayer        no
MAXLEvel = n                      0             no
SMOOTH_steps = n                  0             no
FILL_IN = n                       8             no
```

Meaning of the various subsubkeywords:

SOLVER defines the type of solver. Available types for *s* are:

```
CGS
GMRES
GCR
CGSTAB
MULTIgrid
```

Explanation:

CGS means standard Conjugate Gradients Squared method.

GMRES means GMRES method or GMRESR(m) method. GMRESR(m) is used if Polypreconditioner is used, where m is equal to the parameter n read.

GCR means the special case of GMRESR(1), which for efficiency reasons has been programmed separately. GCR may be regarded as a version of GMRES which allows for both restart and truncation.

CGSTAB means the standard CGSTAB method of Sonneveld and v.d. Vorst.

MULTIGRID means that the linear equations are solved by multigrid. This option has not yet been implemented.

MAXITER defines the maximum number of iterations

ABSACCURACY defines the absolute accuracy, if 0 (default value) a relative accuracy is used

RELACCURACY defines the relative accuracy, default values are:
1d-4 for the transport, turbulence and momentum equations and
1d-6 for the pressure equation.
The relative accuracy is measured by measuring the decrease of the residual. This does not necessarily mean that the relative error of the solver is identical to this number. If both the absolute and relative accuracy are given, the sum of the two is used as termination criterion.

CONDACCURACY makes only sense in the case of the GMRES method. It overrules the options ABSACCURACY and RELACCURACY. In this case the factor *con* means relative accuracy in the common sense.

DIVACCURACY defines a truncation criterion for the pressure equations only. It is only used if `div` > 0. In that case the linear pressure solver stops if

$$\|R^i\| < rel * \|R\| + \frac{\text{div} * \|u\|}{dt} \tag{5.12}$$

If rel $= 0$, we have: $\frac{\|divu\|}{\|u\|} <$ `div`

PRECONDITIONER defines the type of preconditioner. Available values for *pre* are:

```
NONE
DIAGonal
ILUD
ILU
ILU_FILL
TEST
```

Explanation:

in the case of diagonal only a diagonal scaling is used

ILUD uses an ILU decomposition with only the diagonal D updated.

ILU uses the standard ILU(0) preconditioning, where all non-zero elements are adapted.

ILU_FILL uses the an ILU preconditioning, where all non-zero elements are adapted extended with a n extra diagonals. The number of extra diagonals n is given by `FILL_IN = n`

TEST means a user written preconditioner only meant for research purposes.

Default values are:
In case of the momentum equation: ILUD.
In case of the transport or turbulence equations: ILU.
In case of the pressure equation: ILU.

POSTCONDITIONER defines that a postconditioner is used instead of a preconditioner. The possibilities PREConditioner and POSTConditioner exclude each other. For postconditioner the same values as for preconditioner are available.

MODIFY $= \alpha$ is only used if an ILU or ILUD preconditioner is used. It defines whether a classical ILU(D) preconditioner is used or the modified one of Gustafsson, or some convex combination of those two. The factor α defines the weight factor in the following sense:

$$\text{Preconditioner} = \alpha * \text{ ILU} + (1 - \alpha) * \text{ MILU},$$

hence $\alpha = 0$ means standard method, $\alpha = 1$ means Modified ILU.
Default values are:
In case of the momentum equation: $\alpha = 1$.
In case of the transport or turbulence equation: $\alpha = 1$.
In case of the pressure equation: $\alpha = 0.975$.

POLYPRECONDITIONER defines the degree of the polynomials to be taken if a polynomial preconditioner is used.
0 means no polynomial preconditioning If $n > 0$ an outer and an inner loop is used. The resulting method is called GMRESR. n defines the maximal number of iterations in each inner loop. The iteration method to be used in the inner loop is defined by PRECONDITIONER, MODIFY and SOLVER.

At this moment only GMRES is implemented for the inner loop.

Suggestion: POLYPRECONDITIONER should only be used if GMRES is used as inner iteration method. The question whether to use polypreconditioning or not is not simple to answer. A rough rule that could be used is the following:
First try to run the problem without polypreconditioner. Use amount of output to get information about the number of iterations of GMRES. If more than 20 iterations are used by GMRES, it is advised to use polypreconditioning, otherwise do not use it. For more detailed information consult C. Vuik [50]. If polypreconditioning is used n=5 is a good value

AMOUNT_OF_OUTPUT defines the amount of output ($-1 \leq n \leq 2$)

ERROROCCURANCE defines how to react in case of an error. Possible values for *err* are:

```
STOP
RESUME
```

STOP means stop if an error occurs.

RESUME means resume the computation if possible if an error occurs .

GMRESTART defines after how many steps the GMRES or GCR method restarts. In the case of polypreconditioning it defines after how many steps the outer loop of GMRESR restarts.

ORTHOGONAL defines after how many vectors truncation is carried out in GCR or in the case of polypreconditioning it defines after how many steps the outer loop of GMRESR truncates. Remark: if n(ortho) > n(gmrestart) no truncation is carried out.

STARTVECTOR = start defines how the start vector for each iteration must be created. At this moment this possibility is meant for research possibilities only. The following values for *start* are available:

```
ZERO
EXPLicit
PREC
LINear
```

start = ZERO means start with the null vector.

start = EXPLICIT means start with an explicitly given vector. This possibility has not yet been implemented

start = PREC means start with the solution at the preceding multi-block iteration (or time level in the first multi-block iteration). In the case of the pressure equation this means start with the pressure correction of the preceding time level.

start = LINEAR means start with a linear extrapolation between the last two time-steps.

Default values are:
In case of the momentum equation: PREC.
In case of the transport equation: PREC.
In case of the pressure equation: PREC.

Remark: in the case of a pressure equation in combination with LINEAR, the start vector is made equal to $\alpha * (p(n) - p(n-1))$ where α is computed by the solver in such a way that a fast, convergence can be achieved.

RITZVALUES = n, indicates that the linear solver should estimate n Ritz values after the solution has been computed. These values give insight in the solution process as well as in stability properties of the discretization. At this moment this parameter is meant for research purposes only.

Suggestion: approximately 50 Ritz values give sufficient insight.

PRINT_SOLUTION indicates that the solution must be printed in all time steps indicated by PRINT_STEPS. The solution is printed as stored in the program, that is in a staggered way and in the contravariant components that are used.

PRINT_STEPS indicates that the printing defined by the option PRINT_SOLUTION must be carried for the time steps ITIME1, ITIME1+ITSTEP, ITIME1+2×ITSTEP, ... , ITIME2

CG_RELax $= \omega$, defines the minimum value of the normed inner product between search direction and residual vector in the Bi-cgstab process. During the iteration a division by this inner product is performed. Once the value is too small the residual may grow to unacceptable values and loss of figures may be the result. This behaviour is visible in the famous peaks in many of the pictures showing the convergence behaviour of Bi-cgstab. Sleijpen and van der Vorst [42] propose to repair it by defining a minimum value for the inner product. This value must be between 0 and 1, and the default value is 0.7.

CG_INNer $= n$, defines the number of GMRES steps in the Bi-cgstab(l) process. The standard Bi-cgstab process consists of a Bi-CG outer loop and a GMRES(1) inner loop. According to [41] for problems with large advection Bi-cgstab(2) performs much better. l must be smaller than 16, the default value is 1.

NEUMayer Neumayer [42] defined an improvement of the original CGS algorithm, which is more stable. It does not suffer so much from the erratic behaviour one often sees in the convergence pictures of CGS. The default is to use the Neumayer improvement in CGS.

NO_NEUMayer If No_Neumayer is given as keyword, the standard CGS process is performed.

FILL_IN $= n$, defines the number of extra diagonals used to compute the ILU preconditioner in case of ILU_FILL preconditioning.

MAXLEVEL $= n$, defines the maximum number of levels in the case of multigrid preconditioning. If n=0 this number is computed in a suitable way.

SMOOTH_STEPS $= n$, defines the number of smoothing steps in the case of multigrid preconditioning. If n=0 this number is computed in a suitable way.

5.7 The keyword INITIAL_CONDITIONS

The keyword INITIAL_CONDITIONS indicates that the user wants to give initial conditions for some unknowns explicitly. For unknowns that have not been given any initial conditions, the initial condition 0 is assumed. In order to define the initial conditions the following subkeywords may be used:

Keyword	Default value	mandatory
RESTart = t	none	no

INSESSION = sessionname	none	no
U_MOMentum = g	0	no
V_MOMentum = g	0	no
W_MOMentum = g	0	no
TRANsport a = g	0	no
PRESsure = g	0	no
K_TURBulence = g	1e-4	no
EPS_TURBulence = g	1e-4	no
OMEGA_TURBulence = g	1e-4	no
REFINE = n	none	no
LAMTURB = t	none	no

g may take one of the forms number or FUNC=i as described for the velocity boundary conditions. However, instead of a function subroutine USFUNB, the function subroutine usfuni (6.2) is used, which is called by the ISNAS program in the following way:

```
value = USFUNI ( i, x, y, z )
```

INSESSION = *sessionname*, indicates that the computation must be resumed with the results of the session named *sessionname*, in order to distinguish between various sessions.
At this moment *sessionname* is restricted to integer numbers.

RESTART = t, indicates that the starting vector will be read from the restart file. The parameter t indicates the time at which the computation is resumed.

U/V/W_MOMENTUM = g defines the initial condition for u, v and w velocity component (in Cartesian co-ordinates) respectively.

TRANSPORT $a = g$ defines the initial condition for the a^{th} transport quantity.

PRESSURE = g defines the initial condition for the pressure.

K_TURBulence = g defines the initial condition for the turbulent kinetic energy k.

EPS_TURBulence = g defines the initial condition for the ε.

OMEGA_TURBulence = g defines the initial condition for the ω.

REFINE = t assumes that the solution of a coarse grid has been stored in the restart file. Furthermore the mesh has been refined one times since then. The solution on the coarse grid will be interpolated to the fine grid.
The parameter t has the same meaning as in RESTART = t.

LAMTURB = t assumes that the solution of a laminar problem has been stored in the restart file. This laminar solution is used as starting value for the turbulent equations. The parameter t has the same meaning as in RESTART = t.

5.8 The keyword TURBULENCE

The keyword TURBULENCE indicates that a turbulence model will be used. If omitted the flow is assumed to be laminar.
TURBULENCE may be followed by the following subkeywords:

Keyword	Default value	mandatory
MODEL = m	K_EPS	no
LES_MODEL = l	SMAGORINSKY	no
VISCOUS_CORRECTIONS = v	NO	no
ANISOTROPY = a	NONE	no
KAPPA = k	0.41	no
E = e	9.0	no
C_MU = c	0.09	no
SIGMA_K = s	1.0	no
SIGMA_EPS = s	1.3	no
CONE_EPS = c	1.44	no
CTWO_EPS = c	1.92	no
C_D = c	0.08	no
SIGMA_T = s	2.0	no
A = a	26.6	no
E_ROUGH = e	33.0	no
ETA_Zero = e	4.38	no
BETARNG = b	0.012	no
C_S = c	0.1	no
ALPHA = a	0.556	no
BETASTAR = b	0.09	no
BETA = b	0.075	no
SIGMA = s	0.5	no
SIGMASTAR = s	0.5	no
MOD_PRODUCTION = s	0.0	no
CTHREE_EPS = c	0.05	no
CTAU_ONE = c	0.0	no
CTAU_TWO = c	0.0	no
CTAU_THREE = c	0.0	no
MAX_WINDOWS = m	20	no
TIME_INTERVAL = t	1	no

Usually the subkeyword MODEL, defining the type of turbulence model should be sufficient. The default closure constants used are those that are commonly accepted in the literature. However, the user has the option to use his own constants in the turbulence models.

MODEL defines the type of turbulence model to be used. It must be followed by the type of model required. The following models are available:

```
none
```

```
algebraic
K_EPS
RNG_K_EPS
K_OMEGA
LES
EXT_K_EPS
```

none no turbulence model is used, i.e. laminar flow is assumed.

algebraic has not yet been implemented.

K_EPS defines the standard $k-\varepsilon$ model.

RNG_K_EPS defines the RNG $k-\varepsilon$ model.

K_OMEGA defines the Wilcox $k-\omega$ model.

LES means that a large eddy model is used.
If the keyword LES_MODEL is used this is the default value.

EXT_K_EPS defines the extended $k-\varepsilon$ model.

LES_MODEL defines the type of LES turbulence model to be used.
This keyword may only be used if no turbulence model is given or if the turbulence model is set equal to LES.
The following models are available:

```
SMAGORINSKY
```

SMAGORINSKY the SMAGORINSKY model is used.

VISCOUS_CORRECTIONS = v indicates whether viscous corrections must be used or not in the vicinity of a solid wall. The meaning of this subkeyword depends on the choice of the model. In the case of standard k-ε model, low-Reynolds-number effects are incorporated to reproduce the law-of-the-wall correctly. In the case of k-ω model, viscous corrections are employed for the special boundary condition for ω (see also keyword BOUNDARY_CONDITIONS). The following values for v are available:

```
YES
NO
```

YES the equations of k-ε model will be modified using the Lam-Bremhorst damping functions, or the asymptotic behaviour of ω near a wall, which is employed as a boundary condition for k-ω model, will be corrected.

NO the standard k-ε model without any viscous damping functions will be employed, or the asymptotic behaviour of ω near a wall will not be corrected.

ANISTROPY defines the type of anisotropic form of the eddy-viscosity concept to be used. The following models are available:

```
none
SPEziale
RUBinstein_barton
NISizima_yoshizawa
MYOng_kasagi
```

none no anisotropic model is used, i.e. the Boussinesq hypothesis is employed.

SPEZIALE defines the nonlinear model of Speziale.

RUBINSTEIN_BARTON gives the Rubinstein-Barton model arises from the RNG theory.

NISIZIMA_YOSHIZAWA means the Nisizima-Yoshizawa model based on the DIA approach.

MYONG_KASAGI defines the Myong-Kasagi model.

C_MU, SIGMA_K, SIGMA_EPS, CONE_EPS and CTWO_EPS are the empirical constants, which should be used for the standard k-ε model, RNG based k-ε model as well as the extended k-ε model. Details on the determination of these constants can be found in [24], [64] and [17], respectively. The values mentioned above are associated with the standard k-ε model. In case of the RNG model, the following values should be used:

```
C_MU      = 0.085
SIGMA_K   = 0.7179
SIGMA_EPS = 0.7179
CONE_EPS  = 1.42
CTWO_EPS  = 1.68
```

In case of the extended model, the following values should be used:

```
C_MU      = 0.09
SIGMA_K   = 0.75
SIGMA_EPS = 1.15
CONE_EPS  = 1.35
CTWO_EPS  = 1.9
```

The constants will be set according to the above mentioned values as soon as the RNG or extended model is used.

ETA_Zero and BETARNG are also used for the RNG model.

CTHREE_EPS is also used for the extended model.
With respect to the Wilcox k-ω model, the following constants must be employed: ALPHA, BETASTAR, BETA, SIGMA and SIGMASTAR. For details we refer to [63].

KAPPA, E, A, C_D and E_ROUGH are the constants needed for the modeling of turbulent flow near a wall. In case of a smooth wall, the constant E will be employed, otherwise E_ROUGH is used. The reason for specifying these two constants at the same time is, that different type of walls (smooth as well as rough) may be involved in one fluid problem. All of these constants, except C_D and A, must be given to specify the law of the wall. The constant C_D belongs to the one-equation model used in, for example, two-layer model. The constant A is needed for the specification of the so-called Van Driest mixing length. At this moment the two-layer model and Van Driest mixing length have not been implemented yet. The constant KAPPA, the so-called Von Karman constant can also be used for an algebraic model (for example the Prandtl mixing length model).

C_S should be used for the LES Smagorinsky model, which has not been implemented yet.

SIGMA_T should be used when a transport equation of temperature is involved. The constant SIGMA_T is the Prandtl/Schmidt number with respect to the temperature.

MOD_PRODUCTION defines whether the standard expression of production term of turbulent energy is used or the Kato-Launder modification, or some convex combination of those two. The factor MOD_PRODUCTION is the weight factor which lies between zero and unity. Hence, MOD_PRODUCTION = 0 means standard, MOD_PRODUCTION = 1 means Kato-Launder correction. If omitted the default value MOD_PRODUCTION = 0 is used.

CTAU_ONE, CTAU_TWO and CTAU_THREE are the closure constants needed for the nonlinear (anisotropic) stress-strain relationship.

MAX_WINDOWS $= m$ defines the maximum number of time-steps used for the time averaging procedure in the smagorinsky model.
If omitted the default value 20 is used.

TIME_INTERVAL $= t$ defines the time interval used for the time averaging procedure in the smagorinsky model.
Mark that this value together with the present time step define the number of time steps used for the averaging. This number may not exceed the value of MAX_WINDOWS.
If omitted the default value 1 is used.

Although it is recommended not to tune the empirical constants mentioned above, it is possible to change the values of these constants provided that the following bounds on the different constants should be employed:

$$0.40 \leq \kappa \leq 0.42$$

$$
\begin{aligned}
&7.45 \leq E \leq 10.0 \\
&0.01 \leq c_\mu \leq 0.36 \\
&0.70 \leq \sigma_k \leq 1.40 \\
&0.70 \leq \sigma_\varepsilon \leq 1.40 \\
&1.00 \leq c1_\varepsilon \leq 1.55 \\
&1.50 \leq c2_\varepsilon \leq 2.00 \\
&0.04 \leq c_d \leq 0.15 \\
&0.50 \leq \sigma_T \leq 4.00 \\
&20.0 \leq A \leq 30.0 \\
&26.0 \leq E_{rough} \leq 37.0 \\
&2.00 \leq \eta_0 \leq 16.0 \\
&0.01 \leq \beta_{RNG} \leq 0.015 \\
&0.10 \leq C_s \leq 0.25 \\
&0.10 \leq \alpha \leq 1.0 \\
&0.04 \leq \beta^* \leq 0.15 \\
&0.01 \leq \beta \leq 0.1 \\
&0.50 \leq \sigma \leq 2.0 \\
&0.50 \leq \sigma^* \leq 2.0 \\
&0.00 \leq mod_{prod} \leq 1.0 \\
&0.00 \leq c3_\varepsilon \leq 0.40 \qquad (5.13) \\
&-5.0 \leq c_{\tau 1} \leq 5.0 \qquad (5.14) \\
&-5.0 \leq c_{\tau 2} \leq 5.0 \qquad (5.15) \\
&-5.0 \leq c_{\tau 3} \leq 5.0
\end{aligned}
$$

5.9 The keyword MULTI_BLOCK

The keyword MULTI_BLOCK indicates that the user wants to give some extra information about the multi block process. This keyword must be followed by subkeywords containing this extra information. If omitted the standard multi-block parameters are used.
The keyword may be followed by the following subkeywords:

```
SUBDOMAIN_solution = isol
SAVE_PRECOnditioner
TYPE_OF_ALGorithm = itype
MOMentum_equations
TRANSport_equation i or all
PRESsure_equation
TURBulence_equation i or all
ALL_equations
```

SUBDOMAIN_SOLUTION = isol defines the way the subdomain solution is computed/approximated.
The following values for isol are available:

```
ACCurate
INACCurate
ILU
```

ACCURATE means that the subdomains are assumed to be solved accurately (enough). The fact that subdomains are solved accurately means that a reduction of vector length in the acceleration is possible.

INACCURATE means that the subdomains are assumed to be solved inaccurately. It is advised to lower the subdomain solution accuracy as much as possible to say 0.1. The algorithm which assumes accurate solution of subdomains is in general slower. At present, `INACCURATE` is the default.

ILU means that the subdomain solution is approximated by applying the inverse of the subdmain ILU preconditioner to the right-hand side. This is a special case of the INACCURATE option. This method is definitely faster on a single machine than the algorithm which uses accurate solution of subdomains.

SAVE_PRECONDITIONER defines that the preconditioner must be built only once at in the first domain decomposition iteration. This means that the preconditioner is stored for each block and reused at every next domain decomposition iteration. The default is not to remember the preconditioner and to rebuild it each domain decomposition iteration. The default is therefore less efficient but requires less memory.

TYPE_OF_ALGORITHM = itype defines the type of multi-block algorithm to be used. The following values for *itype* are available:

```
SEQuential
PARallel
```

SEQUENTIAL means that the sequential algorithm is applied. If this algorithm is used in the case of parallel computing it means that for each processor the sequential algorithm is used but that of course over the various processors the parallel algorithm is used.

PARALLEL means that the parallel algorithm is applied even if only one processor is available. This algorithm is approximately two times slower than the sequential algorithm and is in fact only available because of research purposes.

The default algorithm is the sequential one.

...EQUATION. defines the type of equation to which the subsequent subsubkeywords should be applied. The meaning of these subkeywords is obvious. They may be followed by the subsubkeywords:

Keyword	Default value	mandatory
METHOD = imethod	accelerated	no
AMOUnt_of_output = out	0	no
MAXITer = n	100	no
KRYLOV_OUter = n	20	no
TRUNCATION_strategy = strategy	JACKSON_robinson	no
RELAXation = r	1	no
RELACcuracy = rel	1e-4	no
REUSE_SEarch = n	0	no
REUSE_VAlues = yes	no	no
ORTHOGONALIZATION = iortho	modified	no

METHOD = *imethod* defines the type of domain decomposition algorithm to be used. The following values of *imethod* are available:

```
ACCelerated
STAndard
```

STANDARD means that the standard multi-block algorithm is applied. In the case of ACCELERATED (default value) the domain decomposition process is accelerated by a GCR method. This parameter is mainly meant for research purposes.
`METHOD = STANDARD` is only applied if the accurate subdomain solution method is chosen.

AMOUNT_OF_OUTPUT = *out*, defines the amount of output. The following values for *out* are available:

- < 0 : No output
- 0 : Only fatal errors will be printed
- 1 : Additional information about the iteration is printed
- 2 : Gives a maximal amount of output concerning the iteration process

MAXITER = n defines the maximum number of multi block iterations.

KRYLOV_OUTER = n defines the maximum number of search directions used in the outer loop of GCR.

TRUNCATION_strategy = *strategy* defines the type of truncation strategy to be used with the accelerated domain decomposition algorithm. The following values of strategy are available:

```
JACKSON_robinson
NONE
```

JACKSON_robinson means that a Jackson and Robinson truncation strategy is used [19]. NONE means that no truncation is used. The GCR method is restarted in an optimal way [59].

RELACCURACY = *rel* defines the relative accuracy to be used for the solution of the interface equations.

REUSE_SEarch = n defines the number of search directions that must be stored for this equation. These search directions are reused in the next time-step. n may be less or equal to the number of outer Krylov iterations.
This gives a much faster solution method for the pressure equation. For the other equations there is no significant decrease in CPU time.

REUSE_VAlues = *yes* indicates that not only the search directions are kept and reused but also the corresponding search values ($v_k = As_k$). This option may only be used if the matrix is constant in time. It makes only sense in combination with REUSE_SEarch > 0.

ORTHOGONALIZATION = *iortho* indicates the type of orthogonalization scheme to be used in the multi-block process (GCR). Possible values for *iortho* are:

```
modified
reorthogonalized
```

modified means the modified Gram-Schmidt process is applied.

reorthogonalized the classical Gram-Schmidt process is applied with reorthogonalization.

Default value: `modified`

5.10 The keyword COMPRESSIBLE

The keyword COMPRESSIBLE indicates that the user wants solve the compressible Navier Stokes equations. The following subkeywords may be used:

Keyword	Default value	mandatory
GAMMA = n	1.4	no
MACH = n	0.2	no
VEL_Sound = n	330	no
ALPha = n	0	no
P_V = n	0.89	no
P_OUT = n	0	no
DENS_UPWind = method	no_dens_upwind	no
NO_DENS_UPWind	no_dens_upwind	no
NO_ENTHALPY	enthalpy	no
NO_SCALING	no_scaling	no
PRES_CORR_METHOD = i	0	no

```
P_REF = p                              0          no
RHO_REF = rho                          1          no
VEL_REF = v                            1          no
ENERGY_EQUATION = e                enthalpy       no
equation_of_state = e              perfect_gas    no
```

These keywords have the following meaning:

GAMMA = a gas constant equal to the specific heat at constant pressure divided by the specific heat at constant volume, in air $\gamma = 1.4$.

MACH = the inlet Mach number.

VEL_SOUND = speed of sound, in air 330 m/s.

ALPHA = inlet flow angle.

P_V = ratio of outlet and inlet pressure: $\frac{p_{out}-p_0}{p_{in}-p_0}$, with p_0 a reference pressure.

P_OUT = outlet pressure.

DENS_UPWIND = method = upwind-biased discretization of the density in the continuity equation, hence in the pressure correction equation, to fulfill the entropy condition.
The subkeyword `method` is used to indicate what kind of upwinding is applied. Possible values:

```
GRADIENT_BASED
MACH_BASED
UNCONDITIONAL
EXPLICIT
IMPLICIT
```

EXPLICIT upwind bias is applied to the continuity equation in an explicit manner:

$$\frac{\rho^{n+1}-\rho^n}{\delta t} + D\sigma^n m^{n+1} = 0 \tag{5.16}$$

$$\sigma^n = \frac{\rho^n_{\text{upwind}}}{\rho^n_{\text{central}}} \tag{5.17}$$

IMPLICIT upwind bias is applied to the continuity equation in an implicit manner

$$\frac{\rho^{n+1}-\rho^n}{\delta t} + D\sigma^{n+1} m^{n+1} = 0 \tag{5.18}$$

$$\sigma^{n+1} = \frac{\rho^{n+1}_{\text{upwind}}}{\rho^{n+1}_{\text{central}}} \tag{5.19}$$

GRADIENT_BASED means that the density ρ is convected such that the TVD property is satisfied. The ISNAS scheme is applied.

MACH_BASED upwinding is applied as soon as the mach number exceeds a the value 0.9.

UNCONDITIONAL A first order upwinding is applied in all cases

If `method` is not given the default `mach_based` is assumed.

NO_DENS_UPWIND = density upwinding is switched off.

NO_ENTHALPY means that no enthalpy equation is solved. It concerns a very special version of the compressible flow equations.

NO_SCALING the dimensional compressible Euler equations are solved. Non-dimensionalisation is switched off.

PRES_CORR_METHOD $= i$ If $i = 0$, the compressible pressure correction method is used.
If $i = 1$, an alternative pressure correction method is used, which better preserves contact discontinuities.

P_REF $= p$ defines a reference pressure. This reference pressure is used to produce a dimensionalised pressure in the postprocessing file.

RHO_REF $= \rho$ defines a reference density. This reference density is used to produce a dimensionalised density in the postprocessing file.

VEL_REF $= u$ defines a reference velocity. This reference velocity is used to produce a dimensionalised velocity in the postprocessing file.

ENERGY_EQUATION $= e$ defines what type of energy equation is used. This implies also what type of primary variable for the energy is utilized. Possible values for e are

ENTHALPY means that the enthalpy h is used as primary energy variable.

TOTAL_ENTHALPY means that the total enthalpy H is used as primary energy variable.

INTERNAL_ENERGY means that the internal energy e is used as primary energy variable.

DENS_TOT_ENTH means that the primary variable is the density times total enthalpy: ρH (only for tudfinvol).

DENS_TOT_ENGY means that the primary variable is the density times total energy: ρE (only for tudfinvol).

EQUATION_OF_STATE $= e$ = defines what type of equation of state is used to express the relation between density, pressure and energy.
Possible values for e are

PERFECT_GAS the perfect gas law is used.

USER_PROVIDED a user provided equation of state is applied. The user must supply some user functions related to the equation of state. These functions are: USDRHODH (6.8), USDRHODP (6.9) and USCALCRHO (6.10).
In the case that the internal energy is used as unknown, also a subroutine USCOMPINTEN must be supplied to compute the internal energy from the temperature. In this way the user may give the temperature as initial condition as well as boundary condition, and not the primary variable e.
USDRHODH computes $\frac{\partial \rho}{\partial h}$, which is used in the pressure correction equation. h may be either the enthalpy h, the total enthalpy H or the internal energy e, depending on the choice of energy equation.
The call to this subroutine is:

```
call usdrhodh(eddy,solut,ni,nj,nk,nvirtual,ndim,ndegfd,drhodh)
```

USDRHODP computes $\frac{\partial \rho}{\partial p}$, which is used in the pressure correction equation.
The call to this subroutine is:

```
call usdrhodp(eddy,solut,ni,nj,nk,nvirtual,ndim,ndegfd,drhodp)
```

USCALCRHO computes ρ, as function of the previously computed solution, including the pressure
The call to this subroutine is:

```
      call uscalcrho ( eddy, solut, ni, nj, nk, nvirtual, ndim,
     +                 ndegfd, ilowloop, iuppploop, jlowloop,
     +                 jupploop, klowloop, kuppploop )
```

USCOMPINTEN computes e, as function of the previously computed solution, usually the temperature
The call to this subroutine is:

```
      call uscompinten ( eddy, solut, ni, nj, nk, nvirtual, ndim, ndegfd )
```

5.11 The keyword CAVITY

The keyword CAVITY indicates that the user wants to solve the compressible Navier Stokes equations combined with a cavity model. This keyword may only be used in combination with the keyword COMPRESSIBLE. The following subkeywords may be used:

Keyword	Default value	mandatory
CLIQUID	1e-6	no
CVAPOUR	1e-6	no
LOWERPRESSTRANSIT	1	no

UPPERPRESSTRANSIT	2	no
PRESSURE_GAUSS_SEIDEL	none	no
START_UP	none	no

These keywords have the following meaning:

CVAPOUR = speed of sound in the vapour phase.

cliquid = speed of sound in the liquid phase

lowerpresstransit = lower transit pressure of phase transition

upperpresstransit = upper transit pressure of phase transition

PRESSURE_GAUSS_SEIDEL If this keyword is found, the pressure equation is solved by a non-linear Gauss-Seidel accelerated GMRES method.

START_UP If this keyword is found, the cavitation calculation is started with a modified equation of state. This means that it is assumed that there is only water no cavitation. This is only necessary in a start up phase.

5.12 The keyword FREE_SURFACE_FLOW

The keyword FREE_SURFACE_FLOW indicates that the problem has at least one free surface boundary. At this moment only one algorithm to update the free boundary has been implemented. It is restricted to a stationary 2d Cartesian free boundary.
The following subkeywords may be used:

Keyword	Default value	mandatory
METHOD = type	NONE	no
RELAXATION = a	1	no

These keywords have the following meaning:

METHOD = *type* = defines the type of method that will be used to update the free boundary after each step.
At this moment the following values for *type* are available:

NONE
PLAIN

These subkeywords have the following meaning:

NONE means that no free surface flow is computed, hence the boundary is not updated.

PLAIN means that the standard method is used to update the free boundary. At this moment this means that at the free boundary the boundary condition $\frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x} = v$ is used, with $h(x)$ the height of the free surface, and $\mathbf{u} = (u, v)$ the Cartesian velocity vector. This boundary condition is discretized using a first order upwind method. Restriction:

The present implementation is far from general. In fact it is assumed that we have only one block and that the region is as sketched in Figure. 5.12.1. So the top boundary is the free surface boundary

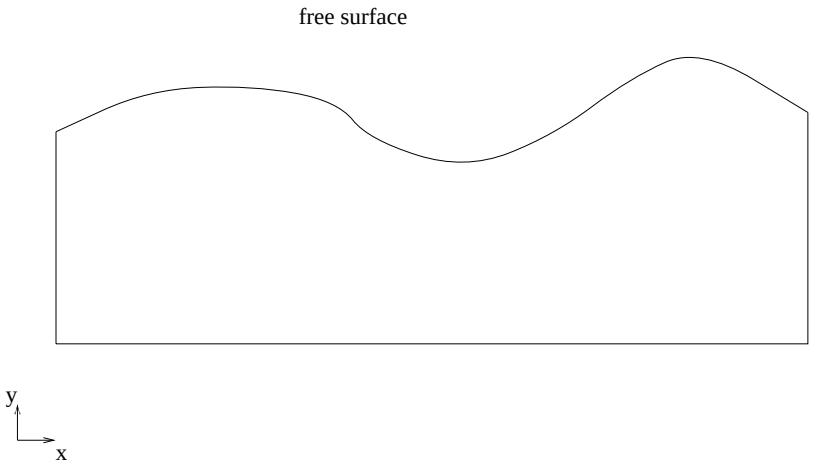


Figure 5.12.1: Region for free-surface flow

and the grid is generated from left to right and from below to the top. This means in terms of a SEPMESH input, that C1 is the lower boundary, C2 the outflow boundary and C3 the free surface boundary. Furthermore it has been assumed that the fluid flows from left to right.

RELAXATION $= \omega$ defines a relaxation factor for updating the free boundary. In order to get convergence it is necessary to define an under-relaxation parameter independent of the time step used.
In our example $\omega = 0.1$ proved to be a suitable choice.

5.13 The keyword MAIN_STRUCTURE

The keyword MAIN_STRUCTURE is only meant for those users that want to experiment with special algorithms. With this keyword it is possible to influence the structure of the main program. For example one can decide if an iteration over sets of equations must be carried out, or that sub-stepping for some equations must be applied. If the keyword MAIN_STRUCTURE is not

found, the structure of the main program is completely defined by the other input parameters. However, when this keyword is used it may be necessary to define things like sub-stepping or iteration that otherwise would have been defined in other input parts.
The following subkeywords may be used:

```
GLOBAL_LOOP
CLUSTER i
```

These keywords have the following meaning:

GLOBAL_LOOP indicates that information about the global loop is defined. This keyword must be followed by subkeywords defining this information.

CLUSTER i defines a new cluster of equations. A cluster is a conglomerate of equations (possibly consisting of one equation), which must be treated as one system with respect to loops time-stepping and so on.
This keyword must be followed by subkeywords defining the cluster and containing information about the loops and so on for the cluster.

Subkeywords for GLOBAL_LOOP the following subkeywords are allowed

Keyword	Default value	mandatory
SEQUENCE_OF_EQUATIONS = (i,j,k,...)	natural sequence	no
ITERATE_INITIAL_CONDITION	no	no
MIN_INITIAL_ITER = m	1	no
MAX_INITIAL_ITER = m	1	no
ABS_INITIAL_ACCURACY = e	0	no
REL_INITIAL_ACCURACY = e	10e-2	no
MIN_STATIONARY_ITER = m	0	no
MAX_STATIONARY_ITER = m	0	no

These keywords have the following meaning:

SEQUENCE_OF_EQUATIONS $= (i, j, k, ...)$ defines in which sequence the equations are solved per time step.

ITERATE_INITIAL_CONDITION If this keyword is found, the program runs with the initial time step, however, without increasing the actual time, until convergence is achieved.
After that the time integration actually starts.

MIN_INITIAL_ITER $= m$ defines the minimum number of iterations with respect to the initial condition iteration.

MAX_INITIAL_ITER $= m$ defines the maximum number of iterations with respect to the initial condition iteration.

ABS_INITIAL_ACCURACY $= e$ defines the absolute accuracy with respect to the initial condition iteration.

REL_INITIAL_ACCURACY $= e$ defines the relative accuracy with respect to the initial condition iteration. The actual accuracy is a linear combination of both absolute and relative accuracy.

MIN_STATIONARY_ITER $= m$ must only be used if a stationary solution must be found. This parameter defines the minimum number of iterations.

MAX_STATIONARY_ITER $= m$ must only be used if a stationary solution must be found. This parameter defines the maximum number of iterations.

Subkeywords for CLUSTER i the following subkeywords are allowed

Keyword	Default value	mandatory
EQUATIONS = (j,k,...)	i	no
STATIONARY	not	no
ABS_STATIONARY_ACCURACY = e	0	no
REL_STATIONARY_ACCURACY = e	0	no
MIN_STATIONARY_ITER = m	0	no
MAX_STATIONARY_ITER = m	0	no
nsubsteps = n	1	no

These keywords have the following meaning:

EQUATIONS $= (j, k, ...)$ defines which equations belong to the cluster. If omitted it is assumed that only equation i is used.

STATIONARY if this keyword is found it is assumed that the present cluster must be iterated until a stationary solution is achieved for each time step.

ABS_STATIONARY_ACCURACY $= e$ defines the absolute accuracy with respect to the iteration for a stationary solution.

REL_STATIONARY_ACCURACY $= e$ defines the relative accuracy with respect to the iteration for a stationary solution. The actual accuracy is a linear combination of both absolute and relative accuracy.

MIN_STATIONARY_ITER $= m$ must only be used if a stationary solution must be found. This parameter defines the minimum number of iterations.

MAX_STATIONARY_ITER $= m$ must only be used if a stationary solution must be found. This parameter defines the maximum number of iterations.

nsubsteps $= n$ means that each time-step for the cluster is subdivided into n subtime-steps. Hence the actual time-step for the cluster is smaller than the global time step.

5.14 The keyword PROFILE_INPUT

This keyword is meant to define some information with respect to a flow around a (two-dimensional) profile.
At this moment it is only implemented in the unstructured finite volume program, not yet in Deft.
The keyword may be followed by subkeywords defining information about the profile.
The following subkeywords may be used:

```
UPPER_PROFILE = Ci
LOWER_PROFILE = Cj
```

Meaning of these subkeywords:

UPPER_PPROFILE = Ci defines the curve number corresponding to the upper part of the profile. Mark that only one curve number may be used. This implies that if the upper part of the profile consists of several curves, these curves must be combined to a new composite curve.
This option is only available if the mesh has been generated by SEPMESH.
Default value: $i = 1$

LOWER_PROFILE = Cj defines the curve number corresponding to the lower part of the profile. See also the remarks with respect to UPPER_PROFILE.
Default value: $i = 2$

With respect to profile flow, the following things must be kept in mind:

- at the inflow boundary, the momentum vector must be prescribed using keywords U_LEN and ANGLE.
- at the outflow boundary, the boundary conditions for momentum must be SIGMANT, SIGMANN given.
- the leading edge must be positioned in the origin, and the trailing edge must be positioned at the x-axis, e.g. in (1,0).
- the boundary condition must be constants, i.e. not a function of time and/or position.
- the upper and lower surface of the profile must each exist of one curve only.

5.15 The keyword FREQUENT_OUTPUT

This is especially useful if some quantities must be followed in time. It concerns a limited number of quantities, complete fields are only written at the time-steps indicated by tout.

At this moment it is only implemented in the unstructured finite volume program, not yet in Deft.
The keyword may be followed by subkeywords defining information about which quantities must be written.
The following subkeywords may be used:

```
FREQUENCY = f
LIFT
MINMAX_MACHNUMBER
NUMBER_OF_SUPERSONIC_VERTICES
POSITION_SONIC_POINTS
DENSITY_RES_ONE
DENSITY_RES_TWO
DENSITY_RES_INF
MOMENTUM_RES_ONE
MOMENTUM_RES_TWO
MOMENTUM_RES_INF
ENTHALPY_RES_ONE
ENTHALPY_RES_TWO
ENTHALPY_RES_INF
```

Meaning of these subkeywords:

FREQUENCY $= f$ defines the frequency with which this output is written to file `sepcomp.freq`. $f \geq 1$ defines the time steps at which the frequent output is written. If $f = 1$ each time step information is written, if $f = 2$ only the odd time steps and so on.
Default value: $f = 1$

LIFT If this subkeyword is found both the lift and the drag of a profile will be written to the output file. This keyword makes only sense in combination with the keyword PROFILE.
If omitted the lift and drag are not written.

MINMAX_MACHNUMBER The minimum and maximum Mach numbers in the region will be written. This keyword makes only sense in combination with the keyword COMPRESSIBLE.
If omitted the minimum and maximum Mach numbers are not written.

NUMBER_OF_SUPERSONIC_VERTICES The number of supersonic vertices in the region will be written. This keyword makes only sense in combination with the keyword COMPRESSIBLE.
If omitted the number will not be written.

POSITION_SONIC_POINTS The position of the sonic points along the profile will be written. Theoretically there are at most 2 sonic points at each side of the profile, hence 4 positions are written.
In each step 4 coordinates are written defining the relative x-position along

the profile, where the profile is scaled from $x = 0$ to $x = 1$. If during a step more than 2 sonic points along a side are found, only the first two found are written. This keyword makes only sense in combination with the keywords COMPRESSIBLE and PROFILE.
If omitted the positions are not written.

DENSITY_RES_ONE The quantity $||\rho^{n+1} - \rho^n||_1$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

DENSITY_RES_TWO The quantity $||\rho^{n+1} - \rho^n||_2$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

DENSITY_RES_INF The quantity $||\rho^{n+1} - \rho^n||_\infty$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

MOMENTUM_RES_ONE The quantity $||m^{n+1} - m^n||_1$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

MOMENTUM_RES_TWO The quantity $||m^{n+1} - m^n||_2$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

MOMENTUM_RES_INF The quantity $||m^{n+1} - m^n||_\infty$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

ENTHALPY_RES_ONE The quantity $||h^{n+1} - h^n||_1$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

ENTHALPY_RES_TWO The quantity $||h^{n+1} - h^n||_2$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

ENTHALPY_RES_INF The quantity $||h^{n+1} - h^n||_\infty$, with n indicating the time-level, is written to file. For definitions of the norm, see below.
If omitted this quantity is not written.

The following definitions of norms, with $u = (u_1, u_2, \ldots, u_n)$, are used:

- 1 norm:
$$||u||_1 = \frac{\sum_{i=1}^{n} |u_i|}{n} \tag{5.20}$$
- 2 norm:
$$||u||_2 = \sqrt{\frac{\sum_{i=1}^{n} u_i^2}{n}} \tag{5.21}$$

- ∞ norm:

$$||u||_\infty = \max(|u_i|) \tag{5.22}$$

Chapter 6

Creating your own main program

In many applications it is sufficient to use the command ISNASEXE and there is no need to create a main program. However, sometimes ISNASEXE does not supply enough flexibility for your purposes. Reasons for creating your own main program are for example:

- It is necessary to add a function subroutine because one of the boundary conditions, one of the coefficients or perhaps the initial conditions depend on space or time.
- The buffer space used by program ISNASEXE is insufficient for your application. If this is the case isnasexe returns with a message.
- You are extending, changing or debugging isnasexe. This is only meant for developers and is described in the Programmers Guide [40].

In Section 6.1 it is described how you make your local main program ISNASEXE.
The function subroutines that must be provided by the user in case of variable coefficients, boundary conditions or initial conditions are described in the Sections 6.2, 6.3, 6.4, 6.5 and 6.6.

6.1 How to create and run a local program ISNASEXE in a serial environment

The creation of a main program in Deft is relatively simple. The name of the main program may be chosen freely. However, there is one exception. In the case of a parallel environment, only the name isnasexe may be used, due to some scripts necessary to use mpi. This restriction is only temporarily. In general the main program has the following shape:

```
program example
implicit none
integer nbuffr
parameter( nbuffr = 5000000 )
integer ibuffr
common ibuffr(nbuffr)

call is_main ( nbuffr )

end


function usfunx ( .... )
end

subroutine usfilx ( .... )
end
```

The program name "example" may be replaced by any other suitable name. The declarations concerning IBUFFR and NBUFFR define the length of the buffer array to be used by Deft. In this example the default length 5000000 has been used. However, if the buffer length is insufficient, this number must be enlarged.
Subroutine IS_MAIN is the actual main Deft subroutine. It requires the declared length of array IBUFFR as only parameter.

If function subroutines must be provided, the simplest way is to put them in the same file as the main program, just behind this main program. Only the subroutines actually written by the user should be supplied. The function $usfunx$ and the subroutine $usfilx$ used in the example above represent these user subroutines.

The actual program isnasexe can be put into your directory by the command:

```
isget isnasexe
```

This command copies the standard isnasexe program into your directory with the name isnasexe.f. The next step is to adapt this program for your own purposes, and add those user subroutines that are required for the application. It is a good practice to rename the file isnasexe.f to a new name that has something to do with the application, for example channel.f. It is advised to use the same name in the program statement.

Once the program has been created it must be compiled and linked. This must

be performed by the command islink in the following way:

```
islink isnasexe
```

where isnasexe stands for the name of the fortran file containing the main program, without the extension .f.
The islink commands compiles the program isnasexe including all user subroutines provided in this file. After successful compilation the program isnasexe is linked with the subroutines provided, all files with the extension .o in the subdirectory, and of course the Deft libraries. The files with extension .o are supposed to be compiled before by a FORTRAN or possibly C-compiler. The file isnasexe.o itself is removed.
The result of the islink command is an executable with the name isnasexe, provided compilation and linking have been carried out successfully. To run this executable, simply type its name, for example:

```
isnasexe
```

This program will run provided the grid has been generated before and the Deft pre-processor has been applied and no errors are generated.
If Deft is run in a parallel environment on several computers, then it is necessary to link isnasexe first and after that run isnasmpi with an input file as described in Section 3.3. In that case the name of the main program is restricted to `isnasexe`.

6.2 Function subroutine usfuni

Description

Only if the initial conditions are not constant throughout the domain it is necessary to provide the user written subroutine USFUNI.

Heading

```
function usfuni ( ichoice, x, y, z )
```

Parameters

integer ichoice

double precision usfuni, x, y, z

usfuni Must get the value of the function in the point x,y,z, depending on the choice parameter ichoice.

ichoice Choice parameter. This parameter may be used to distinguish between several initial conditions.
The parameter is set by Deft and gets the value of the parameter i in `FUNC = i` in the input file for the pre-processor.

x,y,z Co-ordinates of the point in which the initial condition must be evaluated.

Input

The parameters ichoice, x, y and z have gotten a value by the Deft program.

Output

The user must explicitly give usfuni some value.

Example

Suppose the initial condition for the u-velocity is $u = x^2 + y^2$ and the initial condition for the pressure is $p = sin(xy)$. Suppose furthermore that u corresponds to ichoice=1 and p to ichoice=2. Then function subroutine usfuni may have the following form:

```
      function usfuni ( ichoice, x, y, z )
      implicit none
      integer ichoice
      double precision usfuni, x, y, z
      if ( ichoice.eq.1 ) then

c     --- ichoice = 1, u = x^2 + y^2

         usfuni = x**2 + y**2

      else if ( ichoice.eq.2 ) then

c     --- ichoice = 2, p = sin(xy)

         usfuni = sin(x*y)

      end if

      end
```

6.3 Function subroutine usfunb

Description

The user written subroutine USFUNB must be provided, if the boundary conditions are not constant for all space and or time.

Heading

```
function usfunb ( ichoice, x, y, z, t )
```

Parameters

integer ichoice

double precision usfunb, x, y, z, t

usfunb Must get the value of the function in the point x,y,z, depending on the choice parameter ichoice and the time t.

ichoice Choice parameter. This parameter may be used to distinguish between several boundary conditions.
The parameter is set by Deft and gets the value of the parameter i in `FUNC = i` in the input file for the pre-processor.

x,y,z Co-ordinates of the point in which the boundary condition must be evaluated.

t Time at which the boundary condition must be evaluated.

Input

The parameters ichoice, t, x, y and z have gotten a value by the Deft program.

Output

The user must explicitly give usfunb some value.

Example

Suppose the boundary condition for the u-velocity at some boundary is $u = x^2 + y^2$ and the boundary condition for the v-velocity is $v = sin(t)$. Suppose furthermore that u corresponds to ichoice=1 and v to ichoice=2. Then function subroutine usfunb may have the following form:

```
      function usfunb ( ichoice, x, y, z, t )
      implicit none
      integer ichoice
      double precision usfunb, x, y, z, t
      if ( ichoice.eq.1 ) then

c     --- ichoice = 1, u = x^2 + y^2

         usfunb = x**2 + y**2

      else if ( ichoice.eq.2 ) then

c     --- ichoice = 2, v = sin(t)
```

```
      usfunb = sin(t)

    end if

    end
```

6.4 Function subroutine usfunc

Description

The user written subroutine USFUNC must be provided, if the coefficients are not constant throughout the domain for all time.

Heading

```
function usfunc ( ichoice, x, y, z, t )
```

Parameters

integer ichoice

double precision usfunc, x, y, z, t

usfunc Must get the value of the function in the point x,y,z, depending on the choice parameter ichoice and the time t.

ichoice Choice parameter. This parameter may be used to distinguish between several coefficients.
The parameter is set by Deft and gets the value of the parameter i in `FUNC = i` in the input file for the pre-processor.
USFUNC is only used if $0 < i < 100$. For values of i between 100 and 200 USFUNC1 will be used, whereas for $i > 1000$ USFUNC must be programmed.

x,y,z Co-ordinates of the point in which the coefficient must be evaluated.

t Time at which the coefficient must be evaluated.

Input

The parameters ichoice, t, x, y and z have gotten a value by the Deft program.

Output

The user must explicitly give usfunc some value.

Example

Suppose that the viscosity is a function of the time: $\mu = sin(t)$ and this parameter corresponds to ichoice=1. Then function subroutine usfunc may have the following form:

```
      function usfunc ( ichoice, x, y, z, t )
      implicit none
      integer ichoice
      double precision usfunc, x, y, z, t
      if ( ichoice.eq.1 ) then

c     --- ichoice = 1, mu = sin(t)

         usfunc = sin(t)

      end if

      end
```

6.5 Function subroutine usfunc1

Description

The user written subroutine USFUNC1 must be provided, if the coefficients depend on previously computed solutions. In fact USFUNC1 is the most simple extension of USFUNC in the sense that it provides two extra parameters which contain the previously computed solutions in the actual point.

Heading

```
function usfunc1 ( ichoice, x, y, z, t, soluts, ndegfd )
```

Parameters

integer ichoice, ndegfd

double precision usfunc1, x, y, z, t, soluts(ndegfd)

usfunc1 Must get the value of the function in the point x,y,z, depending on the choice parameter ichoice, the time t and the "old" solution.

ichoice Choice parameter. This parameter may be used to distinguish between several coefficients.
The parameter is set by Deft and gets the value of the parameter i-100 in `FUNC = i` in the input file for the pre-processor.
USFUNC1 is only used if $100 < i < 200$.

x,y,z Co-ordinates of the point in which the coefficient must be evaluated.

t Time at which the coefficient must be evaluated.

ndegfd Number of "old" solutions available in the present point.

soluts In this array of length ndegfd the "old" solutions in the present point are stored. The values of these solutions do not have to be the actual values with which the Deft program computes. For example internally Deft uses so-called contra-variant velocity components, whereas in soluts only the standard Cartesian components are stored. Furthermore it is possible that an unknown is not present in the actual point. In that case Deft provides an interpolated value.
The sequence in which the unknowns are stored in soluts is fixed and corresponds to the standard Deft numbering.
This means that the first ndim positions are occupied by the Cartesian velocity components, the next one by the pressure, followed by the NTRANS transport quantities and finally by the turbulence degrees of freedom.

Input

The parameters ichoice, t, ndegfd, x, y and z have gotten a value by the Deft program.
Array soluts has been filled by Deft.

Output

The user must explicitly give usfunc1 some value.

Example

Suppose that the viscosity is a function of the temperature: $\mu = 0.01e^{-0.03T}$ and this parameter corresponds to ichoice=1.
Let the dimension of space (ndim) be 2 and T be the only transport quantity. Suppose furthermore that the flow is laminar. In that case ndegfd = 4 and soluts contains u, v, p and T respectively.
Then function subroutine usfunc1 may have the following form:

```
      function usfunc1 ( ichoice, x, y, z, t, soluts, ndegfd )
      implicit none
      integer ichoice, ndegfd
      double precision usfunc1, x, y, z, t, soluts(ndegfd)
      if ( ichoice.eq.1 ) then

c     --- ichoice = 1, mu = 0.01 exp(-0.03T)

         usfunc1 = 0.01d0 * exp(-0.03*soluts(4))

      end if

      end
```

6.6 Subroutine usfilc

Description

The user written subroutine USFILC must be provided, if the coefficients depend on previously computed solutions and the user wants to have a maximum flexibility to fill the coefficient arrays himself. An important disadvantage of USFILC is that the user must know exactly how the solution arrays are filled. Also he must know something about the fluxes used as unknowns. Hence this possibility is only recommended for users with insight knowledge.
USFILC is called for each coefficient separately.
USFILC is called if the choice parameter for the coefficients (ICHOICE) is larger than 1000 and less than 10000.

Heading

```
      subroutine usfilc ( choice, coefs, ncoefs, i, ni, nj, nk,
     +                    ndim, nvirtual, coor, solut, ndegfd, time )
```

Parameters

integer choice, ncoefs, i, ni, nj, nk, ndim, nvirtual, ndegfd

double precision coefs(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ncoefs)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
coor(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndim)
time

choice Choice parameter to be used to distinguish between several possibilities. This parameter is initialized by program ISNASEXE and gets the value of ICHOICE-1000. Compare with subroutine USFUNC (6.4).

coefs Double precision array, where the first index refers to the "i"-direction, the second one to the "j"-direction and the third one to the coefficient sequence number. If ndim = 3, of course also the "k"-direction must be used.
The user must fill the coefficients himself for the complete field. Each index refers to a cell center. Only one call to usfilcsp per time step is performed, hence all coefficients the user wants to fill with this subroutine must be filled in this call.
Virtual cells do not have to be filled, hence a loop from 1 to ni and from 1 to nj must be used.

ncoefs Number of coefficients for the equation.

i Sequence number of coefficient for the equation.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

ndim Dimension of space (2 or 3).

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

coor Array containing the co-ordinates of the vertices of the cells. The 4 vertices of cell (i,j) have sequence numbers (i,j), (i+1,j), (i+1,j+1), (i,j+1).

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

ndegfd Number of "old" solutions available in the present point.

time Time at which the coefficient must be evaluated.

Input

The parameters choice, i, ncoefs, ni, nj, nk, ndim, nvirtual, ndegfd and time have gotten a value by the Deft program.
The arrays coefs, coor and solut have been filled by Deft.

Output

The user must fill the coefficients in array coefs.

6.7 Subroutine usfilcsp

Description

The user written subroutine USFILCP must be provided, if the coefficients depend on previously computed solutions and also on the Cartesian velocity coefficients In fact USFILCP is at present the most complex subroutine for the user, since the user is supposed to fill a set of coefficients in the complete field in one call.

Heading

```
subroutine usfilcsp ( coefs, ncoefs, ni, nj, nk, ndim,
                      nvirtual, coor, solut, ndegfd,
                      time, veloc )
```

Parameters

integer ncoefs, ndegfd, ndim, ni, nj, nk, nvirtual

double precision coefs(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ncoefs)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
coor(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndim)
veloc(1:ni+1,1+nj+1,1:ndim), time

coefs Double precision array, where the first index refers to the "i"-direction, the second one to the "j"-direction and the third one to the coefficient sequence number. If ndim = 3, of course also the "k"-direction must be used.
The user must fill the coefficients himself for the complete field. Each index refers to a cell center. Only one call to usfilcsp per time step is performed, hence all coefficients the user wants to fill with this subroutine must be filled in this call.
Virtual cells do not have to be filled, hence a loop from 1 to ni and from 1 to nj must be used.

ncoefs Number of coefficients for the equation.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

ndim Dimension of space (2 or 3).

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

coor Array containing the co-ordinates of the vertices of the cells. The 4 vertices of cell (i,j) have sequence numbers (i,j), (i+1,j), (i+1,j+1), (i,j+1).

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

ndegfd Number of "old" solutions available in the present point.

time Time at which the coefficient must be evaluated.

veloc Array containing the Cartesian velocity components in the vertices at the previous time level.

Input

The parameters ncoefs, ni, nj, nk, ndim, nvirtual, ndegfd and time have gotten a value by the Deft program.
The arrays coefs, coor, solut and veloc have been filled by Deft.

Output

The user must fill the coefficients in array coefs.

Example

Suppose that the viscosity (coefficient 1) is a function of the temperature: $\mu = 0.01e^{-0.03T}$ and this parameter corresponds to choice=10000. Let the dimension of space (ndim) be 2 and T be the only transport quantity. Suppose furthermore that the flow is laminar. In that case ndegfd = 4 and soluts contains u, v, p and T respectively.
Then subroutine usfilcsp may have the following form:

```
 subroutine usfilcsp ( coefs, ncoefs, ni, nj, nk, ndim, nvirtual,
+                      coor, solut, ndegfd, time, veloc )
 implicit none
 integer ncoefs, ndegfd, ndim, ni, nj, nk, nvirtual
 double precision coefs(1-nvirtual:ni+1+nvirtual,
+                       1-nvirtual:nj+1+nvirtual,1:ncoefs),
+                 solut( 1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual,1:ndegfd),
+                 coor(1-nvirtual:ni+1+nvirtual,
+                      1-nvirtual:nj+1+nvirtual,1:ndim),
+                 veloc(1:ni+1,1+nj+1,1:ndim),
+                 time
 integer i, j
 do i = 1, ni
    do j = 1, nj
       coefs(i,j,1) = 0.01d0 * exp(-0.03*solut(i,j,4))
    end do
 end do

 end
```

6.8 Subroutine usdrhodh

Description

The user written subroutine USDRHODH must be provided, if the user provides its own equation of state. This subroutine must return the value of $\frac{\partial \rho}{\partial h}$ in all centers of the internal cells.
h may be either the enthalpy h, the total enthalpy H or the internal energy e, depending on the choice of energy equation.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
subroutine usdrhodh ( eddy, solut, ni, nj, nk, nvirtual, ndim, ndegfd, drhodh )
```

Parameters

integer ndegfd, ndim, ni, nj, nk, nvirtual

double precision eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,*)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)

drhodh(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

time Time at which the coefficient must be evaluated.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

ndegfd Number of "old" solutions available in the present point.

drhodh In this array the user must store the values of $\frac{\partial \rho}{\partial h}$ in all internal cells.

Input

The parameters ni, nj, nk, ndim, nvirtual and ndegfd have gotten a value by the Deft program.
The arrays eddy and solut have been filled by Deft.

Output

The user must fill the value of $\frac{\partial \rho}{\partial h}$ in array drhodh.

Example

For a perfect gas the equation of state is $\rho = \frac{\gamma}{(\gamma-1)} \frac{p}{h}$.
So in that case we have $\frac{\partial \rho}{\partial h} = -\frac{\gamma}{(\gamma-1)} \frac{p}{h^2}$ The pressure is stored in solut(.,.,3,1) and the enthalpy in solut(i,j,4,1).
So for a perfect gas the subroutine usdrhodh may look like:

```
      subroutine usdrhodh ( eddy, solut, ni, nj, nk, nvirtual, ndim,
     +                      ndegfd, drhodh )
      implicit none
      integer ndegfd, ndim, ni, nj, nk, nvirtual
      double precision eddy(1-nvirtual:ni+1+nvirtual,
     +                      1-nvirtual:nj+1+nvirtual,*),
```

```
+                 solut( 1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual,1:ndegfd),
+                 drhodh(1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual)
 double precision gamma, constant
 gamma = 1.4d0
 constant = -gamma/(1d0-gamma)
 integer i, j
 do i = 1, ni
    do j = 1, nj
       drhodh(i,j) = constant*solut(i,j,3,1) / solut(i,j,4,1)**2
    end do
 end do

 end
```

of course in this case there is no need to supply a subroutine usdrhodh.

6.9 Subroutine usdrhodp

Description

The user written subroutine USDRHODP must be provided, if the user provides its own equation of state. This subroutine must return the value of $\frac{\partial \rho}{\partial p}$ in all centers of the internal cells.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
subroutine usdrhodp ( eddy, solut, ni, nj, nk, nvirtual, ndim, ndegfd, drhodp )
```

Parameters

integer ndegfd, ndim, ni, nj, nk, nvirtual

double precision eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,∗)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
drhodp(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

time Time at which the coefficient must be evaluated.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

ndegfd Number of "old" solutions available in the present point.

drhodp In this array the user must store the values of $\frac{\partial \rho}{\partial p}$ in all internal cells.

Input

The parameters ni, nj, nk, ndim, nvirtual and ndegfd have gotten a value by the Deft program.
The arrays eddy and solut have been filled by Deft.

Output

The user must fill the value of $\frac{\partial \rho}{\partial p}$ in array drhodp.

Example

For a perfect gas the equation of state is $\rho = \frac{\gamma}{(\gamma-1)} \frac{p}{h}$.
So in that case we have $\frac{\partial \rho}{\partial p} = \frac{\gamma}{(\gamma-1)} \frac{1}{h}$ The enthalpy is stored in solut(i,j,4,1).
So for a perfect gas the subroutine usdrhodp may look like:

```
 subroutine usdrhodp ( eddy, solut, ni, nj, nk, nvirtual, ndim,
+                      ndegfd, drhodp )
 implicit none
 integer ndegfd, ndim, ni, nj, nk, nvirtual
 double precision eddy(1-nvirtual:ni+1+nvirtual,
+                      1-nvirtual:nj+1+nvirtual,*),
+                 solut( 1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual,1:ndegfd),
+                 drhodp(1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual)
 double precision gamma, constant
 gamma = 1.4d0
```

```
constant = gamma/(1d0-gamma)
integer i, j
do i = 1, ni
   do j = 1, nj
      drhodp(i,j) = constant / solut(i,j,4,1)
   end do
end do

end
```

of course in this case there is no need to supply a subroutine usdrhodp.

6.10 Subroutine uscalcrho

Description

The user written subroutine uscalcrho must be provided, if the user provides its own equation of state. This subroutine must return the value of ρ in all centers of the internal cells.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
      subroutine uscalcrho ( eddy, solut, ni, nj, nk, nvirtual, ndim,
     +                       ndegfd, ilowloop, iuppploop, jlowloop,
     +                       jupploop, klowloop, kupploop )
```

Parameters

integer ndegfd, ndim, ni, nj, nk, nvirtual, ilowloop, iuppploop, jlowloop, jupploop, klowloop, kupploop

double precision eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,$*$)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
drhodp(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.
For this subroutine it is important that ρ must be stored in eddy(.,.,2)

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

time Time at which the coefficient must be evaluated.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

ndegfd Number of "old" solutions available in the present point.

ilowloop, iupploop, jlowloop, jupploop, klowloop, kupploop lower and upper bounds for the i, j and k loops with respect to the filling of ρ in eddy.

Input

The parameters ni, nj, nk, ndim, nvirtual, ndegfd, ilowloop, iupploop, jlowloop, jupploop, klowloop, kupploop have gotten a value by the Deft program.
The arrays eddy and solut have been filled by Deft.

Output

The user must fill the value of ρ in array eddy (second array).

Example

For a perfect gas the equation of state is $\rho = \frac{\gamma}{(\gamma-1)}\frac{p}{h}$.
The pressure is stored in solut(.,.,3,1) and the enthalpy in solut(i,j,4,1).
So for a perfect gas the subroutine uscalcrho may look like:

```
 subroutine uscalcrho ( eddy, solut, ni, nj, nk, nvirtual, ndim,
+                       ndegfd, ilowloop, iupploop, jlowloop,
+                       jupploop, klowloop, kupploop )
 implicit none
 integer ndegfd, ndim, ni, nj, nk, nvirtual, ilowloop,
+        iupploop, jlowloop, jupploop, klowloop, kupploop
 double precision eddy(1-nvirtual:ni+1+nvirtual,
+                      1-nvirtual:nj+1+nvirtual,*),
+                 solut( 1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual,1:ndegfd)
 double precision gamma, constant
 gamma = 1.4d0
```

```
constant = gamma/(1d0-gamma)
integer i, j
do i = ilowloop, iupploop
   do j = jlowloop, jupploop
      eddy(i,j,2) = constant * solut(i,j,3,1) / solut(i,j,4,1)
   end do
end do

end
```

of course in this case there is no need to supply a subroutine uscalcrho.

6.11 Subroutine uscompinten

Description

The user written subroutine uscompinten must be provided, if the user uses the internal energy as energy equation in stead one of the enthalpy equations. This subroutine must return the value of ρ in all centers of the internal cells.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
 subroutine uscompinten ( eddy, solut, ni, nj, nk, nvirtual, ndim,
+                         ndegfd, ilowloop, iupploop, jlowloop,
+                         jupploop, klowloop, kupploop )
```

Parameters

integer ndegfd, ndim, ni, nj, nk, nvirtual, ilowloop, iupploop, jlowloop, jupploop, klowloop, kupploop

double precision eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,∗)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
drhodp(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.
For this subroutine it is important that ρ must be stored in eddy(.,.,2)

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

time Time at which the coefficient must be evaluated.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

ndegfd Number of "old" solutions available in the present point.

ilowloop, iupploop, jlowloop, jupploop, klowloop, kupploop lower and upper bounds for the i, j and k loops with respect to the filling of ρ in eddy.

Input

The parameters ni, nj, nk, ndim, nvirtual, ndegfd, ilowloop, iupploop, jlowloop, jupploop, klowloop, kupploop have gotten a value by the Deft program.
The arrays eddy and solut have been filled by Deft.

Output

The user must fill the value of ρ in array eddy (second array).

Example

For a perfect gas the equation of state is $\rho = \frac{\gamma}{(\gamma-1)}\frac{p}{h}$.
The pressure is stored in solut(.,.,3,1) and the enthalpy in solut(i,j,4,1).
So for a perfect gas the subroutine uscompinten may look like:

```
 subroutine uscompinten ( eddy, solut, ni, nj, nk, nvirtual, ndim,
+                         ndegfd, ilowloop, iupploop, jlowloop,
+                         jupploop, klowloop, kupploop )
 implicit none
 integer ndegfd, ndim, ni, nj, nk, nvirtual, ilowloop,
+        iupploop, jlowloop, jupploop, klowloop, kupploop
 double precision eddy(1-nvirtual:ni+1+nvirtual,
+                      1-nvirtual:nj+1+nvirtual,*),
+                 solut( 1-nvirtual:ni+1+nvirtual,
+                        1-nvirtual:nj+1+nvirtual,1:ndegfd)
 double precision gamma, constant
 gamma = 1.4d0
```

```
constant = gamma/(1d0-gamma)
integer i, j
do i = ilowloop, iupploop
   do j = jlowloop, jupploop
      eddy(i,j,2) = constant * solut(i,j,3,1) / solut(i,j,4,1)
   end do
end do

end
```

of course in this case there is no need to supply a subroutine uscompinten.

6.12 Subroutine usfilsrc

Description

The user written subroutine usfilsrc must be provided, if the user defines a coefficient as function with IFUNC = 10001. This subroutine must return the value of the corresponding coefficient in all centers of the internal cells.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
      subroutine usfilsrc ( coefs, ni, nj, nk, ndim, nvirtual,
     +                      coor, solut, ndegfd, time, eddy, axisym )
```

Parameters

integer ndegfd, ndim, ni, nj, nk, nvirtual, axisym

double precision time
coor(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,ndim)
eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,∗)
solut(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,1:ndegfd)
coefs(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

time Time at which the coefficient must be evaluated.

coor double precision array in which the coordinates in the vertices are stored.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.

solut Array containing all solutions at the previous time step. The first ndim vectors refer to the contravariant velocity components in a staggered grid and are therefore hard to interpret. The other unknowns are all defined in the cell centers.

coefs double precision array in which the coefficient in the cell centres must be stored by the user.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

ndegfd Number of "old" solutions available in the present point.

axisym This parameter indicates if the coordinate system is Cartesian (0) or axi-symmetric (1)

Input

The parameters ni, nj, nk, ndim, nvirtual, ndegfd, time and axisym have gotten a value by the Deft program.
The arrays eddy and solut have been filled by Deft.

Output

The user must fill the value of the coefficient in array coefs.

6.13 Subroutine uscompvisc

Description

The user written subroutine uscompvisc must be provided, if the user defines a coefficient as function with IFUNC = 10002. This subroutine must return the value of the corresponding coefficient in all centers of the internal cells.
To write this subroutine it is necessary to have some knowledge of the internal data structure of Deft as described in the Programmers Guide.

Heading

```
      subroutine uscompvisc ( coefs, eddy, ni, nj, nk, nvirtual,
     +                        ndim )
```

Parameters

integer ndim, ni, nj, nk, nvirtual

double precision time
eddy(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual,∗)
coefs(1-nvirtual:ni+1+nvirtual,1-nvirtual:nj+1+nvirtual)
In R^3 of course an extra part `1-nvirtual:nk`1+nvirtual+ is required.

eddy double precision array in which some computed quantities are stored. The storage of eddy is described in the Programmers Guide.

coefs double precision array in which the coefficient in the cell centres must be stored by the user.

ni,nj,nk Number of cells in "i", "j" and "k" direction.

nvirtual Number of virtual cells in each direction. Is only used for the declaration.

ndim Dimension of space (2 or 3).

Input

The parameters ni, nj, nk, ndim, nvirtual have gotten a value by the Deft program.
Array eddy has been filled by Deft.

Output

The user must fill the value of the coefficient in array coefs.

Chapter 7

Post-processing

Once the solution has been computed, post-processing must be applied in order to print or plot the results. In the present version of Deft only the SEPRAN post-processor ISNASPOST is available. In Section 7.1 the input to ISNASPOST is described.

7.1 Post processing with SEPRAN

7.1.1 Introduction

In the post processing part of SEPRAN, the output of the solution and derived quantities is produced in a readable (visible) form. Integrals over quantities, integrals over boundaries etc. may be computed and printed or plotted. The output generated may be produced in either print or plot form. Print output is both written to the screen or to a file for later reproducing on a printer.

The post processing is performed by the main program ISNASPOST. It requires two types of input.

First it uses some files produced by the grid generation part (meshoutput) and the computational part (sepcomp.out and sepcomp.inf).

Secondly it requires input from the standard input file.

The input of ISNASPOST is described in the next sections.

Section 7.1.2 describes the general format of the input, including the so-called compute commands, the define commands and the reset commands, Section 7.1.3 treats the various print commands, Section 7.1.4 the plot commands and Section 7.1.5 is devoted to some special commands with respect to time-dependence.

7.1.2 General input for program ISNASPOST

The input for the post processing part must be opened with the COMMAND POSTPROCESSING and must be closed with the COMMAND END.

COMMAND and DATA records.

Options are indicated between the square brackets [and].

POSTPROCESSING (mandatory)
COMMAND record: opens the input for program ISNASPOST.
Must be followed by DATA records of the shape:

NAME V0 = velocity

NAME V1 = pressure
.
.
These records identify the vectors V0, V1 and so on, with the names velocity, pressure etcetera. These names are used in the output subroutines, for example in the heading of the prints. If no names are given, a blank is printed.

In Deft V0 always corresponds to the velocity, V1 to the pressure, V2 to the stream function and V3 to V(2+NTRANS) to the NTRANS transport degrees of freedom. The vectors V(3+NTRANS) to V(2+NTRANS+NTURB) correspond to the turbulent quantities in the sequence provided by the computational program. For example for a $k-\varepsilon$ model the sequence is k followed by ε. The vectors V(3+NTRANS+NTURB) to V(2+NTRANS+NTURB+3*NDIM) correspond to the following quantities: eddy-viscosity, turbulence intensity, turbulence length scale and Reynolds stresses $\overline{u'_i u'_j}$, in which u'_i represent the Cartesian velocity fluctuations.

The actual post processing records have the following shape:

PRINT Vi .....

PLOT .....

COMPUTE Vi .....

DEFINE .....

RESET .....

TIME = ...

TIME HISTORY .....

END (mandatory)
End of the input for program ISNASPOST.

The actual post processing commands may be given in any order, with the restriction that vectors Vi to be printed or plotted must have been defined before, for example by a compute statement.

The PRINT commands are treated in Section 7.1.3, the PLOT commands in 7.1.4 and the TIME (HISTORY) commands in 7.1.5.

The SET commands, as treated in Section 3.7, may be used anywhere in the input. They become activated from the moment they have been read.

DEFINE and RESET commands

The DEFINE and RESET commands are used to set or reset of some defaults for printing or plotting. Their general syntax is:

define plot parameters = ...
define colour table = ...
reset plot parameters
reset colour table

With the define plot parameters statement, the user defines new defaults for the plot parameters. These defaults remain valid until the user resets plot parameters with the reset command, or a new 'define plot parameters' is read. For a description of the plot parameters the user is referred to 5.4.
Remark: one of the plot parameters: region = (xmin, xmax, ymin, ymax) is also used for the print commands. So if this parameter is also given in the define plot parameters, it affects the print output.

The statement define colour table defines the colour numbers for coloured plots. See 7.1.4.

COMPUTE commands

The COMPUTE command is used to define a vector Vi as function of an already available vector Vj. Using the same number i in a new COMPUTE statement redefines vector Vi.
The general syntax for the compute statements is:

```
compute Vi = velocity profile Vj [,degfd=k]
   [,origin=(O_x, O_y)] [,angle = a ]
compute Vi = intersection Vj [,degfd=k]
   [,origin=(O_x, O_y)] [,angle = a ]
compute Vi = intersection Vj [,degfd=k], [,numbunknowns=n]
   plane(ax+by+cz=d)
```

Meaning of these commands:

compute Vi = velocity profile Vj defines vector Vi as a function given by one of the velocity components (degfd=k, default k=1) along the line with origin (O_x, O_y) (default (0,0)) under an angle of a degrees (default a=0). This possibility is only permitted for two-dimensional vector fields. The intersection of the line with the grid is computed and the solution is interpolated onto this line.

Remark: at this moment the method is sensitive to round off, which means that if a line coincides with the boundary of the grid, only some parts or no part at all may be found in the intersection. In that case it is recommended to shift the line over a small distance.

compute Vi = intersection Vj. If the grid corresponding to Vj is a 2D grid, solution Vj along the line with origin (O_x, O_y) (default (0,0)) under an angle of a degrees (default a=0). k is defined by degfd=k (default k=1). This possibility is only available for functions defined on a two-dimensional grid. Furthermore this possibility is completely identical to the preceding one, including the remark given before.

If the grid corresponding to Vj is a 3D grid, solution Vj in the plane defined by ax+by+cz=d. The 3D region is intersected by the plane and a new 2D grid consisting of linear triangles is created. The vector Vj is interpolated on this new 2D grid, and the interpolation is called Vi. With the function Vi all standard postprocessing commands may be executed including the intersection with a line. Default values for a, b, c and d are zero. ISNASPOST also recognizes planes equal to 1 or -1, depending on the preceding sign. All values a, b, c and d equal to zero is not allowed. k is defined by degfd=k (default k=1).
numbunknowns = n defines the number of degrees of freedom that are interpolated. Hence the degrees of freedom k, $k+1$, ... , $k+n-1$ are interpolated. The default value is $n = 1$.

Compute statements only define the vector Vi, which means that the actual computation is performed only if necessary. At most 26 vectors Vi, including V0 are allowed in ISNASPOST.

7.1.3 Print commands for program ISNASPOST

The general input for the program ISNASPOST is described in Section 7.1.2. This paragraph is devoted to the available print commands.

At this moment only two print commands are available. The syntax of the print commands is:

Options are indicated between the square brackets [and].

PRINT Vi [,sequence = (y)] [, region = ($xmin, xmax, ymin, ymax$)]

PRINT BOUNDARY FUNCTION V*i* [,options] *boundary_description*

The *boundary_description* may take one of the following forms:

CURVES (C_1, C_2, C_3, C_5, ...)
SURFACES (S_1, S_2, S_3, S_5, ...) and the following options are available

degfd=*k*

normal_component

suppress_coordinates

tangential_component

sequence = (*y*)

PRINT V*i* prints the complete vector, together with the corresponding nodal point numbers and the co-ordinates.
If no sequence is given the co-ordinates are ordered in increasing x-sequence and for constant x-value in increasing y-sequence. If sequence = (y) is given, then first increasing y-sequence and then increasing x-sequence is used (2D) or the sequence y, z, x in 3D. Sequence = (z) creates the sequence z, y, x (3D only).

If region = $(xmin, xmax, ymin, ymax)$ is given, only the the points with co-ordinates in the range of $xmin \leq x \leq xmax$ and $ymin \leq y \leq ymax$ are printed or plotted. If $ymin, ymax$ is omitted, then the complete y-range is used.

The region to be printed may also be defined with the statement
DEFINE PLOT PARAMETERS region = (.....) which affects both plots and prints.

PRINT BOUNDARY FUNCTION V*i*, may be used to print a function defined along curves (2D and 3D) or surfaces(3d). The option surfaces may only be used if volume elements are present, the option curves if surface or volume elements exist.
The print along the curves is done in the direction of the curve and in the sequence given by the user. If negative curve numbers are used, the corresponding curve is used in reversed direction.
The print along surfaces is sorted with respect to increasing x, y and z values in the same way as for the command PRINT V*i*. In this case the option sequence = (*y*) may be used to define a different sequence.
If degfd=k is given the k^{th} degree of freedom is printed; otherwise all degrees of freedom are printed.
The standard output is the nodal point sequence number followed by the co-ordinates of the node followed by the values. If the option suppress_coordinates is used, the co-ordinates are not printed.
If the option tangential_component is used, it is supposed that the function

Vi is a vector in the points at the boundary. In that case the tangential component of this vector is computed and printed. The tangential vector is defined in the direction of the curve.
In the same way the normal component is computed and printed if the option normal_component is used. The normal is defined as the vector orthogonal to the tangential vector in clockwise direction.
The options normal and tangential component are available only in R^2.

7.1.4 PLOT commands for program ISNASPOST

The general input for the program ISNASPOST is described in Section 7.1.2. This paragraph is devoted to the available plot commands.

The syntax of the plot commands is:
Options are indicated between the square brackets [and].

Contour plots:

```
PLOT CONTOUR Vi [,degfd = k] [,plot parameters] [,nlevel = n] //
   [,levels = (q1,q2,....)] [,minlevel = min] [,maxlevel = max] //
   [,smoothing factor = s]
PLOT COLOURED LEVELS Vi [,degfd = k] [,plot parameters] [,nlevel = n] //
   [,levels = (q1,q2,....)] [,minlevel = min] [,maxlevel = max]
```

Vector plots:

```
PLOT VECTOR Vi [,degfd1 = k_1 ,degfd2 = ksub_2] [,plot parameters]
```

Function plots:

```
PLOT FUNCTION Vi  [,plot parameters]
PLOT VELOCITY PROFILE Vi [degfd=k] [,plot parameters]//
   [origin = (O_x , O_y)]   [, angle = a]
PLOT INTERSECTION Vi [degfd=k] [,plot parameters] [origin = (O_x , O_y)]//
   [, angle = a]
PLOT BOUNDARY FUNCTION Vi, curves (C1, C2, C3, C5, .. . ,Cn ) //
   [,plot parameters] [,degfd=k], [arc_scales = (smin, smax)]
```

3D plots:

```
3D PLOT Vi  [,plot parameters] [,lindirec=l] [block_mode=m] [intersect_angle=a]//
   [,ground_value=g] [,nstep=n] [,transparent]
3D COLOURED PLOT Vi  [,plot parameters]
```

Mesh plots:

```
PLOT MESH [,skip element groups ( g_1, g_2,... )] [,plot parameters] //
   [,renumbered nodes]
PLOT Vj MESH [,plot parameters]
PLOT CURVES [,plot parameters]
PLOT Vj CURVES [,plot parameters]
PLOT POINTS [,plot parameters]
```

User plot commands:

```
PLOT TEXT [,plot parameters]
PLOT POLYGON, coordinates( (x_1, y_1), (x_2, y_2), . . . , (x_n , y_n) )//
   [,plot parameters]
```

Other plot commands:

```
PLOT FIELD Vi [, plot parameters] [,PSTART = (x,y)] [,BNDPART = (j,k) ]//
   [,FLUX = f ][, FROM] [, TOWARDS]
PLOT TRACK Vi [, plot parameters] [,TMAX = t]//
   PSTART = (x_1,y_1[,z_1], x_2,y_2[,z_2] ... x_n,y_n[,z_n])//
  [,NMARK=m] [,NVIEW=v] [,MESH] [,PRINT TRACK]
```

Special plot commands:

```
OPEN PLOT
CLOSE PLOT
PLOT IDENTIFICATION, TEXT = ' text to be plotted '
```

Meaning of these commands:

Contour plots:

PLOT CONTOUR plots contour lines (lines with constant function value) for the given function.
If degfd=k is given, then the k^{th} degree of freedom in each node is used as definition of the function, otherwise the first degree of freedom is used.
The user may define the number of contour levels either by prescribing nlevel = n or by giving the contour levels explicitly through levels = $(q1, q2, \ldots)$. The default number of levels is 5. Besides prescribing the contour levels explicitly, the minimum and/or maximum level may also be given. If omitted, they are computed by the program.
The smoothing factor defines the kind of smoothing that must be applied to the contour lines. The choice $s = 0$ (default), means no smoothing, the contour lines are piecewise linear. $s = 1$, computes a mean value between three succeeding values to filter some of the possible wiggles (Shuman filtering). For s = 2, 3, 4 and 5 a smooth spline is used to plot the contour lines. The higher the value of s, the smoother the spline. Although these pictures are much nicer for publication, the actual plot is in no way better than that of the non-smooth contours. Values larger than 5 are not permitted for s.

PLOT COLOURED LEVELS Vi makes a coloured contour plot of the array Vi, where the region between two levels is coloured.
If degfd=k is given, then the k^{th} degree of freedom in each node is used as definition of the function, otherwise the first degree of freedom is used.

The user may define the number of contour levels either by prescribing nlevel = n or by giving the contour levels explicitly through levels = $(q1, q2, \ldots)$. The default number of levels is 5. Besides prescribing the contour levels explicitly, the minimum and/or maximum level may also be given. If omitted, they are computed by the program.
The colours used for the plotting are the standard colours defined for your system. These colours may be changed by the statement define colour table. See colour table.

Vector plots:

PLOT VECTOR Vi makes a vector plot of two of the degrees of freedom in each point. These components may be defined by degfd1 = k_1, degfd2 = k_2 respectively. If omitted degfd1 = 1, and degfd2 = 2 is assumed.

Function plots:

PLOT FUNCTION Vi, makes a plot of a one dimensional function. At this moment only vectors defined by COMPUTE Vi = velocity profile or COMPUTE Vi = intersection, (See Section 7.1.2) may be plotted by this command. If the solution corresponds to a one-dimensional mesh, the complete solution is plotted.

PLOT VELOCITY PROFILE Vi combines the commands COMPUTE ... = velocity profile Vi... as described in Section 7.1.2 and the command PLOT FUNCTION Vi.

PLOT INTERSECTION Vi combines the commands COMPUTE ... = intersection Vi .... as described in Section 7.1.2 and the command PLOT FUNCTION Vi.
In fact there is no difference between PLOT VELOCITY PROFILE and PLOT INTERSECTION.

PLOT BOUNDARY FUNCTION Vi, CURVES (C1,..., Cn) may be used to plot a function defined along the curves C1 to Cn, where it is necessary that the end point of the i^{th} curve, is identical to the initial point of the $(i+1)^{th}$ curve. If negative curve numbers are used, the corresponding curve is used in reversed direction.
If degfd=k is given, the kth degree of freedom is plotted; otherwise the first one is plotted.

3D plots:

3D PLOT Vi, makes a three-dimensional plot with hidden lines of a function defined on a two-dimensional mesh. With the parameter LINDIREC the user indicates in which direction the surface lines are drawn. Possibilities:

LINDIREC=1: parallel to y-axis

LINDIREC=2: parallel to x-axis

LINDIREC=3: lines are drawn in both directions

LINDIREC=5: A series of three pictures with the options 1, 2 and 3 is made

The default value for LINDIREC is 3. NSTEP=n indicates how many grid lines are used for the 3D-plot. The number of lines in each direction is equal to $(NSTEP + 1) \times \sqrt{NPOINT}$, with $NPOINT$ the number of points in the mesh. The number of grid lines may influence the quality of the picture, however, the computing time increases considerably for increasing values of NSTEP. The default value for n is 1.

3D COLOURED PLOT Vi, makes a three-dimensional plot with coloured faces of a function defined on a two-dimensional mesh. This possibility may be used only on a display. The three-dimensional surface is plotted from infinity towards the viewer, and because of that, a hidden line (surface) picture arises automatically. The colour of the surfaces indicate their distance with respect to the viewer. On a black and white screen, this option produces a classical hidden line plot, however, due to the fact that all faces are plotted and filled with a colour (or black) this option is much faster than the standard hidden line procedure. As a consequence, 3D COLOURED PLOT can not be used on a plotter. For a plot you need a hard-copy unit.

The position of the viewer may be given by EYE-POINT, the position to which the user looks is given by PROJECTION-POINT. See PLOT PARAMETERS. By changing these parameter the observer is able to view of the picture from different angles.

Mesh plots:

PLOT MESH is used to plot a mesh. With the option SKIP ELEMENT GROUPS (g_1, g_2,...) the element groups g_1, g_2,... are excluded from plotting. The brackets around (g_1, g_2,...) are essential.
With the option renumbered nodes, the renumbered nodal point numbers are plotted in stead of the standard nodal point numbers.

PLOT Vj MESH is used to plot a 2D mesh corresponding to the intersection of a 3D mesh with a plane, defined by
COMPUTE Vj = INTERSECTION Vi, PLANE(ax+by+cz=d).
In this case there is only one element group and no renumbering takes place.

PLOT CURVES is used to plot the curves in the mesh. These curves are defined by the user during the mesh generation.

PLOT Vj CURVES is used to plot the curves in the 2D mesh corresponding to the intersection of a 3D mesh with a plane, defined by
COMPUTE Vj = INTERSECTION Vi, PLANE(ax+by+cz=d).
These curves are created by the intersection program and define the outer boundary of the intersection.

PLOT POINTS is used to plot the user points in the mesh. These user points are defined by the user during the mesh generation.

User plot commands:

The user plot commands offer the user the possibility to add extra information to the standard SEPRAN plots. These commands can only be used in combination with the commands OPEN PLOT and CLOSE PLOT. A typical application is:

OPEN PLOT
PLOT CONTOUR V0
PLOT TEXT, TEXT = '.....', ORIGIN = (o_x, o_y) [,plot parameters]
CLOSE PLOT

PLOT TEXT offers the user the possibility to plot a text anywhere in the picture, provided this command has been preceded by an OPEN PLOT command and at least one of the standard SEPRAN plot commands. The command must be succeeded by (if necessary) extra plot commands and finally the command CLOSE PLOT. PLOT TEXT may never be given before a SEPRAN plot command is given. The plot parameters TEXT = 'text to be plotted ' and ORIGIN = (o_x, o_y) are mandatory. The height of the letters is defined by the parameter HEIGHT (Default: 0.25 cm). The origin must be given in user co-ordinates.

PLOT POLYGON may be used to plot a polygon anywhere in the picture. This command is subject to the same restrictions as the command PLOT TEXT. Combinations of OPEN PLOT, CLOSE PLOT, several SEPRAN plot commands and several USER plot commands (like PLOT TEXT and PLOT POLYGON) are allowed. The polygon to be plotted is defined by the data coordinates((x_1, y_1), (x_2, y_2), . . . , (x_n, y_n)). This defines a polygon from x_1, y_1 to x_2, y_2 , . . . , until x_n, y_n, where n is at least 2. If a closed polygon should be plotted, it is necessary to make the first and last point identical. The co-ordinates must be given in user co-ordinates. The brackets in the data statement coordinates are essential and may not be omitted.

Other plot commands:

PLOT TRACK may be used to compute and plot a particle trace in a velocity field. TMAX indicates the end time for the tracing of particles.
NMARK indicates the number of markers to be placed along a track.
The starting points of the particle trajectories must be given by PSTART

= ...
If MESH is given, not only the trajectories are plotted, but also the mesh. If PRINT TRACK is given, the co-ordinates of the trajectories are printed to the standard output file.
NVIEW defines the type of parallel projection in the three-dimensional case. Possible values are:

1	projection on (x,z) plane from $y = \infty$
2	projection on (y,z) plane from $z = \infty$
3	projection on (x,z) plane from $y = -\infty$
4	projection on (y,z) plane from $z = -\infty$

Special plot commands:

OPEN PLOT is a necessary command if the user wants to plot more than picture in one plot. All plot commands after this statement are plotted in the same plot until s CLOSE PLOT is given. OPEN PLOT may be used to plot several SEPRAN plot commands or to provide SEPRAN plots with extra information, for example by using PLOT TEXT and/or PLOT POLYGON. So in this way it is for example possible to get a contour plot and a vector plot in one picture.

CLOSE PLOT is necessary to close the plot opened by OPEN PLOT.

PLOT IDENTIFICATION may be used to provide all succeeding plots with the same IDENTIFICATION. This command must always be given together with the data command: TEXT = '...'. This text is plotted on each succeeding picture until a new PLOT IDENTIFICATION command is read. To suppress the effect of PLOT IDENTIFICATION, use a blank text: ' '. The position of the start of the plot identification must be given by the user by the function ORIGIN (o_x, o_y). In this special case the ORIGIN is given in centimeters counted from the origin of the plot.

Plot parameters

The following plot parameters may be used at the place formally indicated by [,plot parameters]:

angle = α
axis
bold
boundaries
colour = c
contract
elements
eye point = (x_e, y_e, z_e)
factor = f
height = h

inner
length = l
mark
maxcolour = m_2
mincolour = m_1
ncolour = n
noaxis
nobold
noboundaries
nocontract
node
noelements
noinner
nomark
nonumber
nonode
norotate
number
number format = (n_x, m_x, n_y, m_y)
pict i of n
reference = refval
region = ($xmin,\ xmax,\ ymin,\ ymax$)
rotate
scales = ($x_{under}, x_{upper}, y_{under}, y_{upper}$)
steps = (stepx, stepy)
symbol = s
text = ' .... '
textx = ' .... '
texty = ' .... '
yfact = y

These options may be separated by commas.

angle = α This parameter gives the angle under which the observer sees the plot.
$0 \leq \alpha \leq 360$

axis This parameter is used to indicate that the plot must be provided with an axis with scale. It makes only sense for those pictures that do not plot axis themselves, i.e. all pictures except those indicated by PLOT FUNCTION type commands. If an OPEN PLOT command is given, the axis are plotted only once.

bold indicates that outer boundaries to be plotted are plotted by double lines. bold may be suppressed by nobold. Default: nobold.

boundaries is used in combination with 3D COLOURED PLOT. It indicates that the boundaries of each face must be plotted in the standard colour.

For example on a black and white terminal, the combination boundaries and a black colour gives a classical hidden line plot. Boundaries may be suppressed by including a parameter noboundaries. Default: boundaries.

colour $= c$ Defines the colour number to be used for line plotting.

contract is used in combination with PLOT MESH. It indicates that the elements are contracted by a factor of 0.8 before plotting. As a result all common boundaries of elements are plotted twice. contract may be suppressed by nocontract. Default: nocontract.

element indicates that during the plotting of the mesh also the element numbers are plotted. element may be suppressed by noelement. Default: noelement.

eye point $= (x_e,\ y_e,\ z_e\ )$ defines the point where the observer is positioned. This point is only used in combination with the option 3D COLOURED PLOT. The default value is (0,−10,0).

factor $= f$ defines a multiplication factor. In the case of PLOT VECTOR it defines the multiplication factor of each vector before plotting.
In the case of a function plot, the function is multiplied by f.
Default f=1 in the case of a function plot and automatically scaling in the case of a vector plot. If factor = 0 (default value), this factor is automatically computed, otherwise the length of each vector is multiplied by f before plotting. For the length of the vectors, the physical units are used, where the unit length is made equal to the geometrical unit length as indicated by the co-ordinates.

height $= h$ gives the height of the texts to be plotted by commands involving TEXT = '...' in centimeters.

inner indicates that for plots where the boundary of the region is plotted, not only the outer boundaries are plotted, but also the inner boundaries. inner may be suppressed by noinner. Default noinner.

length $= l$ gives the length of the plot in centimeters. Instead of length also plotfm may be used. The default length is machine dependent but usual values are 20 cm or 15 cm.

mark indicates that during the plotting of the mesh also the node points are marked with a star. mark may be suppressed by nomark. Default: nomark.

maxcolour $= m_2$ gives the last value to be used in the colour table for a specific plot. The default value is mincolour + ncolour.

mincolour $= m_1$ gives the first value to be used in the colour table for a specific plot. The default value is 1.

ncolour $= n$ This parameter defines the number of colours that is used in the coloured plots. In fact this has the same meaning as nlevel $= n$, and both may be interchanged without having any influence. If both are given the first one read is used.
The default value is 20 for coloured levels, and 10 for plotted lines.

noaxis suppresses the option axis.

nobold suppresses the option bold.

noboundaries suppresses the option boundaries.

nocontract suppresses the option contract.

noelement suppresses the option element.

node indicates that during the plotting of the mesh also the node numbers are plotted. node may be suppressed by nonode. Default: nonode.

noinner suppresses the option inner.

nomark suppresses the option mark.

nonode suppresses the option node.

nonumber suppresses the option number.

norotate means that the picture is not rotated.
Default: depending on the size of the picture.

number makes only sense in combination with PLOT CURVES or PLOT POINTS. It indicates that the curves and user points must be provided with numbers. The default is nonumber.

number format $= (\, n_x, m_x, n_y, m_y)$ defines the number of digits of the numbers to be printed along the axis, where nx, ny define the number of digits in front of the decimal point (zero means floating format) and mx, my the number of digits behind the decimal point.
Default: if scales is given (0,2,0,2) otherwise computed by the program.

pict $= i$ of n May be used in combination with the records PLOT FUNCTION, PLOT VELOCITY PROFILE, or TIME HISTORY PLOT. If this statement is used, more than one one-dimensional plot is made in one picture with axes. Statements of this type must be placed consecutively, without other type of statements between. The number i must be given in increasing order from 1 to n. n gives the number of curves to be plotted in one picture.

For example the syntax in the case of $n = 3$ should be:
PLOT FUNCTION Vk_1, ... , pict 1 of 3
PLOT FUNCTION Vk_2, ... , pict 2 of 3
PLOT FUNCTION Vk_3, ... , pict 3 of 3

reference = refval is used to define a reference value for the 3D plot of a function. This reference value defines the reference value for the z-height. If reference is not given, the maximal function value is used as reference value.

region = ($xmin$, $xmax$, $ymin$, $ymax$) is used to define a cut of a two-dimensional region.

rotate means that the picture is rotated over an angle of 90°.

scales = ($x_{under}, x_{upper}, y_{under}, y_{upper}$) define the range of the scales along the axis of a one-dimensional plot, See Figure 7.1.1. (Default: computed by the program).

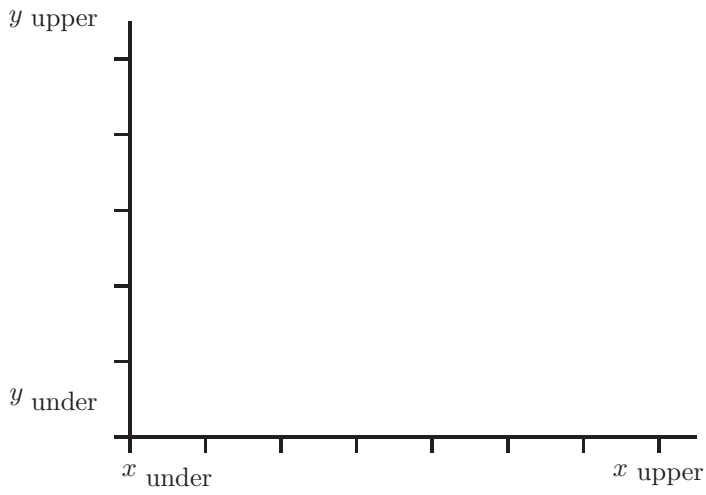


Figure 7.1.1: Definition of x_{under} etc.

steps = (stepx, stepy) defines the number of steps to be used along the axis.
(default: (10,10))

symbol = s defines the number of the symbol to be used for plotting a one-dimensional function (installation dependent).

text = ' .... ' defines a text to be plotted. For the commands PLOT IDENTIFICATION and PLOT TEXT, this is the text as described before. For the other SEPRAN plot commands, except the commands corresponding to the PLOT FUNCTION type, this text is always plotted at the bottom of the picture. Use of this option is independent of OPEN PLOT and CLOSE PLOT. If OPEN PLOT is given the text is plotted only once.

textx = ' .... ', texty = ' .... ' define the texts to be plotted along the axes (default x and y). The part between the quotes is used as text.

yfact = y Scale factor; all y-coordinates are multiplied by y before plotting the mesh.
$y \neq 1$ should be used when the co-ordinates in x and y direction are of different scales, and hence the picture becomes too small. Default value: 1.
$y < 0$ defines the *absolute* height of the picture to be $\mid y \mid$ cm.

The plot parameters defined in a plot record are only valid for that specific plot record. They overwrite defaults locally. Parameters defined by the DEFINE plot parameters command are used for all records.

Colour table

The numbers in the colour table define the colours to be used for the plotting. Which colours are connected with these numbers depends on your local installation.
The default colour table is defined by the numbers 1, 2, 3,...
By the command DEFINE COLOUR TABLE = $(C_1, C_2, C_3, \ldots)$ the user may connect new numbers to the colours 1, 2, 3 etc.

7.1.5 Special commands for time-dependent problems with respect to program ISNASPOST"

The general input for the program ISNASPOST is described in Section 7.1.2. This paragraph is devoted to the available time commands.

The syntax of the time commands is:
Options are indicated between the square brackets [and].

TIME = t_0
TIME = (t_0, t_1)
TIME = (t_0, t_1, istep)
TIME HISTORY [(t_0, t_1)] print min Vi
TIME HISTORY [(t_0, t_1)] print max Vi
TIME HISTORY [(t_0, t_1)] print min abs (Vi)
TIME HISTORY [(t_0, t_1)] print max abs (Vi)
TIME HISTORY [(t_0, t_1)] print point(x,y,z) Vi [,degfd=k]
TIME HISTORY [(t_0, t_1)] plot min Vi
TIME HISTORY [(t_0, t_1)] plot max Vi
TIME HISTORY [(t_0, t_1)] plot min abs (Vi)
TIME HISTORY [(t_0, t_1)] plot max abs (Vi)
TIME HISTORY [(t_0, t_1)] plot point(x,y,z) Vi [,degfd=k]

TIME = (t_0, t_1, istep) is meant for time-dependent problems. All commands after this COMMAND are carried out for the actual times t_0 to t_1 with

integer steps istep. If t_0 and /or t_1 do not coincide with times at which the solution is actually computed, the times closest to t_0 and t_1 are chosen. If t_1 is omitted only $t = t_0$ is used. istep gives the number of time steps minus one between succeeding times (default 1).

TIME HISTORY (t_0, t_1) makes a time history of the quantity from time t_0 to t_1. If (t_0, t_1) is omitted, the complete time interval is used.

plot / print min/max Vi plots or prints the minimum, maximum value of Vi respectively, abs(Vi) does the same for the absolute value of Vi.

plot / print point (x,y,z) Vi makes a time history of the value of Vi in point (x,y,z). At this moment the node closest to (x,y,z) is used instead of the point itself.

Chapter 8

Inspecting the output file and trouble shooting

In this chapter we shall consider the output file produced by `isnasexe` and also treat some of the possible problems that may occur when running Deft and how to solve these problems.
In Section 8.1 the present form of the output file is considered. Trouble shooting is the subject of Section 8.2.

8.1 Inspecting the output file

In the file isnasexe.out a lot of information about the computations can be found. In general most of it is not important for the user and in future versions the amount of output will be reduced considerably. At this moment each time step produces output. For example the last time step of the example treated in Section 9.1 gives the following output:

```
TIME STEP   10    (t =   1.00)



Output of subroutine  ISGMR


The 2-norm of the initial residual is:0.475927E-03
The number of executed iterations in ISGMR  is     3
The 2-norm of the residual is 0.202052E-07
```

```
Output of subroutine  ISGMR


The 2-norm of the initial residual is:0.295993E-03
The number of executed iterations in ISGMR  is     7
The 2-norm of the residual is 0.261574E-10

THE NET MASS OUTFLOW OVER ALL BLOCKS IS   -2.049E-11

STOPPING CRITERION FOR STATIONARY SOLUTION

Equation       Lambda1        Stopcrit.      Maxnorm
   1         0.588151E+00   0.599860E-03   0.121776E-03
   2         0.633784E+00   0.508468E-01   0.165019E-01
```

It starts with the actual time step and time. Next some output of subroutine ISGMR is produced. This is in fact the linear solver. First the output with respect to the velocity is printed and after that with respect to the pressure. This output is self-explaining.
The output ends with the net mass outflow, which should be approximately 0, and some information about the stopping criterion. This information gives information to check whether the solution has become stationary.
The stopping criterion gives information about each equation, where equation 1 refers to the velocity and equation 2 to the pressure. The lambda printed is nothing else than $\frac{\|u^{n+1}-u^n\|}{\|u^n-u^{n-1}\|}$ where the super script denotes the time level. This parameter is an indication of how fast the method is converging to steady state. If lambda is not less than 1. there is no guarantee that you are in the neighbourhood of a steady state. The Stopcrit value indicates how small the norm must be in order that the solution may be considered stationary. It uses an accuracy of 10^{-2}. Maxnorm gives the norm of the difference of the last two iterations. So we see that in this example indeed the stationary state has been reached within the accuracy required.

8.2 Trouble shooting

8.2.1 No convergence

One of the most frequently produced error message concerns the lack of convergence in the linear solver. Another problem might be that the solution does not reach steady state.
In both cases it is in general difficult to find the cause of the problems. In this section we shall do some suggestions about possible reasons and what to do in such cases.

Decrease time-step If all input is correct and the mathematical model is

supposed to converge then the standard solution is always to reduce the time-step. Especially in the case of a transient small time-steps may be necessary for convergence of the solution. Since this is the easiest way to overcome problems, it is always a good practice to start with this method.

Check input In fact checking of the input should always be done at first. It is important that coefficients and boundary conditions are given in a correct way.

Check boundary conditions An important part of the checking of the input is the checking of the boundary conditions. It is necessary that the number of boundary conditions at each boundary is correct. This means that for the momentum equations exactly *ndim* boundary conditions must be given for each outer boundary and for the scalar unknowns exactly one. Furthermore the velocity boundary conditions must be given in independent directions.

Always realize that normal components are directed outwards and that tangential components are always directed in the anti-clockwise direction. So, for example, 'un = 1' does not mean a uniform inflow velocity profile but rather a uniform velocity profile.

Another important item is the prescription of boundary conditions at outflow. In general, prescribing the unknowns at the outflow boundary (Dirichlet boundary conditions), is non-physical and may introduce serious convergence problems.

Finally prescribing the normal velocity at all outer boundaries, implies that the pressure is not unique but fixed upon an additive constant. In that case it is necessary to have an exact mass balance over the outer boundaries.

Check model parameters Another important issue is the checking of the model parameters. It might be possible that the flow is turbulent, whereas you use a laminar model. For example if ρ is too large, μ too small or the velocity too large, the flow may become turbulent and a turbulence model is necessary. Always estimate the Reynolds number in order to be sure that the flow is laminar.

8.2.2 Wiggles

In some cases Deft has produced results that show clear wiggles. If the wiggles occur in the neighbourhood of the outflow boundary this may be caused by inaccurate or incorrect outflow boundaries.
Another possible reason for wiggles is that the grid is not smooth enough. Sharp gradients in the grid may produce wiggles in the solution, especially at large Reynolds numbers. A possible solution is to smooth the grid. Sometimes multiblock is necessary to get a smooth grid. If smoothing of the grid is not possible

or hard to achieve, it is advised to use another type of discretization like the so-called "WesBeek" discretization.

Note that in some rare cases, wiggles may be produced by postprocessing. Wiggles due to postprocessing can be recognized easily since these are always confined within grid cells. Wiggles across different grid cells are probably a result of Deft computation.

Chapter 9

Examples

In this chapter we consider a number of test examples that have been run to test the Deft code. These examples are merely meant to test the code both from a software point of view as well as from a numerical point of view. However, they give also an impression of how a real application may look like.
In Section 9.1 we consider one of the most simple flows, the Poisseuille flow in a straight channel.
Section 9.2 treats the laminar flow in a 90° bend at Reynolds number 100.
In Section 9.3 the flow through an l-shaped region is computed with a staggered arrangement. This example is meant to demonstrate the effect of a very non-smooth region.
In Section 9.4 the flow through an l-shaped region is computed with a collocated arrangement. This example allows to show the behaviour of the collocated scheme on a realistic non-smooth grid.
Section 9.5 shows a more complicated example, the flow over a backward facing step. This example is commonly used as benchmark problem. In our case we compare single block with multiblock.
In Section 9.6 an example of a user function is demonstrated. It concerns an analytic example that has no practical importance but may be used to check the accuracy of the solution method.
Section 9.7 deals with a problem containing an extra transport equation. In this example we consider the flow in a square cavity driven by a temperature difference. As a consequence the momentum equations are coupled with the temperature equation.
An example of a turbulent flow is treated in Section 9.8. In this example we consider a turbulent flow through a tube with a sinusoidal constriction using a k-ε model.
Section 9.9 shows an example of the solution of a transport equation, where the velocity is given. In this case the momentum equations are skipped. The example concerns a well-known benchmark problem, the so-called Molenkamp test.
Section 9.10 shows an example of the solution of the Burgers equation. IN this

case only the momentum equations are solved, the pressure is taken equal to zero.
Finally in Section 9.11 we give a list of all available examples in the Deft directory that can be put into your local directory with the command "isgetex".

9.1 Poisseuille flow in a straight channel

One of the simplest flows is the Poisseuille flow in a straight channel. This flow can be used as a first check on the reliability of the code. The region is given by $0 \leq y \leq 1, \quad 0 \leq x \leq L$. See Figure 9.1.1 for a sketch of the region.

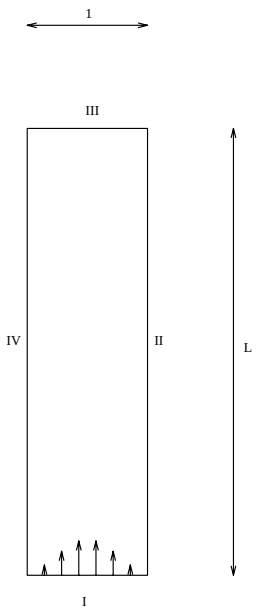


Figure 9.1.1: Definition region for straight channel

At boundary I we have a parabolic inflow condition:

$$\boldsymbol{u} = \begin{pmatrix} 0 \\ 4x(1-x) \end{pmatrix} \tag{9.1}$$

at the boundaries II and IV a no-slip condition and at boundary III we prescribe the parallel outflow condition

$$u_t = 0, \quad \sigma^{nn} = 0 \tag{9.2}$$

The exact solution of the Navier-Stokes equations under these boundary conditions is given by:

$$\boldsymbol{u} = \begin{pmatrix} 0 \\ 4x(1-x) \end{pmatrix}, \quad p = 0.8(L-y) \tag{9.3}$$

In this example the convective terms are equal to zero.
At first sight one may expect (at least for an equidistant grid) that the code solves this problem exactly. However, numerical experiments show that the solution contains a small error. A thorough analysis shows that this error is

due to the approximation of the boundary conditions at the fixed walls. In the Deft code we use a linear extrapolation to satisfy the boundary condition for the tangential velocity. However, this velocity is quadratic and hence the boundary condition is not satisfied exactly. A refinement of the grid shows a $O(h^2)$ convergence to the correct solution.

9.1.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex channel
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  channel
sepmesh  channel.msh
isnaspre channel.prb
isnasexe
isnaspost  channel.pst [ > channel.out ]
sepdisplay
```

The part between the square brackets [] is optional. If it is used the output of the command isnaspost is written to the file channel.out.

9.1.2 Mesh

If we define L = 4, and use 6 cells in the vertical direction and 4 cells in the horizontal direction with equidistant spacing than the following input file for sepmesh might be used to generate the grid:

```
constants
   integers
      nelm1 = 6
      nelm2 = 4
   reals
      B = 1
      H = 4
end
mesh2d
   isnas
   points
      p1=(0,0)
      p2=($B,0)
      p3=($B,$H)
```

```
      p4=(0,$H)
   curves
      c1 = line1(p1,p2,nelm=$nelm1)
      c2 = line1(p2,p3,nelm=$nelm2)
      c3 = line1(p3,p4,nelm=$nelm1)
      c4 = line1(p4,p1,nelm=$nelm2)
   surfaces
      s1 = rectangle5(c1,c2,c3,c4)
   plot
end
```

9.1.3 Problem description

The solution has been defined such that the maximum velocity at inflow is equal to 1. In this example we use a time-step $\Delta t = 0.1$ and an end time $t_1 = 1$, hence 10 time steps are carried out. Since this a stationary problem $\theta = 1$ is recommended. If we define $\rho = 5$ and $\mu = 0.5$, the following file channel.prb might be used to solve the problem.

```
*
Input for the straight channel problem
*
time_integration
   tinit = 0
   tend =  2
   tstep = .1
   theta = 1
   rel_stationary_accuracy = 1d-2
boundary_conditions
   curve 1: inflow 1.0
   curve 2: noslip
   curve 4: noslip
   curve 3: parallel_outflow
coefficients
   momentum_equations
      rho   = 5
      mu    = .5
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      divaccuracy = 0
      startvector = zero
```

9.1.4 Post-processing

If we want to print the velocity, make a vector plot of the velocity, a contour plot of pressure and stream lines, a three-dimensional plot of the pressure and a coloured level plot of the pressure, then the following input file for isnaspost might be used:

```
postprocessing
   name v0 = 'velocity'
   name v1 = 'pressure'
   name v2 = 'stream function'
print vector v0
   plot identification = text = ' Deft  ',origin =(10,10)
   plot vector v0, factor=.2 //
       text='velocity field   Re=10  mesh 6x4  dt=.1  tend=1.0'
   plot contour v1, nlevel=8 //
       text='pressure contour Re=10  mesh 6x4  dt=.1  tend=1.0'
   plot contour v2, nlevel=8 //
       text='streamlines      Re=10  mesh 6x4  dt=.1  tend=1.0'
   3d plot v1, nlevel=20
   plot coloured levels v1, nlevel=8

end
```

9.1.5 Output produced by this example

When running this example each command itself produces some output.

The command sepmesh produces two files: meshoutput and finvol.new. Besides that it echoes the input to the screen as well as some extra information about number of points, number of cells and computation time.

The command isnaspre makes two files isnasinp.cmp and isnaspre.out.

The command isnasexe makes three files sepcomp.inf, sepcomp.out and isnasexe.out. The file isnasexe.out contains the actual output that is readable for the user.
In the file isnasexe.out a lot of information about the computations can be found. In general most of it is not important for the user and in future versions the amount of output will be reduced considerably. The output of the last time step can be found in Section 8.1.

9.2 Flow through a 90 degree bend

A less trivial example is that of a flow through a 90 degrees bend as shown in Figure 9.2.2. The regions defined by the curves 1, 2, 8, 9 and 4, 5, 6, 10 are added to the bend in order to force some kind of fully developed flow at instream and outstream boundary. The boundaries 2, 3, 4 and 6, 7, 8 form the fixed walls. Boundary 1 is an instream boundary, hence boundary 5 is an outlet.
Boundary conditions:

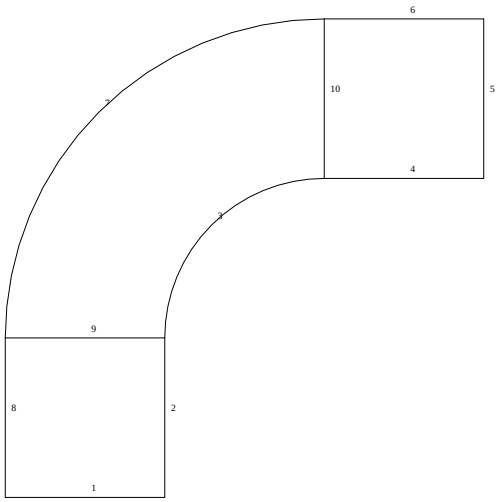


Figure 9.2.2: Definition region of the 90 degree bend

fixed walls (1, 2, 8, 9 and 4, 5, 6, 10) $\quad \boldsymbol{u} = \mathbf{0}$
instream boundary $\boldsymbol{u} = \begin{pmatrix} 0 \\ 4x(1-x) \end{pmatrix}$
outstream boundary $\sigma^{nn} = 0, \quad \sigma^{nt} = 0.$

9.2.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex bend
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  bend
sepmesh  bend.msh
isnaspre bend.prb
isnasexe
isnaspost  bend.pst [ > bend.out ]
sepdisplay
```

9.2.2 Mesh

If we define a grid of 8 × 8 cells in the rectangular regions and a grid of 8 × cells in the bend, then the following input file to create the mesh may be used:

Figure 9.2.3 shows the grid generated by sepmesh.

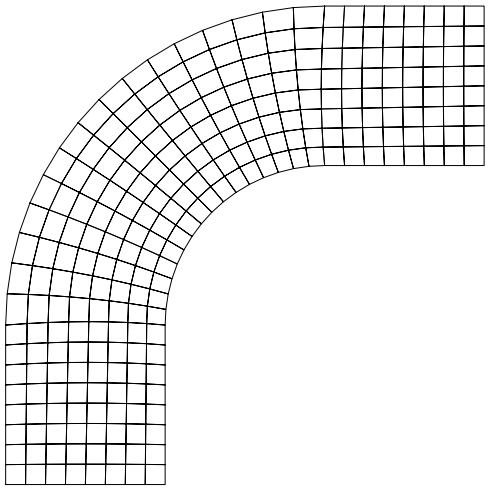


Figure 9.2.3: Mesh for bend problem generated by sepmesh

9.2.3 Problem description

If we define a parabolic inflow profile with maximum velocity 1, a time step $\Delta t = 0.2$, an end time $t_1 = 8$ and as physical parameters $\rho = 50, \mu = 0.5$ then the following input file may be defined to compute the stationary solution:

```
*
Input for the bend problem
*
time_integration
   tinit = 0
   tend =  40
   tstep = .2
   theta = 1
   rel_stationary_accuracy = 1d-2
boundary_conditions
   curve 1: inflow 1.0
   curve 11: noslip
   curve 5: outflow
   curve 12: noslip
coefficients
   momentum_equations
      rho   = 50
      mu    = .5
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      divaccuracy = 0
      startvector = zero
discretization
   momentum_equations
      upwind = none
#      lin_convection = picard
```

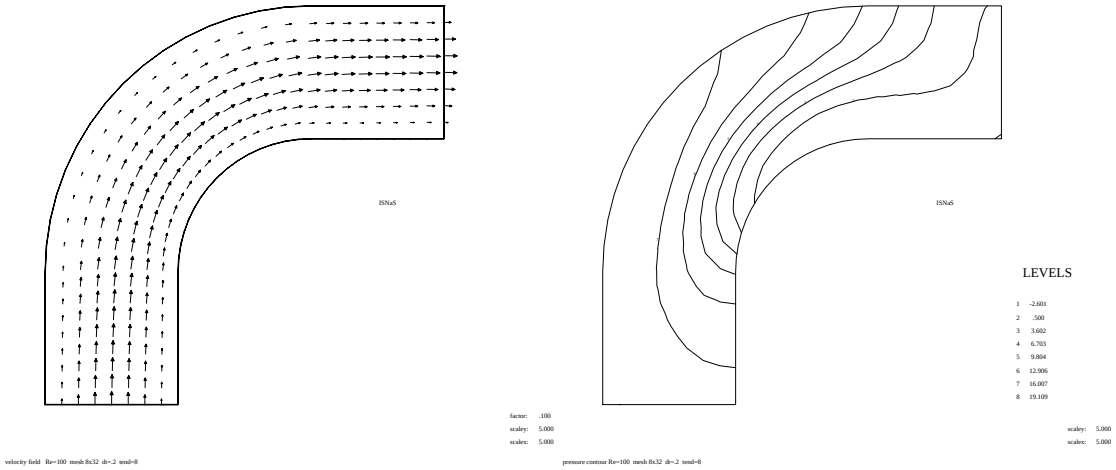
The output file shows that in this case the stationary solution has not yet been reached completely. However, if we require an accuracy of at most 1 %, the solution may be considered as steady state.

9.2.4 Post-processing

The following self explaining input file for isnaspost is used.

```
postprocessing
   plot identification = text = ' Deft  ',origin =(15,10)
   plot mesh
   plot vector v0, factor=.1 //
       text='velocity field   Re=100  mesh 8x32  dt=.2  tend=8'
   plot contour v1, nlevel=8 //
       text='pressure contour Re=100  mesh 8x32  dt=.2  tend=8'
   plot contour v2, nlevel=8 //
       text='streamlines      Re=100  mesh 8x32  dt=.2  tend=8'
   plot coloured levels v1,nlevel=19
end
```

Figure 9.2.4 shows the vector plot of the velocity, as well as the isobars and the stream lines.



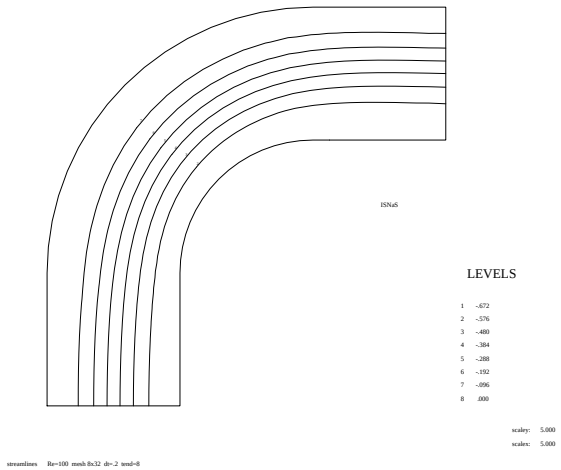


Figure 9.2.4: Vector plot of the velocity, isobars and stream lines in bend problem

9.3 Flow through an L-shape

To investigate the performance of the Deft code for a very non-smooth grid, we consider the flow through an L-shape. Of course such a region is extremely suitable for a multiblock approach, but we will postpone the demonstration of a multiblock example to Section 9.5.
A sketch of the region can be found in 9.3.5.

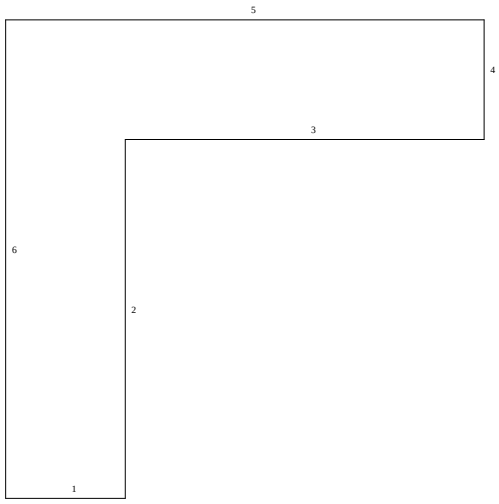


Figure 9.3.5: Definition region of the L-shape

The instream boundary is at the lower side, the outlet at the right-hand side. All other boundaries are assumed to be fixed walls, where we prescribe a no-slip condition $\mathbf{u} = \mathbf{0}$. At the inlet a parabolic velocity field is given and at the outstream boundary we impose the artificial (non-correct) boundary conditions $\sigma^{nn} = 0, u_t = 0$.

9.3.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex lshape
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  lshape
sepmesh  lshape.msh
isnaspre lshape.prb
isnasexe
isnaspost  lshape.pst [ > lshape.out ]
sepdisplay
```

9.3.2 Mesh

The following file may be used to create a grid.

```
constants
   integers
      nelm1=8
end
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(1,0)
      p3=(1,3)
      p4=(4,3)
      p5=(4,4)
      p6=(0,4)
   curves
      c1 = line1(p1,p2,nelm=$nelm1)
      c2 = line1(p2,p3,nelm=$nelm1)
      c3 = line1(p3,p4,nelm=$nelm1)
      c4 = line1(p4,p5,nelm=$nelm1)
      c5 = line1(p5,p6,nelm=$nelm1)
      c6 = line1(p6,p1,nelm=$nelm1)
      c7 = curves(c2,c3)
      c8 = curves(c5,c6)
   surfaces
      s1 = rectangle5(c1,c7,c4,c8)
      plot
end
```

Figure 9.3.6 shows the grid generated by sepmesh.

9.3.3 Problem description

The data for the L-shape problem are respectively $\rho = 5$ and $\mu = 0.5$. The input file for isnaspre might have the following shape

```
*
Input for the lshape problem
```

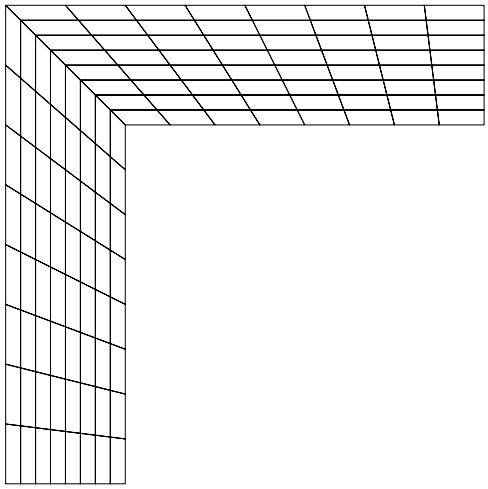


Figure 9.3.6: Mesh for L-shape generated by sepmesh

```
*
time_integration
   tinit = 0
   tend = 3.0
   tstep = .15
   theta = 1
   rel_stationary_accuracy = 1d-2
boundary_conditions
   curve 1: inflow 1.0
   curve 2 to 3: noslip
   curve 4: sigmann=0, ut=0
   curve 5 to 6: noslip
coefficients
   momentum_equations
      rho   = 5
      mu    = .5
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
```

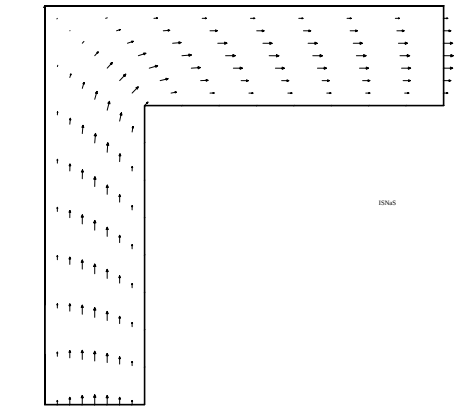
```
      divaccuracy = 0
      startvector = zero
```

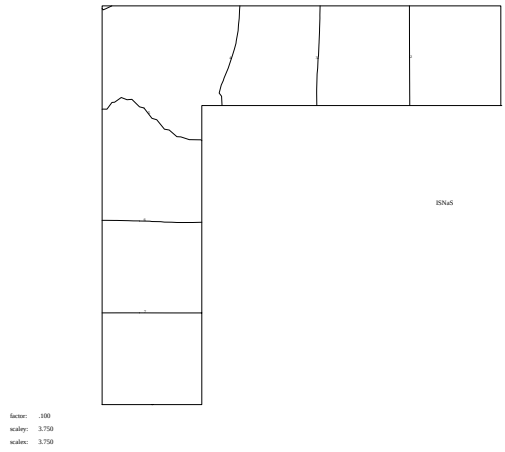
9.3.4 Post-processing

The following self explaining input file for isnaspost is used.

```
postprocessing
   plot mesh
   plot identification = text = ' Deft  ',origin =(15,10)
   plot vector v0, factor=.1//
       text='velocity field   Re=10  mesh 8x16  dt=.15  tend=1'
   plot contour v1, nlevel=8//
       text='pressure contour Re=10  mesh 8x16  dt=.15  tend=1'
   plot contour v2, nlevel=8//
       text='streamlines      Re=10  mesh 8x16  dt=.15  tend=1'
end
```

Figure 9.3.7 shows the vector plot of the velocity, the isobars and the stream lines. From these pictures it is clear that Deft is able to handle fairly non-smooth grids, however, with a certain price. The "discontinuity" in the grid-derivatives is clearly visible in the streamlines. In order to get a smooth solution it is necessary to smooth the grid or to use multi block.





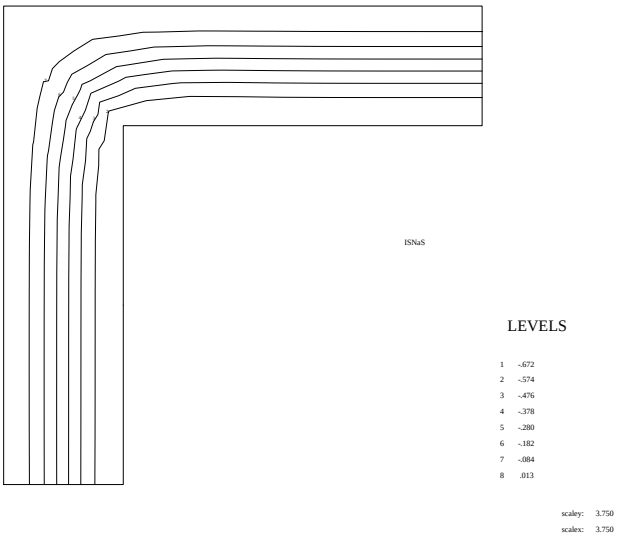


Figure 9.3.7: Vector plot of the velocity, isobars and stream lines in L-shape problem

9.4 Flow through an L-shape. Collocated scheme

To investigate the performance of the Deft code for a very non-smooth grid, we consider the flow through an L-shape with the help of a collocated scheme.
A sketch of the region can be found in 9.4.8.

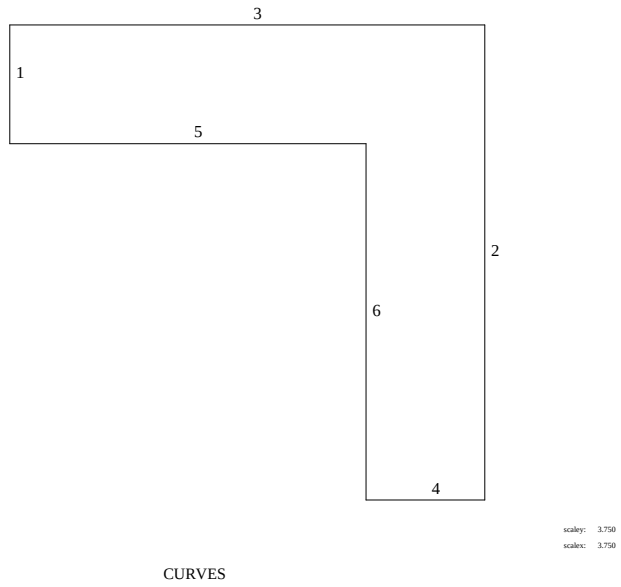


Figure 9.4.8: Definition region of the L-shape

The instream boundary is at the lower side, the outlet at the right-hand side. All other boundaries are assumed to be fixed walls, where we prescribe a no-slip condition $\mathbf{u} = \mathbf{0}$. At the inlet and at the outlet, a parabolic velocity field is given.

9.4.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex lshape_col
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  lshape_col
sepmesh  lshape_col.msh
```

```
isnaspre lshape_col.prb
isnasexe
isnaspost  lshape_col.pst [ > lshape_col.out ]
sepdisplay
```

9.4.2 Mesh

The following file may be used to create a grid.

```
constants
   reals
      right = 1
      top = 4
      left = -3
      walltop = 3
   integers
      nelm1=26
      nelm2=25
      nelm3=29
end
mesh2d
   isnas
   points
      p1=(0,0)
      p2=($right,0)
      p3=($right,$top)
      p4=($left,$top)
      p5=($left,$walltop)
      p6=(0,$walltop)
   curves
      c1 = line1(p1,p2,nelm=$nelm1)
      c2 = line1(p2,p3,nelm=$nelm2,factor=0.5,ratio=1)
      c3 = line1(p3,p4,nelm=$nelm3,factor=1.5,ratio=1)
      c4 = line1(p4,p5,nelm=$nelm1)
      c5 = line1(p5,p6,nelm=$nelm3,factor=0.5,ratio=1)
      c6 = line1(p6,p1,nelm=$nelm2,factor=2.,ratio=1)
      c7 = curves(c2,c3)
      c8 = curves(c5,c6)
   surfaces
      s1 = rectangle5(c1,c7,c4,c8)
      plot
end
```

Figure 9.4.9 shows the grid generated by sepmesh.

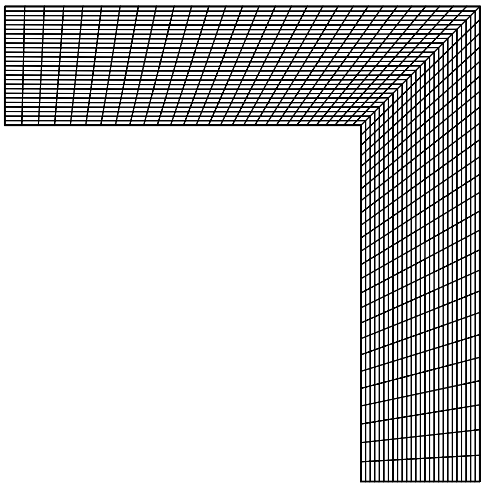


Figure 9.4.9: Mesh for L-shape generated by sepmesh

9.4.3 Problem description

The data for the L-shape problem are respectively $\rho = 1$ and $\mu = 1$. The input file for isnaspre might have the following shape

```
*
Input for the L-shape problem
Collocated arrangement
Wesbeek+bilinear interpolation
*
initial_conditions
time_integration
   tinit = 0
   tend =  5.
   tstep = .01
   theta = 1
   rel_stationary_accuracy = 1d-6
boundary_conditions
   curve 1: u_momentum = dirichlet = 0
            v_momentum = dirichlet = func = 1
   curve 2 to 3: u_momentum = dirichlet = 0
                 v_momentum = dirichlet = 0
   curve 4: u_momentum = dirichlet = func = 2
            v_momentum = dirichlet = 0
```

```
   curve 5 to 6: u_momentum = dirichlet = 0
                 v_momentum = dirichlet = 0
coefficients
   momentum_equations
      rho   = 1
      mu    = 1
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-10
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      divaccuracy = 0
      startvector = zero
discretization
   momentum_equations
   discr_method=bilinear_interpolation
   collocated_grid
end_of_isnas_input
```

9.4.4 Post-processing

The following self explaining input file for isnaspost is used.

```
postprocessing
   name v0 = 'velocity'
   name v1 = 'pressure'
   name v2 = 'stream function'
   plot mesh
   plot identification = text = ' Deft collocated Wesbeek ',origin =(5,10)
   plot vector v0, factor=.2 //
       text='velocity field   Re=1'
   plot contour v1, nlevel=11 //
       text='pressure contour Re=1'
   compute v2 = stream function v0
   name v2 = stream function
   plot contour v2, nlevel=11 //
       text='streamlines      Re=1'
end
```

Figure 9.4.10 shows the vector plot of the velocity, the isobars and the stream lines. From these pictures it is clear that Deft is able to handle fairly non-smooth grids, however, with a certain price. To remove an eventual "discontinuity" in the grid-derivatives, it is necessary to refine the grid (See section 2.2.1).

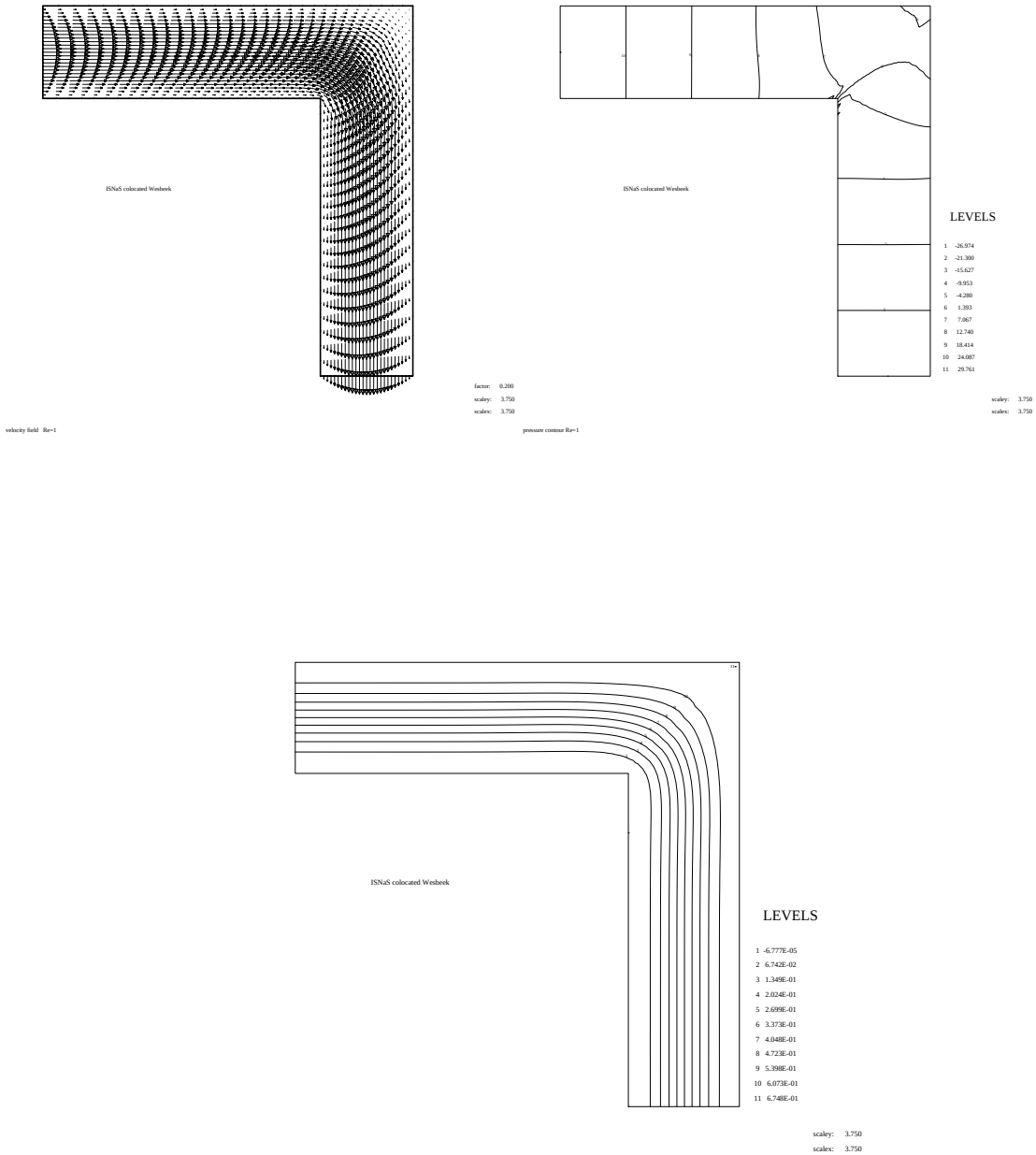


Figure 9.4.10: Vector plot of the velocity, isobars and stream lines in L-shape collocated problem

9.5 Flow over a backward-facing step

The backward facing step belongs to the class of accepted benchmark problem for the incompressible Navier-Stokes equations. Reliable reference solutions can be found in Morgan et al. [26].

Figure 9.5.11 shows the configuration of the region. At boundary 1 (the inlet)

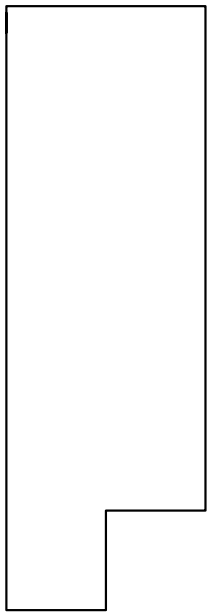


Figure 9.5.11: Definition region of the backward-facing step

we assume a parabolic velocity profile, the boundaries 2, 3, 4, 6, 7 and 8 are fixed walls. At those boundaries we prescribe a no-slip condition. At boundary 5 (the outlet) we prescribe a semi-natural outflow condition, i.e. $\sigma^{nn} = 0, u_t = 0$. The Reynolds number is defined by

$$Re = U_{max}(H - h)/\nu$$

with	U_{max}	the maximum value of the velocity profile at the inlet,
	ν	the kinematic viscosity
	H	the height of the channel after the step
	h	the height of channel above the step

In first instance we shall solve the problem using a smoothed single block grid. After that the multiblock approach will be showed.

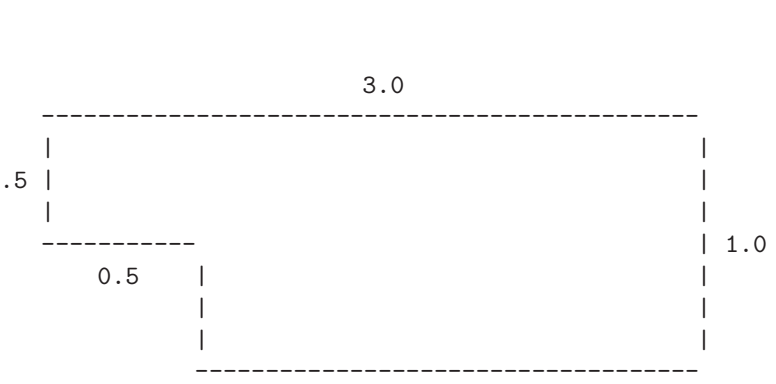
9.5.1 Obtaining the files and running the problem for the single block problem

The relevant files for the single block problem can be copied to the current directory by the following command:

```
isgetex  bfs_sb
sepmesh  bfs_sb.msh
isnaspre bfs_sb.prb
isnasexe
isnaspost  bfs_sb.pst [ > bfs_sb.out ]
sepdisplay
```

9.5.2 Single block mesh

The mesh is generated as one single block. In order to avoid discontinuities due to the abrupt change of the boundary the grid is smoothed using the option smooth in rectangle.




```
constants
   integers
      nelm1=32
   reals
      dim1=3.0
end
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(.5,0)
      p3=(.5,.5)
      p4=(1,0.5)
      p5=(1,$dim1)
```

```
      p6=(0,$dim1)
      p7=(0,1.5)
      p8=(0,1)
   curves
      c1 = line1(p1,p2,nelm=16)
      c2 = line1(p2,p3,nelm=8)
      c3 = line1(p3,p4,nelm=8)
      c4 = line1(p4,p5,nelm=$nelm1)
      c5 = line1(p5,p6,nelm=16)
      c6 = line1(p6,p7,nelm=$nelm1)
      c7 = line1(p7,p8,nelm=8)
      c8 = line1(p8,p1,nelm=8)
      c9 = curves(c2,c3,c4)
      c10 = curves(c6,c7,c8)
   surfaces
      s1 = rectangle5(c9,c5,c10,c1,smooth=2)
      plot
end
```

Figure 9.5.12 shows the grid generated by sepmesh.

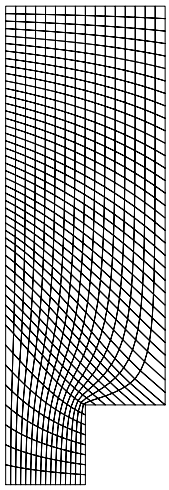


Figure 9.5.12: Single block mesh for backward-facing step generated by sepmesh

9.5.3 Single block problem description

If we define $\rho = 50$ and $\mu = 0.5$ then the following problem file may be used.

```
*
Input for the Backward facing step problem single block,
parabolic inflow boundary condition wit Umax = 1.0 .
*
time_integration
   tinit = 0
   tend =  80
   tstep = .25
   theta = 1
   rel_stationary_accuracy = 1d-2
boundary_conditions
   curve 1: inflow 1.0
   curve 9: noslip
   curve 5: parallel_outflow
#   curve 5: outflow
#   curve 5: inflow -0.5
   curve 10: noslip
coefficients
   momentum_equations
      rho   = 50
#      rho   = 150
      mu    = .5
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      divaccuracy = 0
      startvector = zero
```

9.5.4 Single block post-processing file

The following self explaining input file for isnaspost is used.

```
postprocessing
   plot mesh
   plot identification = text = ' ISNAS 2D backward facing step ',origin =(10,12)
   plot vector v0, factor=.1//
       text='velocity field   Re=50  mesh 16x48  dt=.25  '
   plot contour v1, levels=(-6.2, -4.5, -3.0, -1.0,//
       .1, 2.5, 4.5, 6.0)//
       text='pressure contour Re=50  mesh 16x48  dt=.25  '
   plot contour v2,levels=(-0.015, -0.010, -0.005, 0.000, 0.006,//
     0.016, 0.036, 0.086, 0.136, 0.186, 0.236, 0.286, 0.311, 0.186)//
```

```
       text='streamlines      Re=50  mesh 16x48  dt=.25  '
end
```

Figure 9.5.13 shows the vector plot of the velocity, the isobars and the stream lines. Mark that the step is only slightly visible in the stream lines.

9.5.5 Obtaining the files and running the problem for the multi block problem

The relevant files for the multi block problem can be copied to the current directory by the following command:

```
isgetex  bfs_mb
sepmesh  bfs_mb.msh
isnaspre bfs_mb.prb
isnasexe
isnaspost  bfs_mb.pst [ > bfs_mb.out ]
sepdisplay
```

9.5.6 Multi block mesh

The multi block mesh differs from the single block mesh in the sense that it consists of two blocks and that all cells are rectangular. The input file has the following shape:

```
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(.5,0)
      p3=(.5,.5)
      p4=(1,0.5)
      p5=(1,3)
      p6=(.5,3)
      p7=(0,3)
      p8=(0,.5)
   curves
      c1 = line1(p1,p2,nelm=8)
      c2 = line1(p2,p3,nelm=8)
      c3 = line1(p3,p4,nelm=8)
      c4 = line1(p4,p5,nelm=40)
      c5 = line1(p5,p6,nelm=8)
      c6 = line1(p6,p7,nelm=8)
      c7 = line1(p7,p8,nelm=40)
      c8 = line1(p8,p1,nelm=8)
      c9 = line1(p3,p6,nelm=40)
      c10 = curves(c2,c9)
```

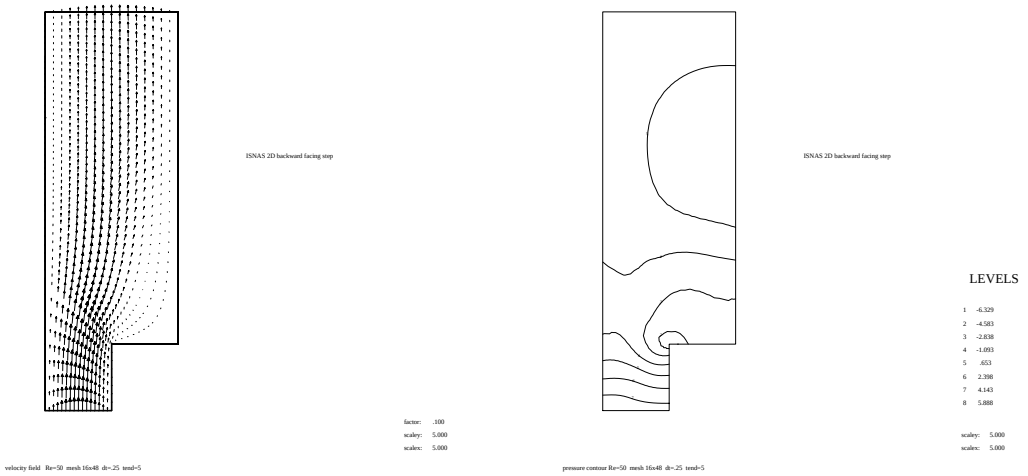


Figure 9.5.13: Vector plot of the velocity, isobars and stream lines in single block backward-facing step

```
      c11 = curves(c7,c8)
   surfaces
      s1 = rectangle5(c10,c6,c11,c1)
      s2 = rectangle5(c4,c5,-c9,c3)
   plot
end
```

Figure 9.5.14 shows the grid generated by sepmesh.

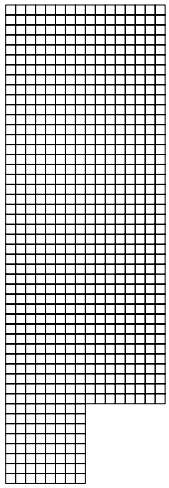


Figure 9.5.14: Multi block mesh for backward-facing step generated by sepmesh

9.5.7 Multi block problem description

The multi block problem file is nearly identical to the single block one, except that the curves have got other names and as a consequence the description of the boundary conditions changes a bit.
Besides that the command number_of_computers = 2 has been added, which implies that not only multi block is applied but also that the multi block process is carried out in parallel at two processors.
The input file becomes:

```
*
Input for the Backward facing step problem multi block
*
number_of_computers = 2
time_integration
```

```
   tinit = 0
   tend  = 5
   tstep = .25
   theta = 1
boundary_conditions
   curve 1: inflow 1.0
   curve 2 to 4: noslip
   curve 5 to 6: parallel_flow
   curve 7 to 8: noslip
coefficients
   momentum_equations
      rho   = 50
      mu    = .5
linear_solver
   momentum_equations
      amount_of_output = 1
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 1
      divaccuracy = 0
      startvector = zero
```

9.5.8 Multi block post-processing

The multi block post processing file is only a little bit different from the single block input file. We give this file without comment.

```
postprocessing
   plot mesh
   plot identification = text = ' ISNAS 2D backward facing step ',origin =(10,12)
   plot vector v0, factor=.1//
       text='velocity field   Re=50  mesh 16x48  dt=.25  tend=5'
   plot contour v1, nlevel=8//
       text='pressure contour Re=50  mesh 16x48  dt=.25  tend=5'
   plot contour v2,levels=(-0.009, -0.004, -0.002, 0.000, 0.006,//
     0.016, 0.036, 0.086, 0.136, 0.186, 0.236, 0.286, 0.311, 0.186)//
       text='streamlines      Re=50  mesh 16x48  dt=.25  tend=5'
end
```

Figure 9.5.15 shows the vector plot of the velocity, the isobars and the stream lines.

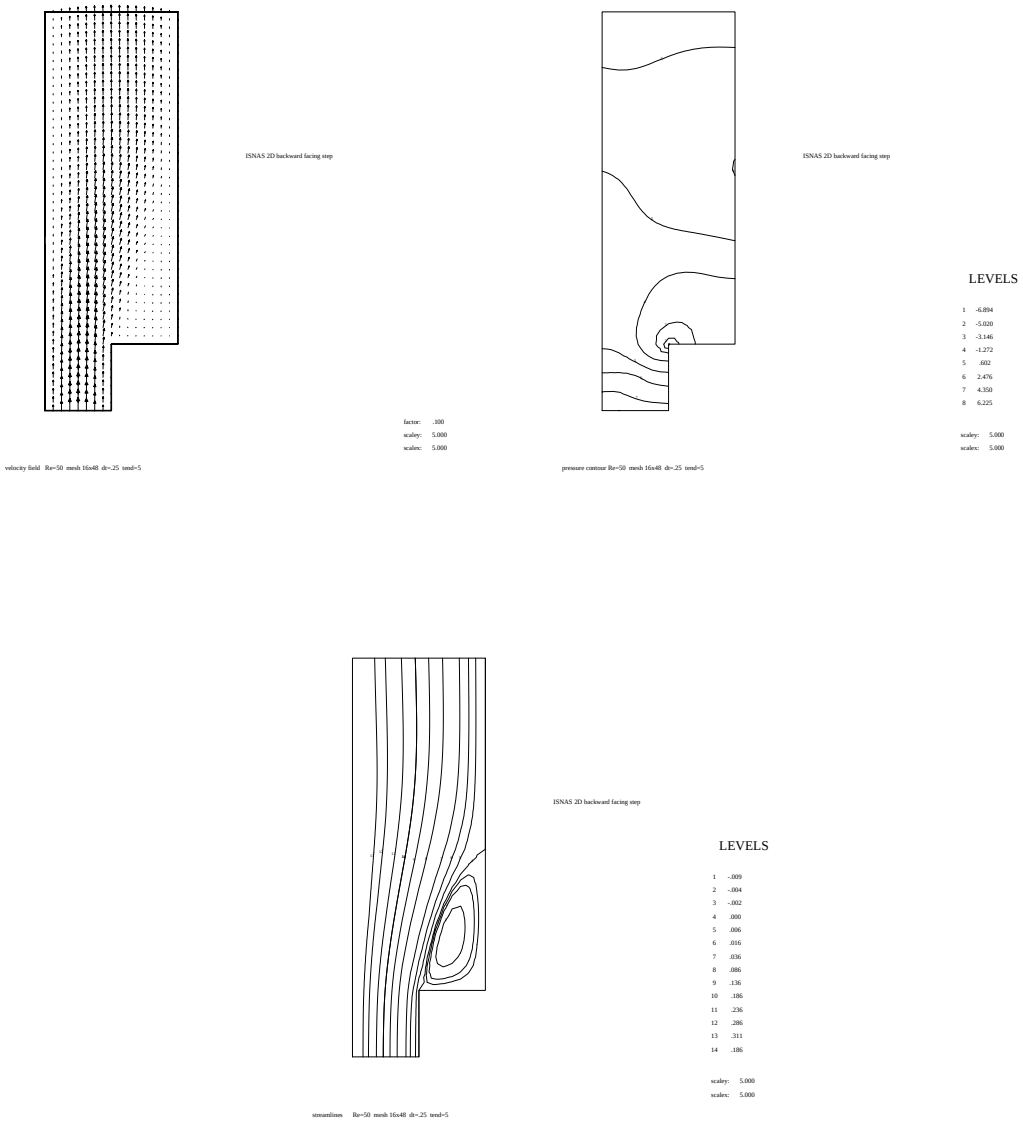


Figure 9.5.15: Vector plot of the velocity, isobars and stream lines in multi block backward-facing step

9.6 An analytic test example

As a simple example using user defined files we consider an artificial mathematical example. This example has no practical meaning but may be used to check the accuracy of the code and the methods used.
At this moment, except on an ad-hoc basis, Deft does not contain means to compute and print the error.

Consider the Navier-Stokes equations with constant values of ρ and μ. Define the exact solution of the Navier-Stokes equations by

$$\begin{aligned} u &= \sin(t)\sin(x)\sin(y) \\ v &= \sin(t)\cos(x)\cos(y) \\ p &= \sin(t)(\sin(x)+\cos(y)) \end{aligned} \tag{9.4}$$

Substitution of (5.4) in the Navier-Stokes equations defines the right-hand side by

$$\begin{aligned} f_1 &= u_t + (uu_x + vu_y) + (p_x - \mu(u_{xx} + u_{yy}))/\rho \\ f_2 &= v_t + (uv_x + vv_y) + (p_y - \mu(v_{xx} + v_{yy}))/\rho \end{aligned} \tag{9.5}$$

with

$$\begin{aligned} u_x &= \sin(t)\cos(x)\sin(y) & v_x &= -\sin(t)\sin(x)\cos(y) \\ u_{xx} &= -u & v_{xx} &= -v \\ u_y &= \sin(t)\sin(x)\cos(y) & v_y &= -\sin(t)\cos(x)\sin(y) \\ u_{yy} &= -u & v_{yy} &= -v \\ u_t &= \cos(t)\sin(x)\sin(y) & v_t &= \cos(t)\cos(x)\cos(y) \\ p_x &= \sin(t)\cos(x) & p_y &= -\sin(t)\sin(y) \end{aligned}$$

9.6.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex analyt
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  analyt
sepmesh  analyt.msh
isnaspre analyt.prb
islink analyt
analyt
isnaspost  analyt.pst [ > analyt.out ]
sepdisplay
```

The part between the square brackets [] is optional. If it is used the output of the command isnaspost is written to the file analyt.out.

9.6.2 Mesh

If we define a rectangular region of size (π, π) and use 20 cells in x and y-direction, the following input file for sepmesh might be used to generate the grid:

```
*
*  Mesh for the analytic test example
*
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(3.1415,0)
      p3=(3.1415,3.1415)
      p4=(0,3.1415)
   curves
      c1 = line1(p1,p2,nelm=20)
      c2 = line1(p2,p3,nelm=20)
      c3 = line1(p3,p4,nelm=20)
      c4 = line1(p4,p1,nelm=20)
   surfaces
      s1 = rectangle5(c1,c2,c3,c4)
end
```

9.6.3 Problem description

The example has Dirichlet boundary conditions, i.e. the velocity is prescribed at all boundaries. In fact this is a very dangerous situation since the pressure is fixed up to an additive constant and hence the problem to be solved is singular. In general it might be necessary to adapt the numerical boundary conditions in such a way that the compatibility condition, implying that net outflow is zero, is satisfied with great accuracy.
In this example however, precautions did not seem to be necessary.

The problem is solved with a Crank-Nicolson scheme ($\theta = 0.5$). Both for the boundary conditions and the right-hand side we need a function subroutine, with two functions.

```
*
Input for the analytic problem
*
time_integration
   tinit = 0
   tend = .5
   tstep = .05
   theta = .5
```

```
boundary_conditions
   curve 1 to 4: ux = time_func=1, uy = time_func=2
coefficients
   momentum_equations
      rho   = 10
      mu    = .5
      force1 = func = 1
      force2 = func = 2
linear_solver
   momentum_equations
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      relaccuracy = 1d-6
      divaccuracy = 0
      startvector = zero
```

In order to run the program we must submit the function subroutines USFUNB and USFUNC. For that reason it is necessary to write our own main program. As an example the following program analyt.f may be used.

```
      program analyt
      implicit none

      integer nbuffr
      parameter( nbuffr = 5000000 )
      integer ibuffr
      common ibuffr(nbuffr)

      call is_main( nbuffr )

      end

      function usfunb ( ichoice, x, y, z, t )

c     User written function subroutine. It gives
c     the user the opportunity to define a
c     boundary condition as a function of space
c     and time.

      implicit none

      double precision usfunb, x, y, z, t
      integer ichoice
```

```
c     x        i    x-coordinate
c     y        i    y-coordinate
c     t        i    actual time
c     ichoice  i    choice parameter given by the user input
c     usfunb   o    computed boundary condition

         if ( ichoice.eq.1 ) then
            usfunb = sin(t) * sin(x) * sin(y)
         else if ( ichoice.eq.2 ) then
            usfunb = sin(t) * cos(x) * cos(y)
         end if

      end

      function usfunc ( ichoice, x, y, z, t )

c     User written function subroutine. It gives
c     the user the opportunity to define a
c     coefficient as a function of space
c     and time.

      implicit none

      double precision usfunc, x, y, z, t
      integer ichoice

c     x        i    x-coordinate
c     y        i    y-coordinate
c     t        i    actual time
c     ichoice  i    choice parameter given by the user input
c     usfunc   o    computed coefficient

      double precision u, ut, ux, uxx, uy, uyy,
     +                 v, vt, vx, vxx, vy, vyy,
     +                 p, px, py,
     +                 mu, rho


      mu  = 0.5d0
      rho = 10d0

      u   =    sin(t) * sin(x) * sin(y)
      ut  =    cos(t) * sin(x) * sin(y)
      ux  =    sin(t) * cos(x) * sin(y)
      uxx =    - u
      uy  =    sin(t) * sin(x) * cos(y)
```

```
      uyy =    - u

      v   =    sin(t) * cos(x) * cos(y)
      vt  =    cos(t) * cos(x) * cos(y)
      vx  =  - sin(t) * sin(x) * cos(y)
      vxx =  - v
      vy  =  - sin(t) * cos(x) * sin(y)
      vyy =  - v

      p   =    sin(t) * (sin(x)+ cos(y))
      px  =    sin(t) * cos(x)
      py  =  - sin(t) * sin(y)


      if ( ichoice.eq.1 ) then
         usfunc = ut +
     +            u*ux +v*uy  +
     +            px / rho  -
     +            mu*(uxx + uyy)/rho
       else if ( ichoice.eq.2 ) then
         usfunc = vt +
     +            u*vx +v*vy  +
     +            py / rho  -
     +            mu*(vxx + vyy)/rho
         end if


      end
```

The program *analyt* must be linked to the Deft libraries with the command islink. After running *analyt* output is written to the screen. The output contains information about the iteration process with respect to the stationary solution. However, since the problem is time-dependent this output makes no sense at all and hence must be neglected.

9.6.4 Post-processing

The following post-processing file is just an example of the type of post-processing possible.

```
postprocessing
   plot identification = text = ' Deft  ',origin =(20,10)
   plot mesh
   plot vector v0, factor=.1 //
       text='velocity field   mesh 20x20  dt=.05  tend=1.55'
   plot contour v1, nlevel=8 //
       text='pressure contour mesh 20x20  dt=.05  tend=1.55'
```

```
   plot contour v2, nlevel=8 //
       text='streamlines      mesh 20x20  dt=.05  tend=1.55'
   plot coloured levels v1,nlevel=19
end
```

Figure 9.6.16 shows the vector plot of the velocity, the isobars and the stream lines.

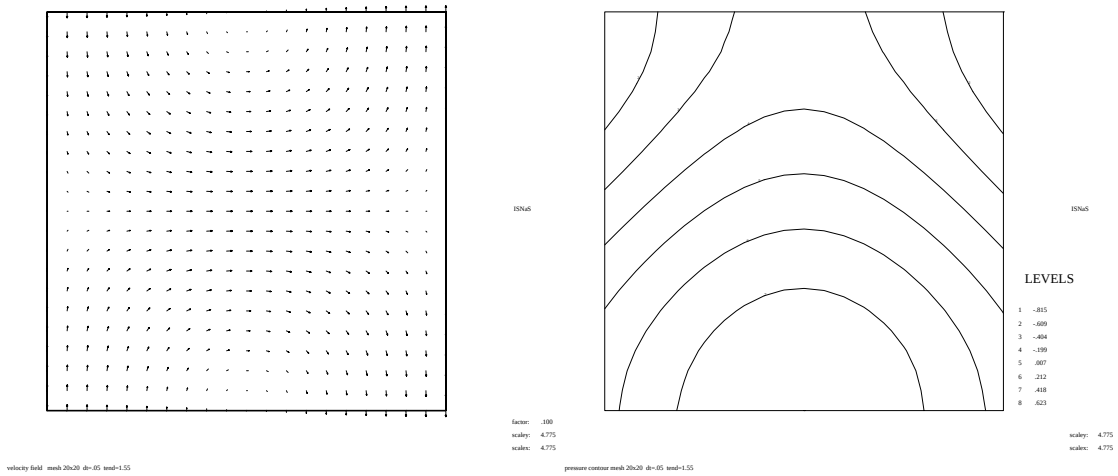


Figure 9.6.16: Vector plot of the velocity, isobars and stream lines in analytic test example

9.7 Natural convection in a square cavity

In this example we introduce the use of extra transport equations. For that purpose we consider a standard benchmark problem for a natural convection flow, see de Vahl Davis et al. [10] (1981).
The domain of reference is a square cavity of unit length as sketched in Figure 9.7.17. The walls of the cavity are fixed, which implies that the velocity satisfies

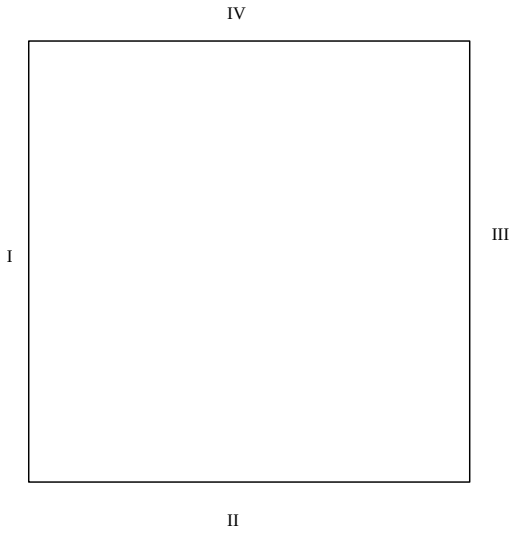


Figure 9.7.17: Definition region for natural convection in a square cavity

no-slip conditions. The temperature at the left side I is held at a constant temperature of one in dimensionless form and at the right side III at zero. The lower and upper sides II and IV are isolated.

The equations to be solved are given by:

$$\begin{aligned} \frac{\partial}{\partial x_i}u_i &= 0 \\ \frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial p}{\partial x_i} - \frac{\partial}{\partial x_j}\tau_{ij} &= \rho g\beta(T - T_0) \\ \rho c_p(\frac{\partial T}{\partial t} + \frac{\partial u_i T}{\partial x_i} - \frac{\partial T}{\partial x_i}\kappa\frac{\partial T}{\partial x_i} &= 0 \end{aligned} \tag{9.6}$$

The dimensionless parameters for this problem are the Reynolds number Re, the Prandtl number Pr and the Rayleigh number Ra, defined by

$$\begin{aligned} Re &= \frac{\rho U L}{\mu} \\ Pr &= \frac{\mu c_p}{\kappa} \end{aligned} \tag{9.7}$$

$$Ra = \frac{bG\rho^2 L^3 \Delta T}{\mu^2} Pr$$

with	U	a specific velocity
	L	a specific length
	μ	the viscosity
	ρ	the density
	c_p	the heat capacity
	κ	the thermal conductivity
	T_0	the reference temperature
	ΔT	a specific temperature difference
	b	the volume expansion coefficient
	G	the acceleration of gravity

9.7.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex bouss
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  bouss
sepmesh  bouss.msh
isnaspre bouss.prb
islink   bouss
bouss
isnaspost  bouss.pst [ > bouss.out ]
sepdisplay
```

The part between the square brackets [] is optional. If it is used the output of the command isnaspost is written to the file bouss.out.

9.7.2 Mesh

If we use 20 cells in the both directions with equidistant spacing then the following input file for sepmesh might be used to generate the grid:

```
mesh2d
   isnas
   points
      p1=(0,0)
      p2=(1,0)
      p3=(1,1)
      p4=(0,1)
   curves
      c1 = line1(p1,p2,nelm=20)
```

```
      c2 = line1(p2,p3,nelm=20)
      c3 = line1(p3,p4,nelm=20)
      c4 = line1(p4,p1,nelm=20)
   surfaces
      s1 = rectangle5(c1,c2,c3,c4)
end
```

9.7.3 Problem description

The solution of the natural convection problem requires one extra transport equation. Furthermore the right-hand-side vector for the momentum equations depends on the temperature. Since Deft solves the transport equations decoupled from the momentum equation, the temperature at the preceding time-level is used to compute the right-hand side. In this case it is necessary to use a function subroutine USFUNC1 to give the right-hand side. As a consequence the value of i in FUNC $= i$, must be between 100 and 200.
The following problem input file may be used for the Boussinesq problem:

```
*
Input for the Boussinesq benchmark problem
(square cavity)
Free convection flow
*
number_of_transport_equations = 1
initial_conditions
time_integration
   tinit = 0
   tend =  6
   tstep = .05
   theta = 1
   rel_stationary_accuracy = 1d-2
boundary_conditions
   curve 1: noslip, transport 1  = neumann = 0
   curve 2: noslip, transport 1  = dirichlet = 0
   curve 3: noslip, transport 1  = neumann = 0
   curve 4: noslip, transport 1  = dirichlet = 1
coefficients
   momentum_equations
      rho   = 1
      mu    = 1
      force2 = func=101
   transport_equation 1
      capacity = 1
      diffusion = 1.408
linear_solver
   momentum_equations
```

```
      amount_of_output = 0
      relaccuracy = 1d-4
      divaccuracy = 0
   pressure_equations
      amount_of_output = 0
      divaccuracy = 0
      startvector = zero
   transport_equations all
      amount_of_output = 0
      relaccuracy = 1d-6
```

In order to run the program we must submit the function subroutine USFUNC1. For that reason it is necessary to write our own main program. As an example the following program bouss.f may be used.

```
      program bouss
      implicit none

      integer nbuffr
      parameter( nbuffr = 5000000 )
      integer ibuffr
      common ibuffr(nbuffr)

      call is_main( nbuffr )

      end

      function usfunc1 ( ichoice, x, y, z, t, soluts, ndegfd )

c     User written function subroutine. It gives
c     the user the opportunity to define a
c     coefficient as a function of space, time and previously computed
c     solutions.

      implicit none

      integer ichoice, ndegfd
      double precision usfunc1, x, y, z, t, soluts(ndegfd)

c     x        i    x-coordinate
c     y        i    y-coordinate
c     t        i    actual time
c     ichoice  i    choice parameter given by the user input
c     soluts   i    array containing the solution at the previous level
c                   in the node
c     ndegfd   i    Length of array soluts
c     usfunc1  o    computed coefficient
```

```
c     temp          temperature

      double precision temp

c     temp          temperature


         if ( ichoice.eq.1 ) then
            temp = soluts(4)
            usfunc1 = 1408d0 * temp
         end if

      end
```

The program *bouss* must be linked to the Deft libraries with the command islink. After running *bouss*, output is written to the screen. The output contains information about the iteration process with respect to the stationary solution. However, since the problem is time-dependent this output makes no sense at all and hence must be neglected.

9.7.4 Post-processing

The following input file for isnaspost plots the velocity vectors, the isobars, stream lines and isotherms. Of the stream function and temperature also a coloured level plot is made.

```
postprocessing
   plot identification = text = ' Deft  ',origin =(18,10)
   plot vector v0 //
     text='velocity field  Ra=1d4 Pr=.71 mesh 20x20  dt=.05  tend=1.55'
   plot contour v1, nlevel=8 //
     text='pressure contour Ra=1d4 Pr=.71  mesh 20x20  dt=.05  tend=1.55'
   plot contour v2, nlevel=8 //
     text='streamlines     Ra=1d4 Pr=.71  mesh 20x20  dt=.05  tend=1.55'
   plot contour v3, nlevel=8 //
     text='temperature contour Ra=1d4 Pr=.71  mesh 20x20  dt=.05  tend=1.55'
   plot coloured levels v2, nlevel=19
   plot coloured levels v3, nlevel=19
end

end
```

Figure 9.7.18 shows the vector plot of the velocity, the isobars, the stream lines and the isotherms.

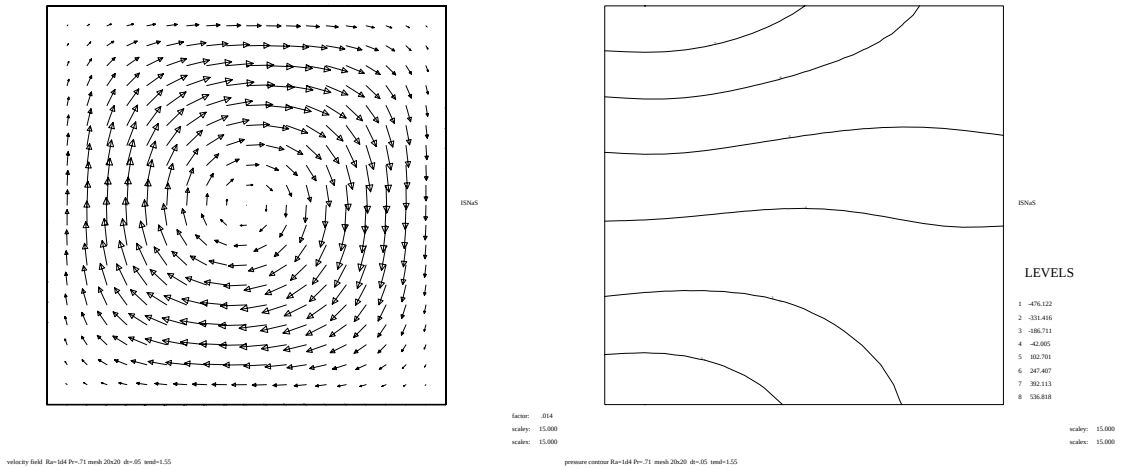


Figure 9.7.18: Vector plot of the velocity, isobars, stream lines and isotherms in natural convection flow

9.8 Turbulent flow through a tube

With the Deft code it is possible to compute complex turbulent flows in two or three dimensions. At this moment, four turbulence models are implemented: the standard k-ε, RNG based k-ε, the extended k-ε and Wilcox's k-ω models. In this section the code has been applied to the prediction of turbulent flow through a tube with a sinusoidal constriction, as shown in Figure 9.8.19. This

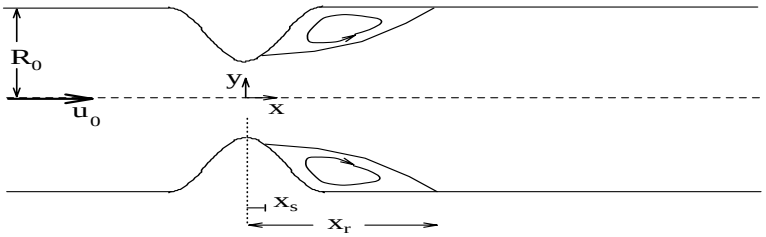


Figure 9.8.19: Region for turbulent flow through a tube

flow has been studied experimentally by Deshpande and Giddens [12].

As an example, the RNG form of k-ε model in conjunction with wall functions is employed. The height of the duct is 50.8 mm and the Reynolds number based on that height and the average inlet velocity is 15,000. The height and the base length of the constriction are $\frac{1}{2}R_0$ and $4R_0$, respectively, where R_0 is the half height of the duct. Due to symmetry, only the lower half of the domain needs to be considered. The inlet profiles for the velocity and turbulence quantities were specified at the plane $x = -4R_0$. Following Deshpande and Giddens, at the inlet a fully-developed power-law profile ($n \approx 6.4$) is assumed for the streamwise velocity:

$$u_{in} = u_0(1 + \frac{y}{R_0})^{1/6.4} \tag{9.8}$$

where $u_0 = 0.342$ m/s is the centerline velocity. For the turbulence quantities k and ε, the following inlet profiles are assumed:

$$k_{in} = 1.5I_{\text{T}}^2 u_{in}^2, \qquad \varepsilon_{in} = \frac{c_\mu^{3/4} k_{in}^{3/2}}{l} \tag{9.9}$$

Here, I_{T} is the turbulence intensity, taken to be 3% and l is the mixing length given by:

$$l = \min(\kappa y, 0.1R_0) \tag{9.10}$$

These inlet conditions are prescribed in routine $usfunb.f$. In addition, symmetry and outstream conditions are imposed in the usual way.

9.8.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex contube
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  contube
sepmesh  contube.msh
isnaspre contube.prb
islink   contube
contube
isnaspost  contube.pst [ > contube.out ]
sepdisplay
```

The part between the square brackets [] is optional. If it is used the output of the command isnaspost is written to the file contube.out.

9.8.2 Mesh

The following input file for sepmesh might be used to generate the grid:

```
*
mesh for 2D turbulent flow through a constricted tube
*
mesh2d
   isnas

   points
      p1  = (-0.1016 , 0.00       )
      p2  = (-0.0508 , 0.00       )
      p3  = (-0.04445, 0.000483365)
      p4  = (-0.0381 , 0.00185988 )
      p5  = (-0.03175, 0.00391996 )
      p6  = (-0.0254 , 0.00635    )
      p7  = (-0.01905, 0.00878004 )
      p8  = (-0.0127 , 0.0108401  )
      p9  = (-0.00635, 0.0122166  )
      p10 = ( 0.0    , 0.0127     )
      p11 = ( 0.00635, 0.0122166  )
      p12 = ( 0.0127 , 0.0108401  )
      p13 = ( 0.01905, 0.00878004 )
      p14 = ( 0.0381 , 0.00185988 )
      p15 = ( 0.04445, 0.000483365)
      p16 = ( 0.0508 , 0.00       )
      p17 = ( 0.3556 , 0.00       )
      p18 = ( 0.3556 , 0.0254     )
      p19 = ( 0.0508 , 0.0254     )
      p20 = (-0.0508 , 0.0254     )
      p21 = (-0.1016 , 0.0254     )
```

```
   curves
      c1 = line1(p1, p2, nelm = 7)
      c2 = spline1(p2, p3, p4, p5, p6, p7, p8, //
                   p9, p10, p11, p12, p13, p14, p15, p16, nelm = 15)
      c3 = line1(p16, p17, nelm = 28)
      c4 = line1(p17, p18, nelm = 20)
      c5 = line1(p18, p19, nelm = 28)
      c6 = line1(p19, p20, nelm = 15)
      c7 = line1(p20, p21, nelm =  7)
      c8 = line1(p21, p1 , nelm = 20)
      c9 = curves(c1,c2,c3)
      c10= curves(c5,c6,c7)

   surfaces
      s1 = rectangle5(c9,c4,c10,c8,smooth=2)

end
```

Figure 9.8.20 shows the grid generated by sepmesh.

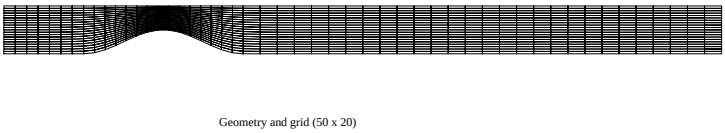


Figure 9.8.20: Mesh for turbulent flow through a tube generated by sepmesh

9.8.3 Problem description

The following file contube.prb might be used to solve the problem.

```
*
2D turbulent flow through a constricted tube
*
turbulence
   model = rng_k_eps
discretization
```

```
  turbulence_equations all
     upwind = isnas
time_integration
   tinit = 0
   tend = 6
   tstep =  0.01
   theta = 1
   rel_stationary_accuracy = 1d-2
initial_conditions
   k_turb = 1d-4
   eps_turb = 1d-4
boundary_conditions
   curve 1 to 3:
     wall_functions = smooth
   curve 4:
     parallel_outflow
     k_neumann = 0
     eps_neumann = 0
   curve 5 to 7:
     freeslip
     k_neumann = 0
     eps_neumann = 0
   curve 8:
     un, func = 1
     ut = 0
     k_dirichlet, func = 2
     eps_dirichlet, func = 3
coefficients
   momentum_equations
      rho   = 1d3
      mu    = 1d-3
linear_solver
   momentum_equations
      maxiter = 1000
      amount_of_output = 0
      relaccuracy = 1d-3
   pressure_equations
      amount_of_output = 0
      maxiter = 1000
      relaccuracy = 1d-4
      divaccuracy = 0
      startvector = zero
   turbulence_equations all
      maxiter = 1000
      amount_of_output = 0
      relaccuracy = 1d-3
```

In order to run the program we must submit the function subroutine USFUNB. For that reason it is necessary to write our own main program. As an example the following program contube.f may be used.

```
      program contube
      implicit none

      integer nbuffr
      parameter( nbuffr = 5000000 )
      integer ibuffr
      common ibuffr(nbuffr)

      call is_main( nbuffr )

      end

      function usfunb ( ichoice, x, y, z, t )

c     User written function subroutine. It gives
c     the user the opportunity to define a
c     boundary condition as a function of space
c     and time.

      implicit none

      double precision usfunb, x, y, z, t
      integer ichoice

c     x        i    x-coordinate
c     y        i    y-coordinate
c     t        i    actual time
c     ichoice  i    choice parameter given by the user input
c     usfunb   o    computed boundary condition

      double precision u, u0, tke, eps, cmu, kappa,
     +                 lscale, it, h

c     cmu           an empirical constant
c     eps           dissipation rate of turbulent energy
c     h             distance between wall and symmetry
c     it            turbulence intensity
c     kappa         von Karman constant
c     lscale        length scale
c     tke           turbulent kinetic energy
c     u             tangential velocity
c     u0            centreline velocity
```

```
cmu    = 9d-2
kappa  = 41d-2

u0     = 0.342d0
It     = 3.13d-2
H      = 0.0254d0

u = u0*((y/H)**1.5625d-1)

tke    = 15d-1*u*u*It*It
if ( tke .eq. 0d0 ) tke = 1d-4

lscale = min(kappa*y, 0.13*H)

if ( lscale .eq. 0d0 ) then
  eps = 1d4
else
  eps = (cmu**75d-2)*(tke**15d-1)/lscale
end if

if ( ichoice .eq. 1 ) then
  usfunb = -u
else if ( ichoice .eq. 2 ) then
  usfunb =  tke
else if ( ichoice .eq. 3 ) then
  usfunb =  eps
end if

end
```

9.8.4 Post-processing

With the post-processings file contube.pst we activate isnaspost to perform the following actions:

- Plot the mesh.
- Make a vector plot of the velocity field.
- Plot the isobars.
- Plot the stream lines.
- Make a contour plot of the turbulent kinetic energy k.

contube.pst has the following shape:

```
postprocessing

   plot identification = text = 'Geometry and grid (50 x 20)',origin =(7,1)
   plot mesh, yfact = 1.0
   plot identification = text = 'Flow through a constricted tube '//
      origin =(6,6)
   plot vector v0, factor = 0.04, yfact = 1.0//
      text='        velocity field        Re=15000  mesh 50x20'
   plot contour v1, yfact = 1.0//
      text='        pressure contour      Re=15000  mesh 50x20'
   plot contour v2, yfact = 1.0//
      levels = (-0.00015 0.0 0.0003 0.0007//
                0.0015 0.0024 0.004 0.0058 0.008)//
      text='        streamlines           Re=15000  mesh 50x20'
   plot contour v3, yfact = 1.0//
      text='        turbulent energy      Re=15000  mesh 50x20'
end
```

Figure 9.8.21 shows the vector plot of the velocity, the isobars and the stream lines. Figure 9.8.22 shows the contour plot of the turbulent kinetic energy.

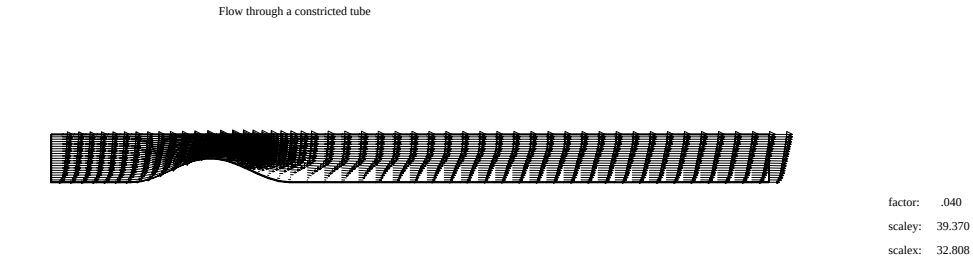


Figure 9.8.21: Vector plot of the velocity, isobars and stream lines

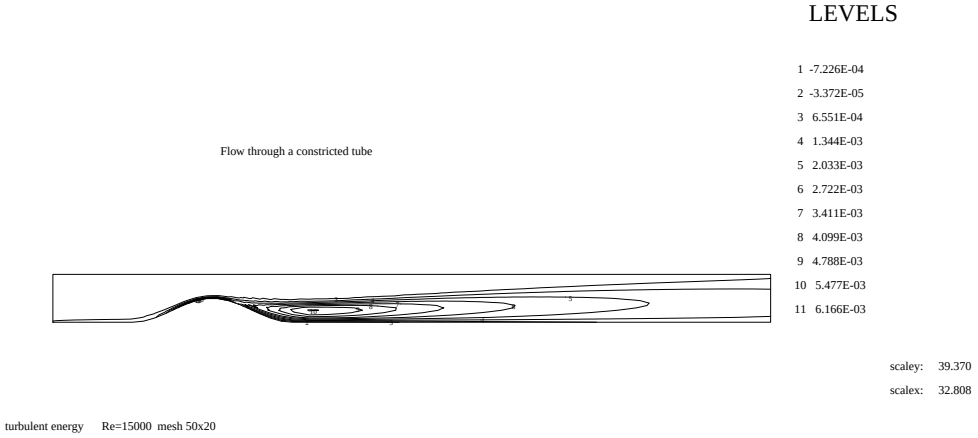


Figure 9.8.22: Contour lines of turbulent kinetic energy k

9.9 The solution of a single transport equation

In this example we assume that the velocity is given and that the sole equation to be solved is a transport equation. For that purpose we consider a standard benchmark problem for a convection problem, the so-called Molenkamp test, see Vreugdenhil and Koren (1993) [54].
Consider a square region with co-ordinates $-1 \leq x \leq 1, -1 \leq y \leq 1$. In this example we consider pure convection. A "cloud" of material is transported without change of form. In this example, a smooth shape of the cloud has been chosen to avoid accuracy problems due to discontinuous derivatives. The scaled advection equation is

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = 0, \tag{9.11}$$

where the velocity field describes a pure rigid-body rotation

$$u = -\omega y, \quad v = \omega x, \quad \omega = 2\pi. \tag{9.12}$$

The initial condition is a Gaussian distribution which does extend outside the domain but only very slightly.

$$c(x, y, 0) = 0.01^{4r^2}, r = \sqrt{(x + \frac{1}{2})^2 + y^2}. \tag{9.13}$$

Boundary conditions are required only at inflow, where the exact solution is imposed:

$$c(x, y, t) = 0.01^{4r^2}, r = \sqrt{(x + \frac{1}{2}cos(\omega t))^2 + (y + \frac{1}{2}sin(\omega t))^2}. \tag{9.14}$$

9.9.1 Obtaining the files and running the problem

The relevant files for this problem can be copied to the current directory by the following command:

```
isgetex cone
```

The problem can be run and the results viewed by giving the commands:

```
isgetex  cone
sepmesh  cone.msh
isnaspre cone.prb
islink   cone
cone
isnaspost  cone.pst [ > cone.out ]
sepdisplay
```

The part between the square brackets [] is optional. If it is used the output of the command isnaspost is written to the file cone.out.

9.9.2 Mesh

The following input file for sepmesh might be used to generate the grid:

```
mesh2d
   isnas
   points
      p1=(-1,-1)
      p2=( 0,-1)
      p3=( 1,-1)
      p4=( 1, 0)
      p5=( 1, 1)
      p6=( 0, 1)
      p7=(-1, 1)
      p8=(-1, 0)
   curves
      c1 = line1(p1,p2,nelm=40)
      c2 = line1(p2,p3,nelm=40)
      c3 = line1(p3,p4,nelm=40)
      c4 = line1(p4,p5,nelm=40)
      c5 = line1(p5,p6,nelm=40)
      c6 = line1(p6,p7,nelm=40)
      c7 = line1(p7,p8,nelm=40)
      c8 = line1(p8,p1,nelm=40)
      c9 = curves(c1,c2)
      c10= curves(c3,c4)
      c11= curves(c5,c6)
      c12= curves(c7,c8)
```

```
   surfaces
      s1 = rectangle5(c9,c10,c11,c12)
end
```

9.9.3 Problem description

The solution is time-dependent. The output will be created only at t = 0.01. In this specific case the initial conditions depend on space and as a consequence a user written function subroutine USFUNI must be provided. Since the velocity is given, the computation of the momentum equations is skipped. Furthermore the so-called "isnas" upwind scheme has been applied for the convection equation.
The file cone.prb used has the following form:

```
*
Unsteady rotation of a cone-shaped scalar field
*
number_of_transport_equations = 1
time_integration
   tinit = 0
   tend = .01
   tstep = 0.001
   theta = 0.5
initial_conditions
   u_momentum = func = 1
   v_momentum = func = 2
   pressure = 0
   transport 1 = func = 3
boundary_conditions
   curve 1: transport 1 = neumann = 0
   curve 2: transport 1 = dirichlet = time_func = 3
   curve 3: transport 1 = neumann = 0
   curve 4: transport 1 = dirichlet = time_func = 2
   curve 5: transport 1 = neumann = 0
   curve 6: transport 1 = dirichlet = time_func = 4
   curve 7: transport 1 = neumann = 0
   curve 8: transport 1 = dirichlet = time_func = 1
coefficients
   transport_equation 1
      capacity = 1
      diffusion = 0
linear_solver
   transport_equations all
      amount_of_output = 0
      relaccuracy = 1d-6
discretization
```

```
   momentum_equations
      skip
   transport_equations 1
      upwind = isnas
end_of_isnas_input
```

In order to run the program we must submit the function subroutines USFUNI and USFUNB. For that reason it is necessary to write our own main program. As an example the following program cone.f may be used.

```
      program cone
      implicit none

      integer nbuffr
      parameter( nbuffr = 5000000 )
      integer ibuffr
      common ibuffr(nbuffr)

      call is_main( nbuffr )

      end

      function usfunb ( ichoice, x, y, z, t )

c     User written function subroutine. It gives
c     the user the opportunity to define a
c     boundary condition as a function of space
c     and time.

      implicit none

      double precision usfunb, x, y, z, t
      integer ichoice

c     x        i    x-coordinate
c     y        i    y-coordinate
c     t        i    actual time
c     ichoice  i    choice parameter given by the user input
c     usfunb   o    computed boundary condition

      double precision omega, a, b, power

      omega = 2d0*3.1415926535d0

      if ( ichoice .eq. 1 ) then
        a = -1
        b = y
```

```
      else if ( ichoice .eq. 2 ) then
        a = 1
        b = y
      else if ( ichoice .eq. 3 ) then
        a = x
        b = -1
      else if ( ichoice .eq. 4 ) then
        a = x
        b = 1
      end if

      power = (a+5d-1*cos(omega*t))**2 + (b+5d-1*sin(omega*t))**2
      usfunb = 1d-2**(4*power)

      end

      function usfuni ( ichoice, x, y, z )

c     User written function subroutine. It gives
c     the user the opportunity to define an
c     initial value  as a function of space.

      implicit none

      double precision usfuni, x, y, z
      integer ichoice

c     x        i    x-coordinate
c     y        i    y-coordinate
c     z        i    z-coordinate
c     ichoice  i    choice parameter given by the userinput
c     usfuni   o    computed boundary condition

      double precision omega, power

      omega = 2d0*3.1415926535d0
      power = (x+5d-1)**2 + y**2

      if ( ichoice.eq.1 ) then
        usfuni = -omega*y
      else if ( ichoice.eq.2 ) then
        usfuni = omega*x
      else if ( ichoice.eq.3 ) then
        usfuni = 1d-2**(4*power)
      end if
```

```
end
```

9.9.4 Post-processing

The following input file for isnaspost might be used:

```
postprocessing
   plot contour v3//
      levels = (0.00001 0.10001 0.20001 0.30001 0.40001 0.50001 0.60001//
                0.70001 0.80001 0.90001)
   3d plot v3
end
```

In this case isnaspost produces two pictures. Figure 9.9.23 shows the contour lines of the concentration and Figure 9.9.24 the three-dimensional plot of the concentration.

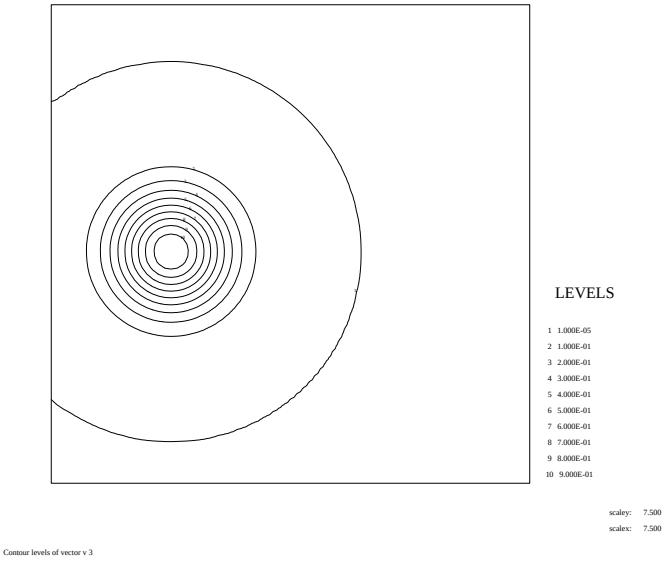


Figure 9.9.23: Contour plot of concentration

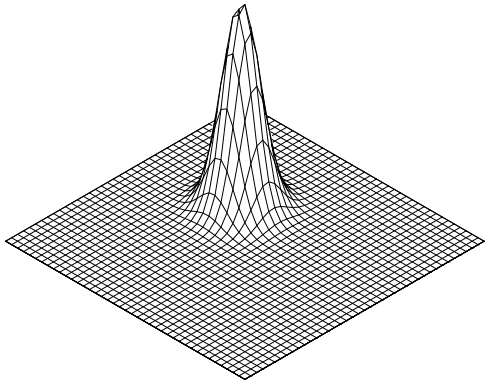


Figure 9.9.24: Contour plot of concentration

9.10 The solution of the one-dimensional Burgers equation

9.11 An overview of all examples that are available through the command isgetex

In this Section we give a short overview of all examples that are available by using the command isgetex. These examples can be put into your local directory by the command:

```
isgetex name_example
```

where name_example is the name of the example.

To run the examples follow the following list:

```
isgetex  name_example
sepmesh  name_example.msh
isnaspre name_example.prb
```

If the file name_example.f exists then

```
islink   name_example
name_example
```

else

```
isnasexe

isnaspost  name_example.pst [ > name\_example.out ]
sepdisplay
```

The following examples are available:

- channel flow

  channel Flow in a straight channel. See 9.1.

  gravity_channel This example considers a very simple channel flow with a uniform velocity. Special in this example is the fact that gravity is used as driving force. As a consequence the pressure depends on the height y.
  The pressure at outflow is prescribed as a function.

  chan_expli_mb 2D plane channel flow multi-block, explicit time integration given by theta=0

  chan_expli_mb_left 2D plane channel flow multi-block, explicit time integration given by theta=0

  chan_expli_mb_par 2D plane channel flow multi-block and parallel, explicit time integration given by theta=0

  chan_expli_mb_pari 2D plane channel flow multi-block and parallel, explicit time integration given by theta=0

chan_infl straight channel problem, inflow boundary conditions over two segments

chan_infl_2 channel flow with inflow at a part of the boundary

chan_mb_inacc_par channel problem, multi block parallel, number_of_computers = 2, subdomain_solution = inaccurate

chan_mb_pr test problem multi block parallel, number_of_computers = 2, subdomain_solution = accurate

chan_mb_pri test problem multi block, parallel, number_of_computers = 2, subdomain_solution = inaccurate type_of_algorithm = par

chanchoup Input for the straight channel with bump Euler compressible, mach = .675d0, upwind = first_order

chancomp test for Euler compressible problem using scaled parameters

chancomp_noscal test for Euler compressible problem using physical parameters

chancomp_rd test for Euler compressible problem read initial conditions from restart file

chancomp_wrt test for Euler compressible problem write solution to restart file

chanexpli straight channel problem, explicit time integration

chanjump Flow in a straight channel, where the grid contains a sudden jump in grid size. This example is used to demonstrate the effect of sudden grid size changes.

chanjump_wb Straight channel problem with jump in grid size wesbeek discretization

channel1 straight channel problem

channel2 straight channel problem

channel3 straight channel problem

channel4 straight channel problem

channel5 straight channel problem

channel6 straight channel problem

channel7 straight channel problem

channel_iblu multi1 problem, one block with a different orientation

channel_mb straight channel problem, multi block

channel_mb1 straight channel problem, multi block

channel_mb2 straight channel problem, multi block

channel_mb3 straight channel problem, multi block

channel_mb4 straight channel problem, multi block

channel_mb5 straight channel problem, multi block

channel_mb6 straight channel problem, multi block

channel_mb7 straight channel problem, multi block

channel_mb8 straight channel problem, multi block

channel_mb_wb straight channel problem, multi block Wesbeek discretization

channel_mbliss straight channel problem, multi block

channel_pic straight channel problem, picard linearization convection

channel_rd straight channel problem restart from restart file

channel_rd_r straight channel problem restart from restart file with refine option

channel_sn straight channel problem, boundary condition sigmann given at inflow

channel_wrt straight channel problem write to restart file

channel_wrt_r straight channel problem write to restart file with refine option(output =cartesian)

channelliss straight channel problem

channelmassfr straight channel problem multi_phase_gas_flow

channpr1 Without preconditioner in order to test the orientation of the channel flow problem (this flow is from left to right. See also channpr2.*)

channpr2 Without preconditioner in order to test the orientation of the channel flow problem (this flow is from right to left. See also channpr1.*)

channpr3 Without preconditioner in order to test the orientation of the channel flow problem (this flow is from bottom to top. See also channpr4.*)

channpr4 Without preconditioner in order to test the orientation of the channel flow problem (this flow is from top to bottom. See also channpr3.*)

chanskco Flow in a straight channel, where the grid has been made deliberately skewed. The input velocity is constant. This example is used to demonstrate the effect of non-orthogonal grids.

- gravity_force

  gravity_channel This example considers a very simple channel flow with a uniform velocity. Special in this example is the fact that gravity is used as driving force. As a consequence the pressure depends on the height y.
  The pressure at outflow is prescribed as a function.

- general

2dcilinder 2D flow around a cylinder, single block, using periodical boundary conditions, inflow parallel with respect to the periodical boundary.

2dcilinder_skew 2D flow around a cylinder, single block, using periodical boundary conditions, inflow skewed with respect to the periodical boundary.

3d 3D channel flow, with dirichlet boundary conditions on all sides, using the classical discretization

3d- See 3d, however, now the flow is in opposite direction

3d2 See 3d, however, now the flow is in another direction

3d2- See 3d2, however, now the flow is in another direction

3d2lin See 3dlin, however, now the flow is in another direction

3d2par See 3dpar, however, now the flow is in another direction

3d3 See 3d, however, now the flow is in opposite direction

3d3- See 3d, however, now the flow is in opposite direction

3d3lin See 3dlin, however, now the flow is in another direction

3d3par See 3dpar, however, now the flow is in another direction

3d_cavity 3d cavity problem, all dirichlet boundary conditions

3d_pic 3d test problem for picard linearization of convection term

3d_skew_wb 3D channel flow, all dirichlet boundary conditions
skew grid, wesbeek discretization

3d_wb_curved_h 3D channel flow, all dirichlet boundary conditions
curved grid, wesbeek discretization

3dbend 3d, 90 degree bend problem, outflow boundary condition: sigmann=0 ut=0

3dbendp 3d bend problem, with periodic boundary conditions

3dbfs 3d backward facing step problem

3dbfs_mb 3d bfs flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip
multiblock, subdomain solution accurate

3dbfs_mb_inacc 3d bfs flow, outflow boundary condition: sigmann=0 and ut=0
side walls: noslip
multiblock, subdomain solution inaccurate

3dbfs_mb_par 3d bfs flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip
multiblock, parallel, number of computers=3, subdomain solution accurate

3dbfs_mb_pari 3d bfs flow, outflow boundary condition: sigmann=0 and ut=0
side walls: noslip
multiblock parallel, number of computers = 3, subdomain solution inaccurate

3dcavskew Driven cavity flow in three dimensions with angle = 45 deg

3dcilinder_skew 3D flow around cylinder, single block, using periodical boundary conditions

3dlin 3d channel flow, all dirichlet boundary conditions boundary condition ux=z, linear velocity field

3dliss 3D channel flow, all dirichlet boundary conditions

3dpar 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip

3dpar_mb 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock subdomain_solution = accurate

3dpar_mb_4 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock 4 blocks, subdomain_solution = accurate

3dpar_mb_4_par 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock parallel, number_of_computers = 4, subdomain_solution = accurate

3dpar_mb_4_pari 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock, parallel,number_of_computers = 4, subdomain_solution = inaccurate

3dpar_mb_inacc 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock , subdomain_solution = inaccurate

3dpar_mb_inacc_p 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock, parallel,number_of_computers = 2, subdomain_solution = inaccurate

3dpar_mb_par 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock, number_of_computers = 2, subdomain_solution = accurate

3dpar_mb_pari 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip multiblock, parallel, number_of_computers = 2 subdomain_solution = inaccurate

3dparliss 3d channel flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip

3dparper as 3dpar problem now with periodic boundary conditions

3dperiod1 3d test for periodic boundary conditions

3dperiod12 3d test for periodic boundary conditions

3dperiod2 3d test for periodic boundary conditions

3dperiod3 3d test for periodic boundary conditions

3dsmagor 3D channel flow, all dirichlet boundary conditions large eddy, smagorinsky , viscous_correction

3dt 3D transport equation

3dtperiod 3D transport equation with periodic boundary conditions

3dturb three-dimensional straight channel flow with turbulence

3duct_lam 3D developing flow in a curved rectangular duct

3dunsnt 3d test for boundary condition: un=0 and sigmant=0

3dunsnt_per as 3dunsnt problem now with periodic boundary conditions

3dunsntall as 3dunsnt problem now on all sidewalls freeslip boundary condition

3dupwind 3D cavity with moving lid To test first order upwind scheme Restriction: Picard linearization must be used !

analyt An artificial analytic example to demonstrate the use of user defined functions. See 9.6.

analyt_fth An artificial analytic example to demonstrate the fractional θ-method for the time integration.

analyt_gth An artificial analytic example to demonstrate the generalized θ-method for the time integration.

aniso Turbulent flow through a square duct computed with the anisotropic model of Speziale variant
This example demonstrates the capability of the anisotropic models to predict the secondary flow which has been missing from the Boussinesq hypothesis
Compare the results with the results obtained from '3dturb' in the test bank

axicom Axisymmetric channel , compressible problem mach=.001 wesbeek discr.

axtest0 axisymmetric straight channel problem

axtest1 analytical axisymmetric problem u=r, v=-2z, p=0 noconvection

axtest2 analytical axisymmetric problem u=r, v=-2z, p=r+3z noconvection

axtest3 axisymmetric flow in a diverging channel

axtest4 analytical axisymmetric problem u=r, v=-2z, p=r+3z with convection

bend Laminar flow through a ninety degrees bend. See 9.2.

bend180 as bend360_mb problem, mesh generated now with Liss

bend360_mb 2d, 360 degree bend problem using multi block

bend360_mb_liss

bend_couette bend problem, couette flow

bend_expli bend problem , explicit time integration given by theta=0

bend_kappa bend problem higher order upwind, kappa=.75

bend_mpl1kappa bend problem upwind = tvd, limiter = mplone_kappa_limiter

bend_mpl2kappa bend problem upwind = tvd, limiter = mpltwo_kappa_limiter

bend_mrkappa bend problem upwind = tvd, limiter = mr_kappa_limiter

bend_muscl bend problem upwind = muscl

bend_noconv bend problem without convection

bend_plkappa bend problem upwind = tvd, limiter = pl_kappa_limiter

bend_rkappa bend problem upwind = tvd, limiter = r_kappa_limiter

bend_splkappa bend problem upwind = tvd, limiter = symm_pl_kappa_limiter

bend_sratio bend problem upwind = tvd, limiter = symm_ratio_limiter

bend_sweby bend problem upwind = tvd, limiter = sweby_phi_limiter

bend_vdt Laminar flow with Reynolds number = 300 through a ninety degrees bend, using 3 different time steps $\triangle t = .05, .1,$ and $.2$.

bend_wb bend problem, Wesbeek discretization

bendcons bend problem standard discretization, upwind first order conservative

bfs_mb Multi-block backward-facing step. See 9.5.

bfs_mb_inacc Backward facing step problem multi block Inaccurate solution of subdomains is used.

bfs_mb_np Backward facing step problem multi block

bfs_mb_rd Backward facing step problem multi block restart from restart file

bfs_mb_rd_r Backward facing step problem multi block restart from restart file with refine option parallel, number_of_computers = 2, subdomain_solution = accurate

bfs_mb_rd_ri Backward facing step problem multi block restart from restart file with refine option parallel, number_of_computers = 2, subdomain_solution = inaccurate

bfs_mb_rdi Backward facing step problem multi block restart from restart file parallel, number_of_computers = 2, subdomain_solution = inaccurate

bfs_mb_turb Turbulent flow over a backward-facing step
Reference: Kim et al, "Investigation of a reattaching turbulent shear layer: flow over a backward-facing step", ASME Journal of Fluids Eng., vol. 102, pp. 302-308, 1980

bfs_mb_wb Backward facing step problem multi block, Wesbeek discretization.

bfs_mb_wrt Backward facing step problem multi block write to restart file

bfs_mb_wrt_r Backward facing step problem multi block write to restart file with refine option (output=cartesian)

bfs_mb_wrt_ri Backward facing step problem multi block write to restart file with refine option (output=cartesian) parallel, number_of_computers = 2, subdomain_solution = inaccurate

bfs_mb_wrti Backward facing step problem multi block write to restart file parallel, number_of_computers = 2, subdomain_solution=inaccurate

bfs_sb Single-block backward-facing step. See 9.5.

bfs_sb_wb Backward facing step problem single block, parabolic inflow boundary condition wit Umax = 1.0 . Wesbeek discretization

bocht 2d, 90 degrees bend problem

bouss Natural convection flow in a square cavity. See 9.7.

bouss_col Boussinesq benchmark problem (square cavity) Free convection flow Collocated arrangement

bouss_mb Boussinesq benchmark problem (square cavity) Free convection flow multi block (4 blocks)

bouss_pr Boussinesq benchmark problem (square cavity) Free convection flow test for printing

bouss_rd Boussinesq benchmark problem (square cavity) Free convection flow test reading restart file

bouss_rd_r Boussinesq benchmark problem (square cavity) Free convection flow restart from restart file with refine option

bouss_wb Boussinesq benchmark problem (square cavity) Free convection flow using wesbeek discretization and a randomized grid

bouss_wb2 Free convection flow in cavity using Wesbeek discretization. The mesh used here was introduced by D.S. Kershaw, J. Comput. Phys., 39, 375 (1981).

bouss_wrt Boussinesq benchmark problem (square cavity) Free convection flow test writing restart file

bouss_wrt_r Boussinesq benchmark problem (square cavity) Free convection flow write to restart file with refine option(output =cartesian)

bump1 laminar flow in a duct with obstruction To illustrate the effect of the mesh to the solution (here good mesh)

bump2 laminar flow in a duct with obstruction To illustrate the effect of the mesh to the solution (here wrong mesh)

bump3 laminar flow in a duct with obstruction (2D version) To illustrate the effect of the mesh to the solution (here good mesh)

bump4 laminar flow in a duct with obstruction (2D version) To illustrate the effect of the mesh to the solution (here wrong mesh)

bump5 laminar flow in a duct with obstruction
Use periodic conditions in order to compare with 2D solution (see bump3.prb) To illustrate the effect of the mesh to the solution (here good mesh)

bump6 laminar flow in a duct with obstruction
Use periodic conditions in order to compare with 2D solution (see bump4.prb) To illustrate the effect of the mesh to the solution (here wrong mesh)

chanskew Flow in a straight channel channel is positioned under an angle of 30 degrees

chanskpa Flow in a straight channel, where the grid has been made deliberately skewed. The only difference with chanskco is that the input velocity is parabolic.

chncav_wb_c test for cavitating flow with shocktube first order upwind conservative discretization = wesbeek

chncav_wb_nc test for cavitating flow with shocktube first order upwind non-conservative discretization = wesbeek

chnma.001 channel , compressible problem mach=.001 Re = 2.3d2, wesbeek discr.

chnma.5 channel with bump, compressible problem mach=.5 Euler, wesbeek discr.

chnma.675 channel with bump, compressible problem mach=.675 now the max machnumber in the flow will be 1.3 the keyword 'pres_corr_method = 1' has to be chosen for convergence

collocated test collocated discretization on curved grid

conc concentric cylinder problem

cone Pure advection without momentum equations; Molenkamp test. See 9.9.

contd compressible with special pressure correction method

contube Turbulent flow through a tube with a sinusoidal constriction. The RNG $k - \varepsilon$ model is used. See 9.8.

convect Test example for pure convection equation (Discontinuous field). This example is used to test upwind schemes.

convrot Test example for pure convection equation (Smith and Hutton test case). This example is used to test upwind schemes.

couette1 Couette1 flow: un, ut given on all boundaries

couette10 Couette10 flow: sigmant, sigmann given

couette11 Couette11 flow: ut, sigmann given

couette12 Couette12 flow: un, sigmant given on all boundaries

couette12_wb Couette12 flow: un, sigmant given on all boundaries

couette13 Couette13 flow: un, ut given on all boundaries

couette14 Couette14 flow: sigmant, sigmann given

couette15 Couette15 flow: ut, sigmann given

couette16 Couette16 flow: un, sigmant given on all boundaries

couette16_wb Couette16 flow: un, sigmant given on all boundaries

couette17 Couette flow: un, ut given on all boundaries

couette18 Couette flow: sigmant , sigmann given

couette19 Couette19 flow: ut, sigmann given

couette2 Couette2 flow: sigmant, sigmann given

couette20 Couette20 flow: un, sigmant given

couette20_wb Couette20 flow: un, sigmant given

couette21 Couette21 flow: un, ut given on all boundaries

couette22 Couette22 flow: sigmant , sigmann given

couette23 Couette23 flow: ut, sigmann given

couette24 Couette24 flow: un, sigmant given

couette24_wb Couette24 flow: un, sigmant given

couette25 Couette25 flow: un, ut given on all boundaries

couette26 Couette26 flow: sigmant, sigmann given

couette27 Couette27 flow: ut, sigmann given

couette28 Couette28 flow: un, sigmant given

couette28_wb Couette28 flow: un, sigmant given

couette29 Couette29 flow: un, ut given on all boundaries

couette3 Couette3 flow: ut, sigmann given

couette30 Couette30 flow: sigmant, sigmann given

couette31 Couette31 flow: ut, sigmann given

couette32 Couette32 flow: un, sigmant given

couette3d Couette flow: un, sigmant given on all boundaries

couette4 Couette4 flow: un, sigmant given on all boundaries

couette4_wb Couette4 flow: un, sigmant given on all boundaries

couette5 Couette5 flow: un, ut given on all boundaries

couette6 Couette6 flow: sigmant, sigmann given

couette7 Couette7 flow: ut, sigmann given

couette8 Couette8 flow: un, sigmant given on all boundaries

couette8_wb Couette8 flow: un, sigmant given on all boundaries

couette9 Couette9 flow: un, ut given on all boundaries

crack Couette flow: un, ut given on all boundaries, multiblock

crack1 Couette flow: un, ut given on all boundaries, multiblock

crack2 Couette flow: un, ut given on all boundaries, multiblock

curvduct Developing flow in a 90 deg curved rectangular duct based on the experimental study of W.J. Kim and V.C. Patel, "Origin and decay of longitudinal vortices in developing flow in a curved rectangular duct", J. Fluids Engng., vol. 116, p. 45-52, 1994. This computation has been presented at the Fifth ERCOFTAC-IAHR Workshop on Refined Flow Modelling, organized by EDF in Chatou (Paris), April 1996. Remark: to compute this flow problem, use restart option, as follows: - First, compute with tstep = 0.0001 and endtime = 0.05 (this file) - restart the computation with tinit=0.05, tstep = 0.01 and endtime can be 0.85 (insession = 2).

curved_h Input for the straight channel problem, discr_method=wesbeek curved grid

curved_h_col Input for the straight channel problem Collocated arrangement Wesbeek+bilinear interpolation

curved_v Input for the straight channel problem, discr_method=wesbeek curved grid

dune Turbulent flow over sand dunes in a river Experimental data from J.C.C. de Ruiter, "Turbulence measurements above artificial dunes", Report Q789, Delft Hydraulics/TOW-Rijkswaterstaat, 1988 The bottom surface is covered with sand particles; average roughness height: 0.0015 m

expansion

fluidbed Input for the bend problem

frsfsub Input for the freesurface channel problem subcritical flow with Fr=0.43

frsfsuper Input for freesurface channel problem supercritical flow with Fr=2.05

gravity Test example for a flow only driven by gravity. The mesh is non orthogonal. The computed flow should be zero, but due to inaccuracies a flow might arise.

gravity_mb Input for the test gravity problem, multi block

hill Wake flows behind two-dimensional model hills (ERCOFTAC Workshop 1995)

intface INTERFACE PROBLEM for testing WESBEEK discretization

kershaw Solving a diffusion equation on the unit square with constant diffusion coefficient, using the integration-path method as proposed in P. van Beek, R.R.P. van Nooyen and P. Wesseling, J. Comput. Phys., 117, 364 (1995). The mesh used here was introduced by D.S. Kershaw, J. Comput. Phys., 39, 375 (1981).

laplax1 Axisymmetric Transport equation. Momentum equation is not solved.

laplax2 Axisymmetric Transport equation. Momentum equation is not solved.

laplax3 Axisymmetric Transport equation. Momentum equation is not solved.

linsol3d_dia_post 3d channel problem, postconditioning for lin. solver

linsol3d_dia_prec 3d channel problem, diag. preconditioning linear solver

linsol3d_ilud_post 3dchannel problem, postconditioning linear solver

linsol3d_ilud_prec 3d channel problem, preconditioning linear solver

linsol3d_noprec 3d channel problem, no preconditioner linear solver

linsol_bicgstab Input for the bend problem, preconditioner linear solver

linsol_cgs Input for the bend problem, preconditioner linear solver

linsol_dia_post Input for the bend problem, postconditioner for linear solver

linsol_dia_prec Input for the bend problem, preconditioner linear solver

linsol_ilu_post Input for the bend problem, postconditioner linear solver

linsol_ilu_prec Input for the bend problem, preconditioner linear solver

linsol_ilud_post Input for the bend problem, postconditioner linear solver

linsol_ilud_prec Input for the bend problem, preconditioner linear solver

linsol_multigrid_post Input for the bend problem, preconditioner linear solver

linsol_multigrid_prec Input for the bend problem, preconditioner linear solver

linsol_noprec Input for the bend problem, no preconditioner linear solver

logo Demonstration flow for multi-block. The flow around the letters ISNAS is computed. The grid must be generated by Liss in the following way:

```
liss pre pin
l2i
```

After that the standard Deft commands may be given.

lowkeps Turbulent flow through channel to test Lam-Bremhorst k-eps model. A very fine mesh has been used.

lshape Flow through an l-shape channel. Example of a very non-smooth grid. See 9.3.

lshape_col Input for the L-shape problem Collocated arrangement Wesbeek+bilinear interpolation

lshape_mb Input for the lshape problem, multi block

lshape_mb_wb Input for the lshape problem, multi block, Wesbeek discretization.

naca0012 Input for naca0012 airfoil, viscous laminar

naca0012_112x32_eu Input for naca0012 airfoil, Euler

naca0012_mclw Input for naca0012 airfoil, viscous laminar, This problem is the same as naca0012, only now with the meshcurves ordered clockwise

naca0021_mb Input for naca0012 airfoil, viscous laminar multiblock, subdomain_solution = accurate

neutrnsp Test problem to check the Neumann or mixed boundary conditions for a transport equation. The momentum equations are skipped.

neutrnsp_mb Input for test of ROBBINS (NEUMANN) boundary condition for TRANSPORT-equation Momentum equation is not solved Multi block (4 blocks)

nozzle Input for the nozzle problem

outstream Couette flow: un, ut given on all boundaries

pol3d Transport of a pollutant mass by convection and diffusion in a 3D flow field

presshole Input for the pressurehole problem, multiblock parallel

presshole_8 Input for the pressurehole problem, multiblock parallel 8 blocks, subdomain_solution = accurate

presshole_8_wb Input for the pressurehole problem, multiblock parallel 8 blocks, subdomain_solution = accurate, discr_method=wesbeek

presshole_8_wbi Input for the pressurehole problem, multiblock parallel 8 blocks, discr_method=wesbeek, subdomain_solution=inaccurate

presshole_8i Input for the pressurehole problem, multiblock parallel 8 blocks, subdomainsolution = inaccurate

presshole_wb Input for the pressurehole problem, multiblock parallel discr_method=wesbeek, subdomain_solution = accurate

presshole_wbi Input for the pressurehole problem, multiblock parallel discr_method=wesbeek, subdomain_solution=inaccurate

pressholei Input for the pressurehole problem, multiblock parallel subdomain_solution = inaccurate

pvmtest 2D plane channel flow multi-block and parallel, testing mpi (pvm)

rectanglecol

ruitequi Example of a skew cavity with "equidistant" grid size.

ruitjump Example of a skew cavity with a jump in the grid.

shockt test for shocktube

shocktnc test for cavitating flow with shocktube

shocktnc_ex test for cavitating flow with shocktube explicit discretization with density bias

shocktnc_exdb test for cavitating flow with shocktube explicit discretization with density bias

shocktnc_gs test for cavitating flow with shocktube making use of nonlinear Gauss-Seidel for solving the pressure equation

shocktnc_houpw test for cavitating flow with shocktube higher order upwind in momentum and continuity

shocktnc_nwt test for cavitating flow with shocktube newton linearisation of momentum equation upwind classical discretization supersonic scheme with defect correction

shocktnc_prit test for cavitating flow with shocktube with iterative solution procedure for the pressure correction

shocktnc_st_c test for cavitating flow with shocktube standard discretization conservative

shocktnc_st_nc test for cavitating flow with shocktube standard discretization non-conservative

shocktnc_sup test for cavitating flow with shocktube supersonic scheme

shocktnc_wb_c test for cavitating flow with shocktube wesbeek discretization conservative

shocktnc_wb_nc test for cavitating flow with shocktube wesbeek discretization non-conservative

sigmant0_x_wb Input for the straight channel problem, wesbeek discretization

sigmant0_y_wb Input for the straight channel problem, wesbeek discretization

stress1 Example of a straight channel problem with skew outflow section, signt = 0 and sign = 2 -4x -4y

stress1_wb Input for the straight channel problem, with skew outflow section : signt = 0 and sign = 2 -4x -4y Wesbeek discretization

stress2 Example of a straight channel problem with skew outflow section , right side signt = 0 and sign = 2 -4x -4y, left side signt = 0 and sign = -2 +4x -4y.

stress2_wb Input for the straight channel problem, with skew outflow section :right side signt = 0 and sign = 2 -4x -4y left side signt = 0 sign = -2 +4x -4y Wesbeek discretization

tchannel Fully developed turbulent flow in a straight channel. The standard $k - \varepsilon$ model is used.

tchannel1 2D turbulent fully-developed plane channel flow (from left to right)

tchannel1_l2t tchannel1_l2t computation of a turbulent channel flow. As initial condition the solution of a laminar problem is read from the restartfile. The laminar solution is written to the restartfile by the tchannel1_lam problem.

tchannel1_lam tchannel1_lam Laminar channel flow , the solution of this problem is written to the restartfile. The tchannel1_l2t.prb problem, which computes a turbulent flow, takes the laminar solution from the restartfile as initial condition.

tchannel1_subst 2D turbulent fully-developed plane channel flow (from left to right)

tchannel1_wb 2D turbulent fully-developed plane channel flow (from left to right)

tchannel2 2D turbulent fully-developed plane channel flow (from right to left)

tchannel3 2D turbulent fully-developed plane channel flow (from bottom to top)

tchannel4 2D turbulent fully-developed plane channel flow (from top to bottom)

tchannel_mb 2D turbulent fully-developed plane channel flow multi-block

tchannel_mb1 2D turbulent fully-developed plane channel flow multi-block

tchannel_mb1_pari 2D turbulent fully-developed plane channel flow multi-block, same as tchannel_mb1 but now parallel

tchannel_mb_pari 2D turbulent fully-developed plane channel flow multi-block, same as tchannel_mb but now parallel with subdomain_solution = inaccurate

tchannelt 2D turbulent fully-developed plane channel flow

tchannelt2 Turbulent flow through an open channel (tilted flume) based on experiments of Nezu and Rodi (1986) An anisotropic model is used to compute the normal stresses more accurately.

testperiod1 test problem periodical boundary conditions

testperiod2 Test problem for periodical boundary conditions

testperiod3 Test problem for periodical boundary conditions

testperiod4 Test problem for periodical boundary conditions

tomega Turbulent flow through channel to test Wilcox's k-omega model. Because k-omega model is a low-Reynolds-number two-equation model, a very fine mesh has been used. Here, no viscous corrections have been used.

transper1 Input for test of periodic boundary conditions for one TRANSPORT-equation. Momentum equation is not solved.

transper2 Input for test of periodic boundary conditions for one TRANSPORT-equation. Momentum equation is not solved.

tube2d_100 Input for tube2d problem, Re=100

tube2d_100_wb Input for tube2d problem, Re=20, wesbeek discretization

tube2d_100_wb_reuse Input for tube2d problem, Re=20, wesbeek discretization

tube3d tube3d flow, outflow boundary condition: sigmann=0 and ut=0 side walls: noslip

ubend Two dimensional turbulent flow through U bend with heat transfer Use multiblock grid of 3400 cells within 3 blocks

ubend_rd Two dimensional turbulent flow through U bend with heat transfer Use multiblock grid of 3400 cells within 3 blocks

upwind Input for the cavity with moving lid To test first order upwind scheme Restriction: Picard linearization must be used !

warmte Input for the 2D turbulent channel flow with heat transfer

wbtrnsp Input for test of WESBEEK discretization for TRANSPORT-equation Momentum equation is not solved

wbtrnsp2 Input for test of WESBEEK discretization for TRANSPORT-equation with discontinuous diffusion coefficient Momentum equation is not solved

wbtrnsp3 Input for test of WESBEEK discretization for TRANSPORT-equation Momentum equation is not solved Using special grid generated with sine functions

wbtrnsp4 Input for test of WESBEEK discretization for TRANSPORT-equation Momentum equation is not solved Using special grid generated with random functions

wbupwcon Test problem wesbeek discretization, first order conservative upwind

Bibliography

1. P. Arminjon and A. Dervieux. Construction of TVD-like artificial viscosities on two-dimensional arbitrary FEM grids. *J. Comp. Phys.*, 106:176–198, 1993. 2.2.2, 2.2.2

2. H. Bijl and P. Wesseling. A unified method for computing incompressible and compressible flows in boundary-fitted coordinates. *J. Comp. Phys.*, 141:153–173, 1998. 2.5, 2.5

3. E. Brakkee. Using L_iSS grids for ISNaS. Report 93-46, Faculty of Technical Mathematics and Informatics, Delft University of Technology, Delft, 1993. 1

4. E. Brakkee. *Domain decomposition for the incompressible Navier-Stokes equations*. PhD thesis, Delft University of Technology, The Netherlands, April 1996. 2.8, 2.8.1

5. E. Brakkee, A. Segal, and C.G.M. Kassels. A parallel domain decomposition algorithm for the incompressible Navier-Stokes equations. *Simulation Practice and Theory*, 3:185–205, 1995. 2.8.4

6. E. Brakkee, C. Vuik, and P. Wesseling. Domain decomposition for the incompressible Navier-Stokes equations: solving subdomain problems accurately and inaccurately. *Int. J. Num. Meth. in Fluids*, 26:1217–1237, 1998. 2.8.3

7. E. Brakkee and P. Wilders. The influence of interface conditions on convergence of Krylov-Schwarz domain decomposition for the advection-diffusion equation. *J. of Scientific Computing*, 12:11–30, 1997. 2.8.1

8. W.L. Chen, F.S. Lien, and M.A. Leschziner. Computational modelling of turbulent flow in turbomachine passage with low-Re two-equation models. In S. Wagner, E.H. Hirschel, J. Périaux, and R. Piva, editors, *Computational Fluid Dynamics '94*, pages 517–524, Chicester, 1994. Wiley. 2.1.5, 2.1.5

9. Y.-S. Chen and S.-W. Kim. Computations of turbulent flows using an extended k-ε turbulence closure model. Report NASA CR-179204, NASA-Marshall Space Flight Center, Alabama, USA, 1987. 2.1.5, 2.1.5

10. G. de Vahl Davis and I.P. Jones. Natural convection in a square cavity - a comparision exercise. In R.W. Lewis, K. Morgan, and B.A. Schrefler, editors, *Num. Methods in Thermal Problems, Vol. II*, pages 552–572, Swansea, U.K., 1981. Pineridge Press. 9.7

11. I.A. Demirdžić. *A finite volume method for computation of fluid flow in complex geometries.* PhD thesis, University of London, 1982. 5.2

12. M.D. Deshpande and D.P. Giddens. Turbulence measurements in a constricted tube. *J. Fluid Mech.*, 97:65–89, 1980. 9.8

13. S.C. Eisenstat. Efficient implementation of a class of preconditioned conjugate gradient methods. *SIAM J. Sci. Stat. Comput.*, 2:1–4, 1981. 2.7.2

14. S.C. Eisenstat, H.C. Elman, and M.H. Schultz. Variable iterative methods for nonsymmetric systems of linear equations. *SIAM J. Num. Anal.*, 20:345–357, 1983. 2.7.1, 2.8.3

15. J. Frank and C. Vuik. Parallel implementation of a multiblock method with approximate subdomain solution. Report 98-11, Faculty of Technical Mathematics and Informatics, Delft University of Technology, Delft, 1998. 2.8.4

16. P.H. Gaskell and K.C. Lau. Curvature-compensated convective transport: SMART, a new boundedness-preserving transport algorithm. *Int. J. Num. Meth. in Fluids*, 8:617–641, 1988. 2.2.2

17. V. Haroutunian. Simulation of vortex shedding past a square prism using three two-equation turbulence models. In *Sixth Int. Symp. on CFD*, volume 1, pages 408–414, Lake Tahoe, Nevada, 1995. A collection of technical papers. 2.1.5, 5.8

18. C. Hirsch. *Numerical Computation of Internal and External Flows. Vol.2: Computational Methods for Inviscid and Viscous Flows.* Wiley, Chichester, 1990. 2.2.2, 2.2.2, 2.5

19. C.P. Jackson and P.C. Robinson. A numerical study of various algorithms related to the preconditioned conjugate gradient method. *Internal Journal for Numerical Methods in Engineering*, 21:1315–1338, 1985. 5.9

20. M. Kato and B.E. Launder. The modelling of turbulent flow around stationary and vibrating square cylinders. In *Proc. Ninth Symposium on Turbulent Shear Flows*, volume 9, page 10.4.1, Kyoto, Japan, 1993. 2.1.5

21. B. Koren. A robust upwind discretization method for advection, diffusion and source terms. In C.B. Vreugdenhil and B. Koren, editors, *Numerical Methods for Advection-Diffusion Problems*, pages 117–137, Braunschweig, 1993. Vieweg. Notes on Numerical Fluid Mechanics 45. 2.2.2

22. C.K.G. Lam and K. Bremhorst. A modified form of the k-ε model for predicting wall turbulence. *ASME J. Fluids Engng.*, 103:456–460, 1981. 2.1.7

23. B.E. Launder and D.B. Spalding. *Lectures on Mathematical Models of Turbulence*. Academic Press, London, 1972. 2.1.5

24. B.E. Launder and D.B. Spalding. The numerical computation of turbulent flows. *Comp. Meth. Appl. Mech. Eng.*, 3:269–289, 1974. 2.1.5, 2.1.6, 2.1.6, 2.1.6, 5.8

25. F.S. Lien and M.A. Leschziner. Upstream monotonic interpolation for scalar transport with application to complex turbulent flows. *Int. J. Num. Meth. in Fluids*, 19:527–548, 1994. 2.2.2

26. K.J. Morgan, J. Périaux, and F. Thomasset, editors. *Analysis of Laminar Flow over a Backward Facing Step*, Braunschweig, 1984. GAMM Workshop held at Bièvres (Fr.), Vieweg. 9.5

27. C. Moulinec, P. Wesseling, A. Segal, and C.G.M. Kassels. Colocated discretization of the navier-stokes equations on highly non-smooth grids. In *Lecture Notes in Physics*, 1998. To appear. 5.2

28. H.K. Myong and N. Kasagi. unknown. *J. Fluids Engng.*, 112:521, 1990. 2.1.5

29. S. Nisizima and A. Yoshizawa. Turbulent channel and Couette flows using an anisotropic k-ε model. *AIAA J.*, 25:414–420, 1987. 2.1.5

30. C.C. Paige and M.A. Saunders. LSQR: an algorithm for sparse linear equations and sparse least square problem. *ACM Trans. Math. Softw.*, 8:44–71, 1982. 2.7.1

31. G. Papadakis and G. Bergeles. A locally modified second order upwind scheme for convection terms discretization. *Int. J. Num. Meth. Heat Fluid Flow*, 5:49–62, 1995. 2.2.2

32. A. Pascau, C. Perez, and D. Sanchez. A well-behaved scheme to model strong convection in a general transport equation. *Int. J. Num. Meth. Heat Fluid Flow*, 5:75–87, 1995. 2.2.2

33. S.V. Patankar and D.B. Spalding. A calculation procedure for heat and mass transfer in three-dimensional parabolic flows. *Int. J. Heat and Mass Transfer*, 15:1787–1806, 1972. 2.2.2

34. V.C. Patel, W. Rodi, and G. Scheuerer. Turbulence models for near-wall and low Reynolds number flows: a review. *AIAA J.*, 23:1308–1319, 1985. 2.1.7

35. R. Rubenstein and J.M. Barton. Non-linear Reynolds stress models and the renormalisation group. *Phys. Fluids A*, 2:1472, 1990. 2.1.5

36. Y. Saad and M.H. Schultz. GMRES: a generalized minimal residual algorithm for solving non-symmetric linear systems. *SIAM J. Sci. Stat. Comp.*, 7:856–869, 1986. 2.7.1

37. H. Schlichting. *Boundary Layer Theory.* McGraw Hill, New York, 1969. 2.1.6

38. G. Segal, K. Vuik, W. Kuppen, and M. Zijlema. ISNaS - incompressible flow solver. mathematical manual. Report 93-96, Delft University of Technology, Faculty of Technical Mathematics and Informatics, Delft, The Netherlands, 1993. 1, 2, 2.2, 2.2

39. Guus Segal. *SEPRAN manuals.* Leidschendam, 1984. 1, 1

40. Guus Segal. Programmers guide of the ISNaS incompressible solver. Internal report Delft University of Technology, 1994. 1, 3.2, 6

41. G.L.G. Sleijpen and D.R. Fokkema. BiCGstab(l) for linear equations involving unsymmetric matrices with complex spectrum. *Electronic Transactions on Numer. Anal. (ETNA)*, 1:11–32, 1993. 5.6

42. G.L.G. Sleijpen and H.A. van der Vorst. Hybrid Bi-Conjugate Gradient methods for CFD problems. Preprint 902, Department of Mathematics, University of Utrecht, Utrecht, 1995. 5.6, 5.6

43. P. Sonneveld. CGS: a fast Lanczos-type solver for nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.*, 10:36–52, 1989. 2.7.1

44. D.B. Spalding. A novel finite difference formulation for differential expressions involving both first and second derivatives. *Int. J. Num. Meth. in Eng.*, 4:551–559, 1972. 2.2.2

45. S.P. Spekreijse. Multigrid solution of second order discretizations of hyperbolic conservation laws. *Math. Comp.*, 49:135–155, 1987. 2.2.2

46. C.G. Speziale. On nonlinear k-l and k-ε models of turbulence. *J. Fluid Mech.*, 178:459–475, 1987. 2.1.5

47. P.K. Sweby. High resolution schemes using flux-limiters for hyperbolic conservation laws. *SIAM J. Num. Anal.*, 21:995–1011, 1984. 2.2.2, 2.2.2, 2.2.2

48. P.C.W. van Beek and P. Wesseling. Finite volume discretization of the incompressible Navier-Stokes equations in non-smooth boundary-fitted coordinates in two dimensions. Report 93-57, Faculty of Technical Mathematics and Informatics, Delft University of Technology, Delft, 1993. 1.2, 2.2, 5.2

49. H.A. van der Vorst. Bi-CGSTAB: a fast and smoothly converging variant of Bi-CG for solution of non-symmetric linear systems. *SIAM J. Sci. Stat. Comp.*, 13:631–644, 1992. 2.7.1, 2.7.1

50. H.A. van der Vorst and C. Vuik. GMRESR: a family of nested GMRES methods. *Num. Lin. Alg. Appl.*, 1:369–386, 1994. 2.7.1, 2.8.3, 5.6

51. J.J.I.M. van Kan, C.W. Oosterlee, A. Segal, and P. Wesseling. Discretization of the incompressible Navier-Stokes equations in general coordinates using contravariant velocity components. Report 91-09, Faculty of Technical Mathematics and Informatics, Delft University of Technology, Delft, 1991. 2.2, 5.2

52. B. van Leer. Towards the ultimate conservative difference scheme. V. A second-order sequel to Godunov's method. *J. Comp. Phys.*, 32:101–136, 1979. 2.2.2

53. B. van Leer. Upwind-difference methods for aerodynamic problems governed by the Euler equations. *Lectures in Appl. Math.*, 22:327–336, 1985. 2.2.2

54. C.B. Vreugdenhil and B. Koren, editors. *Numerical Methods for Advection-Diffusion Problems*, volume 45, Braunschweig, 1993. Vieweg. Notes on Numerical Fluid Mechanics. 9.9

55. C. Vuik. Termination criteria for GMRES-like methods to solve the discretizet incompressible navier-stokes equations. Report 92-50, Faculty of Technical Mathematics and Informatics, Delft University of Technology, Delft, 1992. 2.7, 2.7.2

56. C. Vuik. Further experiences with GMRESR. *Supercomputer*, 55:13–27, 1993. 2.8.3

57. C. Vuik. The solution of a one-dimensional stefan problem. In J.M. Chadam & H. Rasmussen, editor, *Free Boundary Problems Involving Solids; Proceedings of the International Colloquium "Free Boundary Problems: Theory and Applications", Montreal, Canada, 1990*, pages 149–155, Harlow, 1993. Longman Scientific & Technical. 2.7, 2.7.2

58. C. Vuik. Solution of the discretized incompressible Navier-Stokes equations with the GMRES method. *Int. J. Num. Meth. in Fluids*, 16:507–523, 1993. 2.7, 2.7.2

59. C. Vuik. Some historical notes about the Stefan problem. *Nieuw Archief voor Wiskunde, 4e serie*, 11:157–167, 1993. 5.9

60. C. Vuik. New insights in GMRES-like methods with variable preconditioners. *J. Comp. Appl. Math.*, 61:189–204, 1995. 2.8.3

61. C. Vuik. Fast iterative solvers for the discretized incompressible Navier-Stokes equations. *Int. J. Num. Meth. in Fluids*, 22:195–210, 1996. 2.8.3

62. N.P. Waterson and H. Deconinck. A unified approach to the design and application of bounded higher-order convection schemes. In C. Taylor and P. Durbetaki, editors, *Proc. Ninth Int. Conf. on Numer. Meth. Laminar and*

Turbulent Flow, pages 203–214, Pineridge Press, Swansea, 1995. 2.2.2, 2.2.2, 2.2.2, 2.2.2

63. D.C. Wilcox. *Turbulence Modeling for CFD*. DCW Industries Inc., La Canada, California, 1993. 2.1.5, 2.1.7, 5.8

64. V. Yakhot, S.A. Orszag, S. Thangam, T.B. Gatski, and C.G. Speziale. Development of turbulence models for shear flows by a double expansion technique. *Phys. Fluids A*, 4:1510–1520, 1992. 2.1.5, 5.8

65. J. Zhu. A low-diffusive and oscillation-free convection scheme. *Comm. Appl. Num. Meth.*, 7:225–232, 1991. 2.2.2

66. J. Zhu and W. Rodi. A low dispersion and bounded convection scheme. *Comp. Meth. Appl. Mech. Eng.*, 92:87–96, 1991. 2.2.2

67. M. Zijlema. Finite volume discretization of the k-ε turbulence model in general coordinates. Report 93-90, Delft University of Technology, Faculty of Technical Mathematics and Informatics, Delft, The Netherlands, 1993. 5.2

68. M. Zijlema. *Computational modeling of turbulent flows in general domains*. PhD thesis, Delft University of Technology, The Netherlands, April 1996. 2.2.2

69. M. Zijlema. On the construction of a third-order accurate monotone convection scheme with application to turbulent flow in general coordinates. *Int. J. Num. Meth. in Fluids*, 22:619–641, 1996. 2.2.2

70. M. Zijlema and P. Wesseling. Higher-order flux-limiting schemes for the finite volume computation of incompressible flow. *Int. J. Comp. Fluid Dyn.*, 9:89–109, 1998. 2.2.2, 2.2.2