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On the Design of Nonconforming High-Resolution Finite Element Schemes for Transport Problems

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Motivation

Algebraic Flux Correction, abbr. **AFC**, family of high-resolution schemes for convection-dominated transport and anisotropic diffusion problems.

- universal stabilization approach based on algebraic design criteria
- approved for conforming (multi-)linear finite element schemes
- found complicated to extend to higher-order finite elements

Objective: apply AFC schemes to nonconforming finite elements

- Do the algebraic design criteria apply to nonconforming elements?
- Is the accuracy of solutions comparable to P_1/Q_1 approximations?
- How to implement essential boundary conditions?
- Is there any benefit from using nonconforming elements?

Model problem

- Convection-diffusion equation

$$\int_\Omega w\left[\dot{u}+\nabla\cdot\mathbf{f}(u)\right]\,\mathrm{d}\mathbf{x}=0,\qquad \mathbf{f}(u)=\mathbf{v}u-d\nabla u$$

- Fletcher's group representation

$$u(\mathbf{x},t)\approx\sum\nolimits_j\varphi_j(\mathbf{x})u_j(t),\qquad \mathbf{f}(u)\approx\sum\nolimits_j\varphi_j(\mathbf{x})\mathbf{f}(u_j)$$

- Semi-discrete high-order scheme

$$\boxed{\sum\nolimits_j m_{ij}\dot{u}_j=\sum\nolimits_j k_{ij}u_j+\sum\nolimits_j s_{ij}u_j}$$

$$k_{ij}=-\mathbf{v}_j\cdot\int_\Omega\varphi_i\nabla\varphi_j\,\mathrm{d}\mathbf{x},\qquad s_{ij}=-d\int_\Omega\nabla\varphi_i\cdot\nabla\varphi_j\,\mathrm{d}\mathbf{x}$$

Model problem

- Convection-diffusion equation

$$\int_\Omega w\left[\dot{u} + \nabla\cdot\mathbf{f}(u)\right]\,\mathrm{d}\mathbf{x} = 0, \qquad \mathbf{f}(u) = \mathbf{v}u - d\nabla u$$

- Fletcher's group representation

$$u(\mathbf{x},t) \approx \sum\nolimits_j \varphi_j(\mathbf{x})u_j(t), \qquad \mathbf{f}(u) \approx \sum\nolimits_j \varphi_j(\mathbf{x})\mathbf{f}(u_j)$$

- Semi-discrete high-order scheme

$$\boxed{\sum\nolimits_j m_{ij}\dot{u}_j = \sum\nolimits_{j\neq i} k_{ij}(u_j - u_i) + \delta_i u_i}$$

$$\mathbf{M_C}\dot{\mathbf{u}} = \mathbf{K}\mathbf{u}$$

$$k_{ij} = -\mathbf{v}_j\cdot\int_\Omega \varphi_i\nabla\varphi_j\,\mathrm{d}\mathbf{x}, \qquad \delta_i = \sum\nolimits_j k_{ij}$$

Family of AFC schemes

Kuzmin et al.

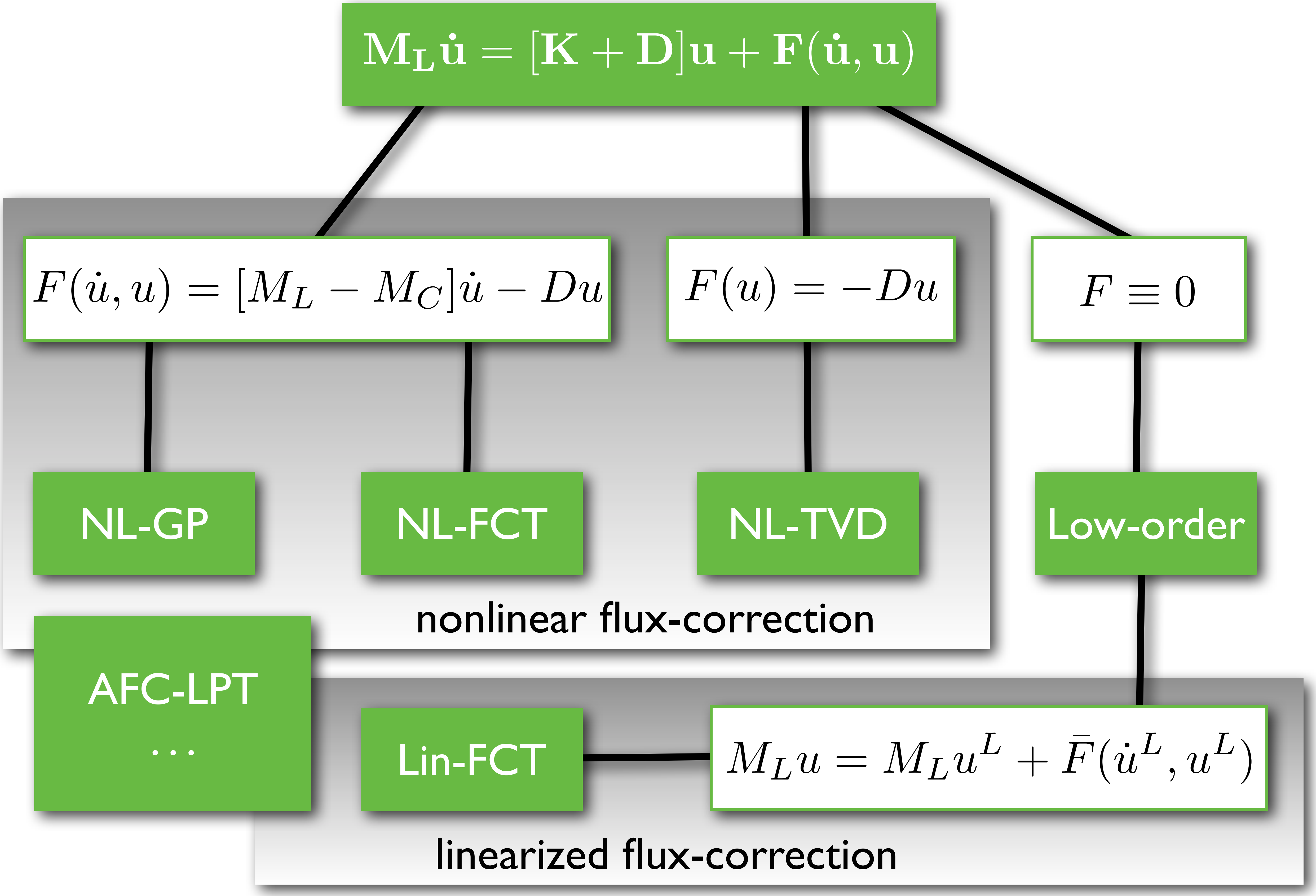
$$\mathbf{M_L}\dot{\mathbf{u}} = [\mathbf{K} + \mathbf{D}]\mathbf{u} + \mathbf{F}(\dot{\mathbf{u}}, \mathbf{u})$$

lumped mass matrix

antidiffusive correction

artificial diffusion operator

Family of AFC schemes *Kuzmin et al.*



$$\mathbf{M_L \dot{u}} = [\mathbf{K} + \mathbf{D}]\mathbf{u} + \mathbf{F}(\dot{\mathbf{u}}, \mathbf{u})$$

$$F(\dot{u}, u) = [M_L - M_C]\dot{u} - Du$$

$$F(u) = -Du$$

$$F \equiv 0$$

$$M_L u = M_L u^L + \bar{F}(\dot{u}^L, u^L)$$

Review of algebraic design principles

- Jameson's Local Extremum Diminishing criterion

IF

$$\underset{\substack{\uparrow\\ \text{positive}}}{m_i}\dot{u}_i = \sum_{j\neq i} \underset{\substack{\uparrow\\ \text{not negative}}}{\sigma_{ij}}(u_j - u_i)$$

THEN local solution maxima/minima do not increase/decrease

- Semi-discrete high-resolution AFC scheme

$$m_i\dot{u}_i = \sum_{j\neq i}\underset{\substack{\text{not negative by}\\ \text{construction}}}{\underline{(k_{ij}+d_{ij})}}(u_j - u_i) + \delta_i u_i + \sum_{j\neq i}\underset{\substack{\text{controlled by}\\ \text{flux limiter}}}{\underline{\alpha_{ij} f_{ij}}}$$

$$\boxed{m_i = \sum\nolimits_j m_{ij}}$$

need to check the positivity of mass matrix coefficients for each finite element by hand!

Finite element spaces

- Parametric quadrilateral finite elements

$$\mathcal{Q}(T) = \{q = \hat{q} \circ \Psi_T^{-1},\, \hat{q} \in \hat{\mathcal{Q}}(\hat{T})\}$$

- Bilinear one-to-one mapping

$$\Psi_T \,:\, \hat{T} := [-1,1] \times [-1,1] \mapsto T \in \mathcal{T}_h$$

$Q_1(T)$	$\hat{Q}_1(\hat{T}) = \mathrm{span}\langle 1, \hat{x}, \hat{y}, \hat{x}\hat{y}\rangle$
$Q_1^{\mathrm{rot}}(T)$ Rannacher & Turek '92	$\hat{Q}_1^{\mathrm{rot}}(\hat{T}) = \mathrm{span}\langle 1, \hat{x}, \hat{y}, \hat{x}^2 - \hat{y}^2\rangle$ $Q_{1,\mathrm{npar}}^{\mathrm{rot}}(T) = \mathrm{span}\langle 1, \xi, \eta, \xi^2 - \eta^2\rangle$

Nonconforming shape functions

$$\hat{\varphi}_1(\hat{\mathbf{x}}) = \frac{1}{4} - \frac{1}{2}\hat{y} - \beta(\hat{x}^2 - \hat{y}^2), \quad \hat{\varphi}_3(\hat{\mathbf{x}}) = \frac{1}{4} + \frac{1}{2}\hat{y} - \beta(\hat{x}^2 - \hat{y}^2)$$

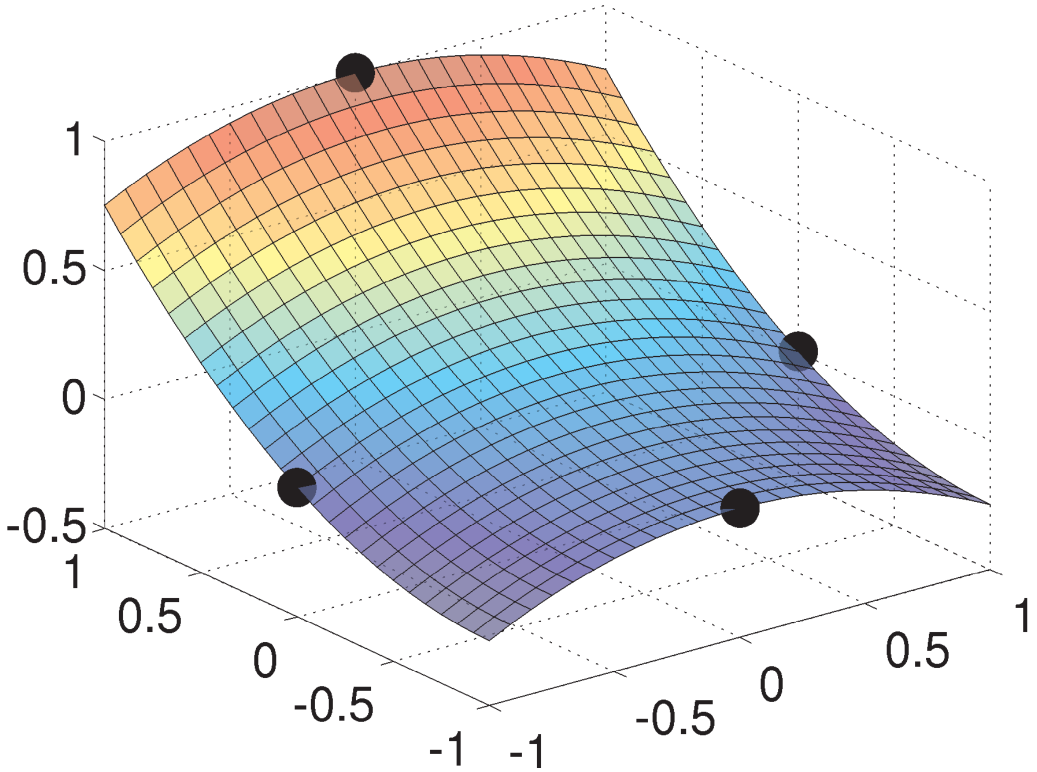
$$\hat{\varphi}_2(\hat{\mathbf{x}}) = \frac{1}{4} + \frac{1}{2}\hat{x} + \beta(\hat{x}^2 - \hat{y}^2), \quad \hat{\varphi}_4(\hat{\mathbf{x}}) = \frac{1}{4} - \frac{1}{2}\hat{x} + \beta(\hat{x}^2 - \hat{y}^2)$$

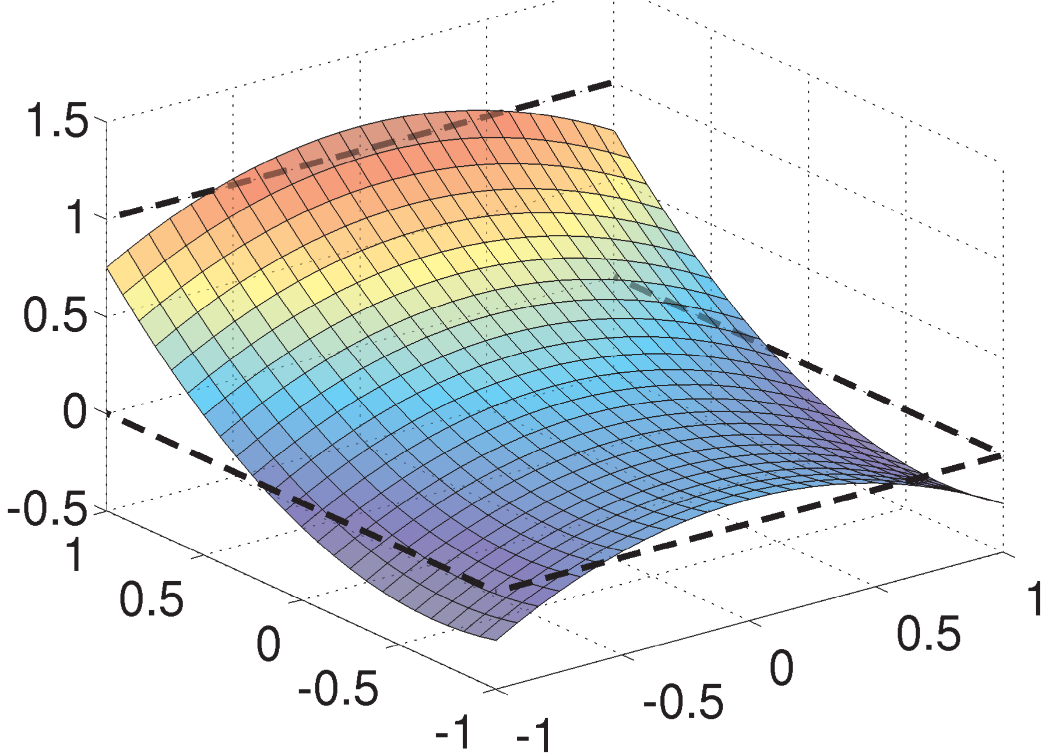
- Midpoint based variant

$$\beta = \frac{1}{4} : \hat{\varphi}_i(\hat{\mathbf{m}}_j) = \delta_{ij}$$

- Mean value based variant

$$\beta = \frac{3}{8} : |\hat{\gamma}_j|^{-1} \int_{\hat{\gamma}_j} \hat{\varphi}_i(\hat{\mathbf{x}})\, \mathrm{d}\gamma = \delta_{ij}$$





Matrix analysis - part I

- Consistent mass matrix on reference element

$$\hat{M} = \begin{pmatrix} \frac{16}{45}\beta^2 + \frac{7}{24} & -\frac{16}{45}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 - \frac{1}{24} & -\frac{16}{24}\beta^2 + \frac{1}{8} \\ -\frac{16}{24}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 + \frac{7}{24} & -\frac{16}{45}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 - \frac{1}{24} \\ \frac{16}{45}\beta^2 - \frac{1}{24} & -\frac{16}{24}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 + \frac{7}{24} & -\frac{16}{45}\beta^2 + \frac{1}{8} \\ -\frac{16}{45}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 - \frac{1}{24} & -\frac{16}{24}\beta^2 + \frac{1}{8} & \frac{16}{45}\beta^2 + \frac{7}{24} \end{pmatrix}$$

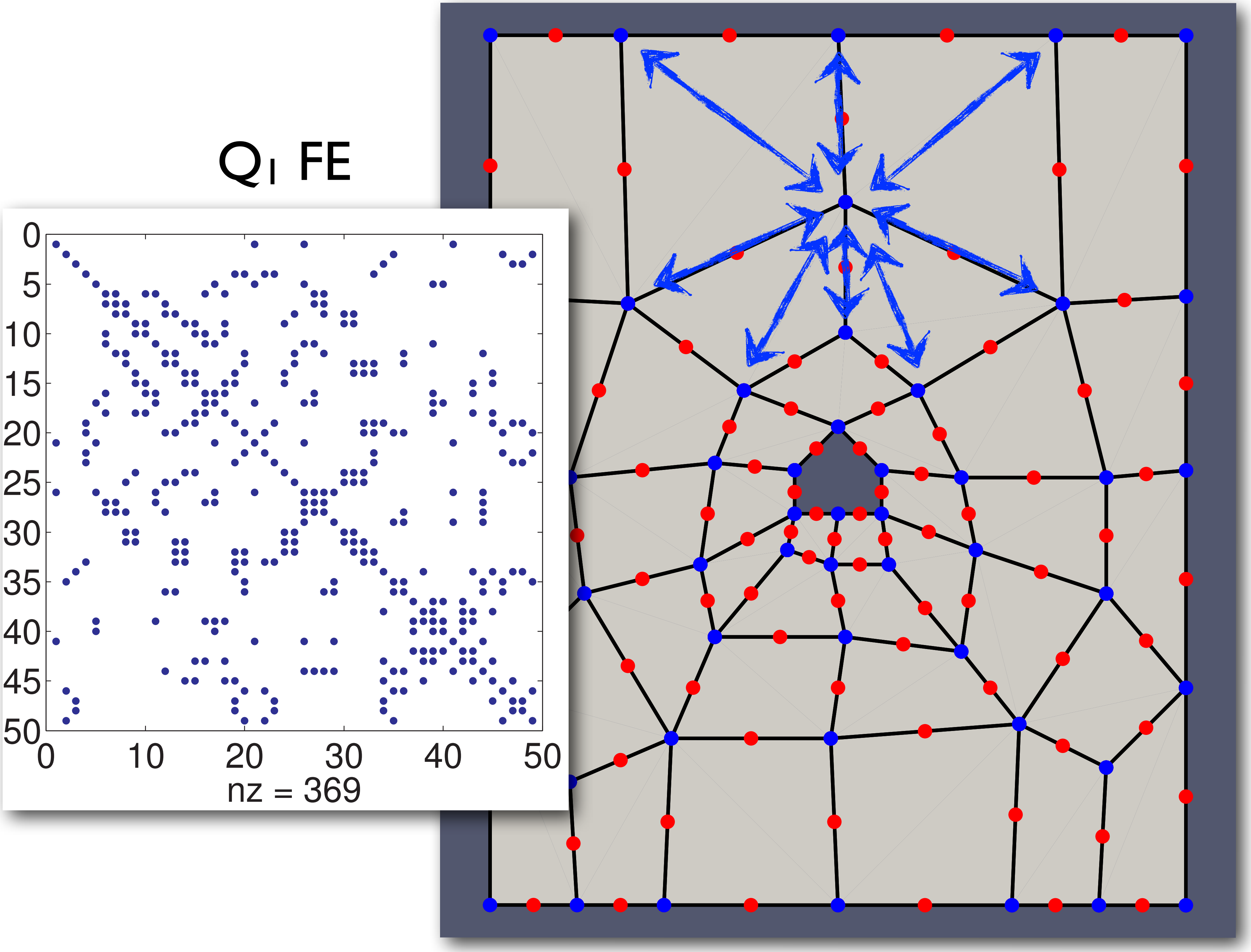
- Positivity criterion

$$0.3423 \approx \frac{1}{16}\sqrt{30} < |\beta| < \frac{3}{16}\sqrt{10} \approx 0.5929$$

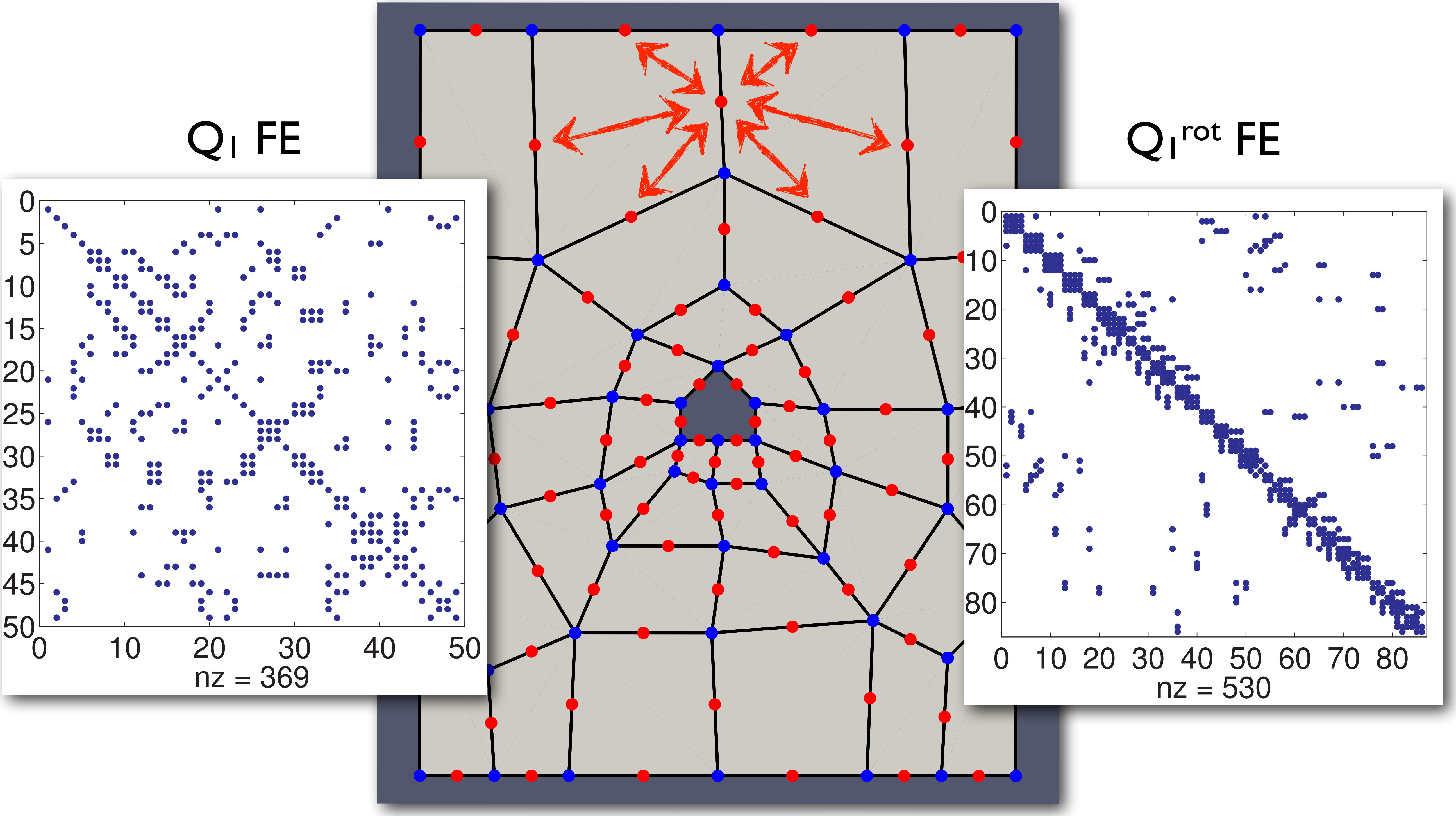
  - midpoint based variant ($\beta = \frac{1}{4}$) has negative matrix coefficients
  - mean value based variant ($\beta = \frac{3}{8}$) has positive matrix coefficients
  - lower bound is invariant to shape of quadrilateral element

Matrix analysis - part 2

Q_1 FE



Matrix analysis - part 2

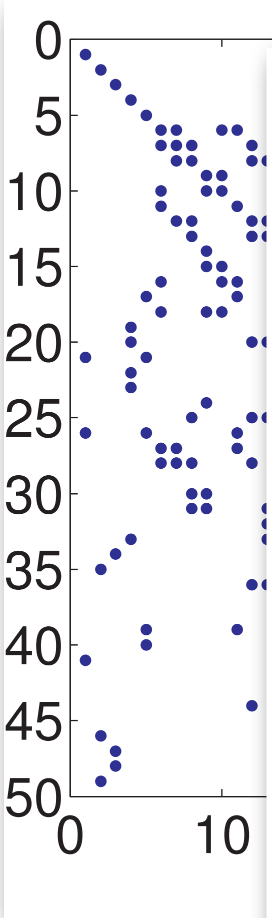

Q_1 FE

Q_1^{rot} FE

Matrix analysis - part 2

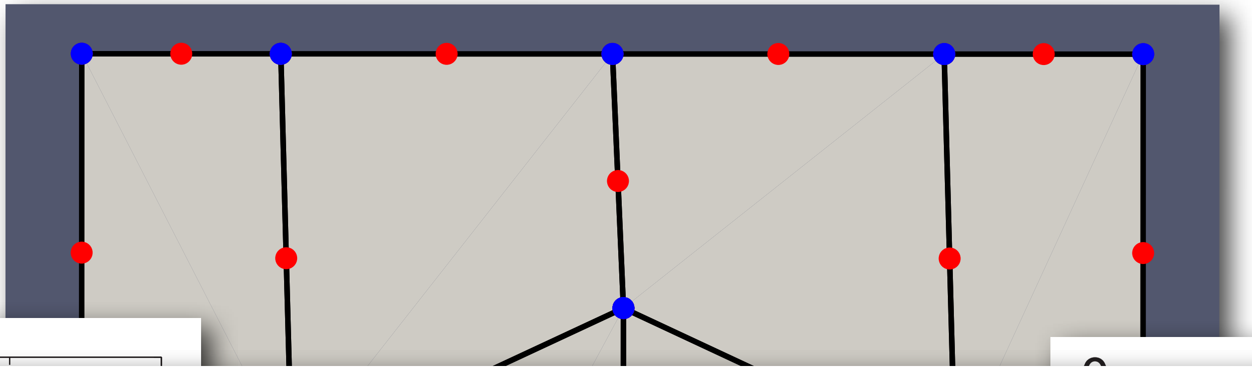
Storage format:
- CRS, CCS

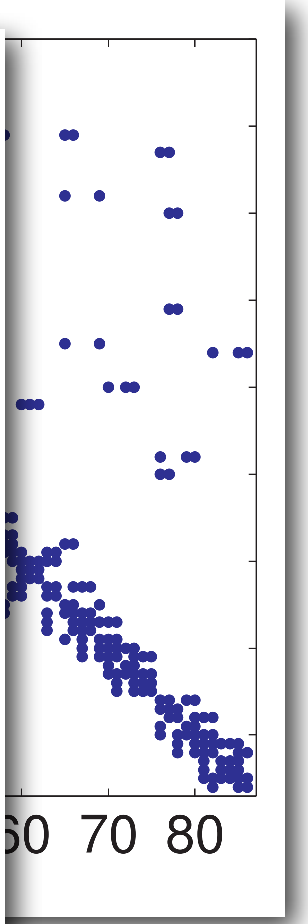
Q_1 FE

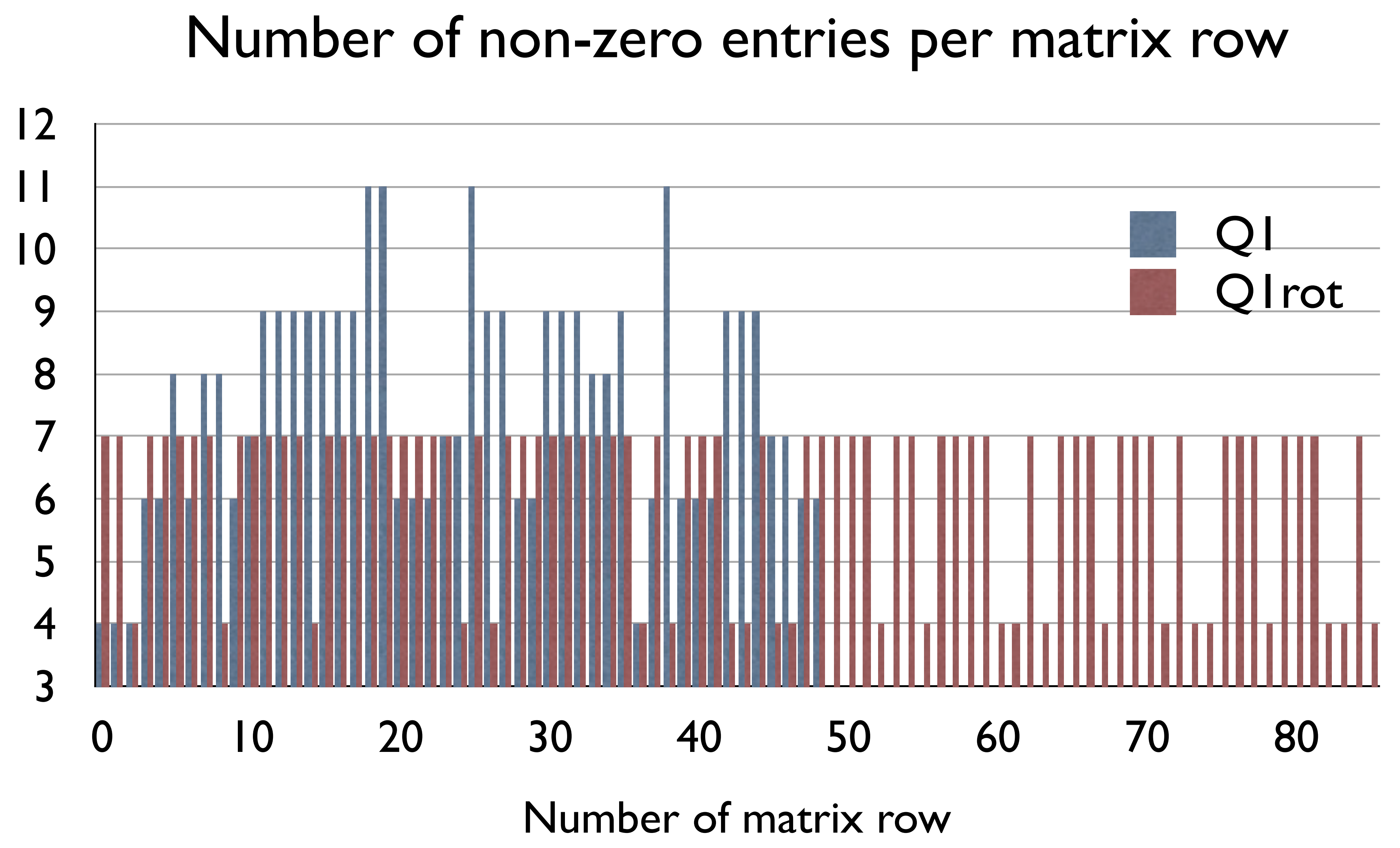


Storage format:
- ELLPACK

Q_1^{rot} FE

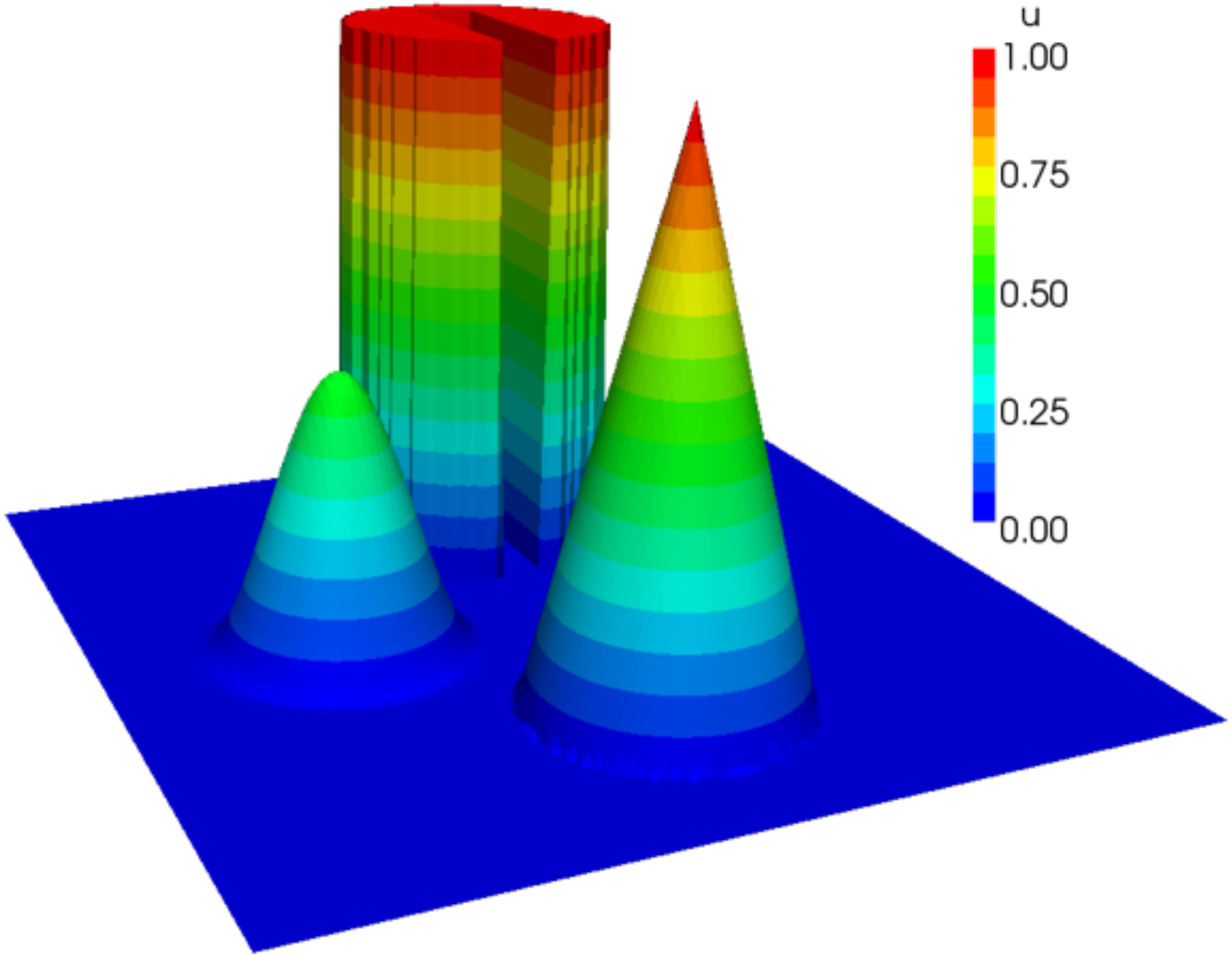





Number of non-zero entries per matrix row

Solid body rotation

$$\begin{aligned} \dot{u} + \nabla \cdot (\mathbf{v}u) &= 0 \ \text{ in } (0,1)^2 \\ u &= 0 \ \text{ on } \Gamma_{\text{inflow}} \end{aligned}$$



- Velocity field

  $\mathbf{v}(x,y) = (0.5 - y, x - 0.5)$

- Grid size

  $h = 1/2^l, l = 5, 6, \ldots$

- Stochastic grid disturbance

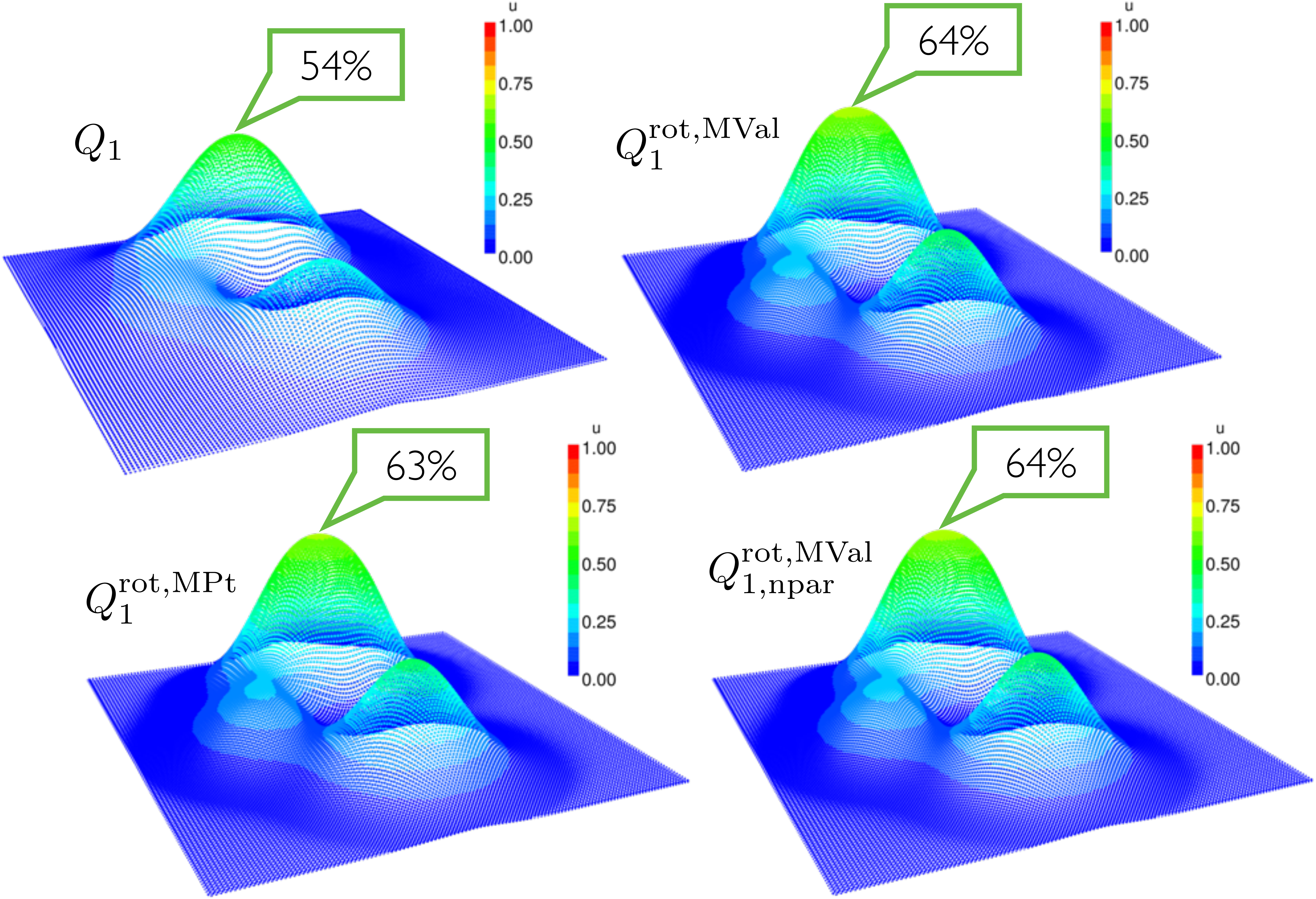
  $\delta \in \{0\%, 1\%, 5\%\}$

- Time step in Crank-Nicolson $\Delta t = 1.28 \cdot h$

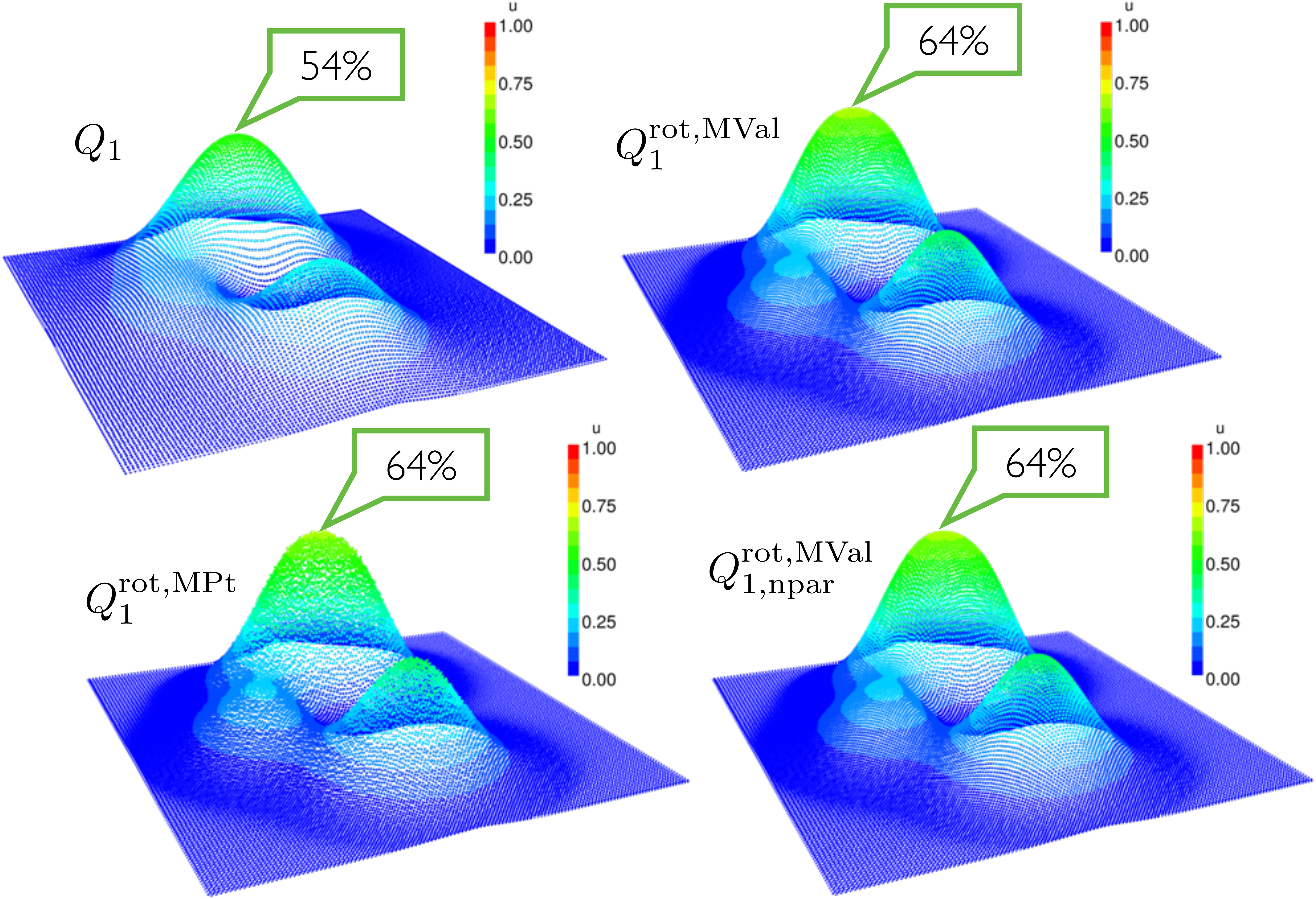
- Initial = exact solution at

  $t = 2\pi k,\ k \in \mathbb{N}$

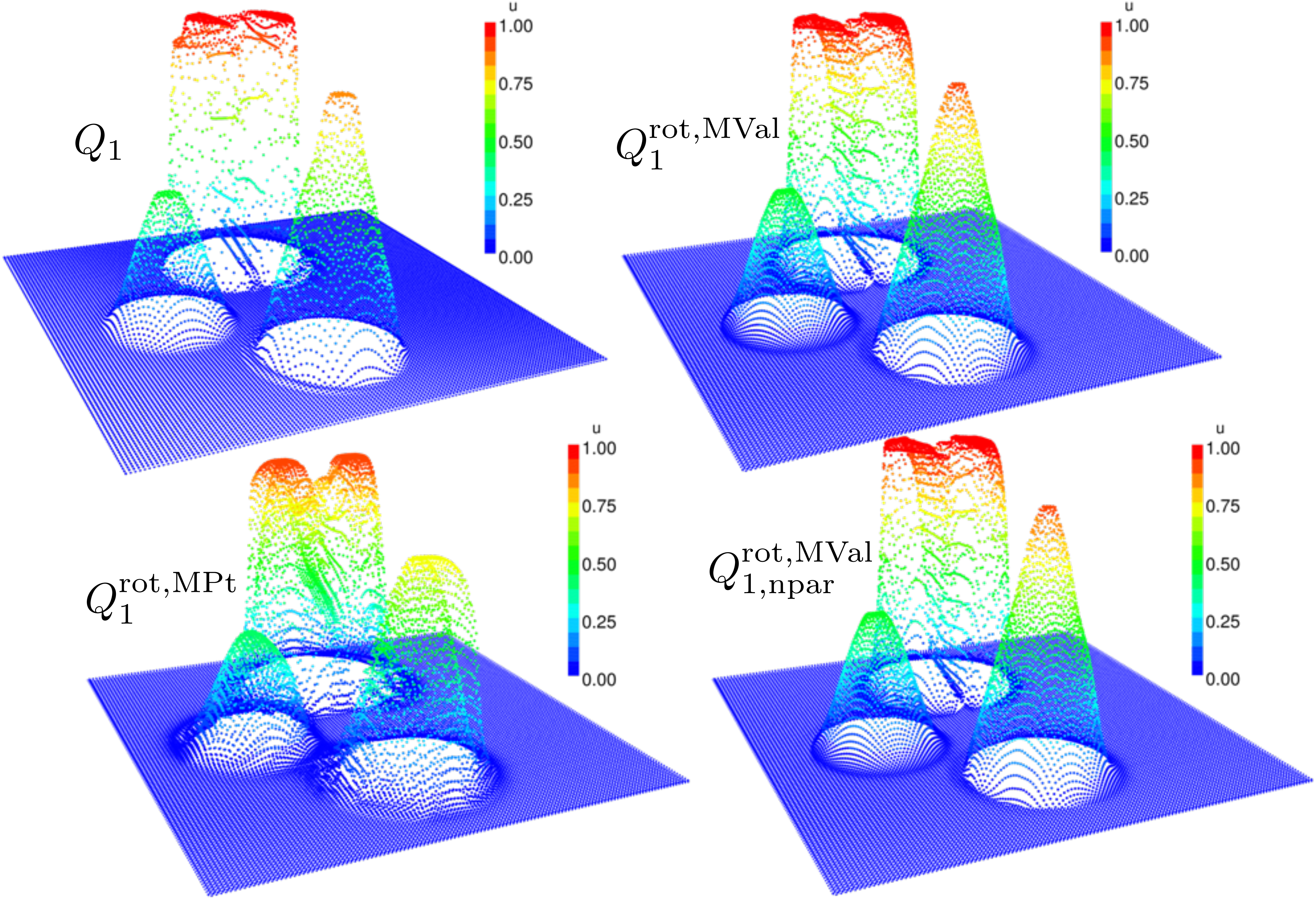
SBR: *low-order solutions (0% mesh perturbation)*



SBR: *low-order solutions (5% mesh perturbation)*



SBR: *NL-FCT solutions (0% mesh perturbation)*



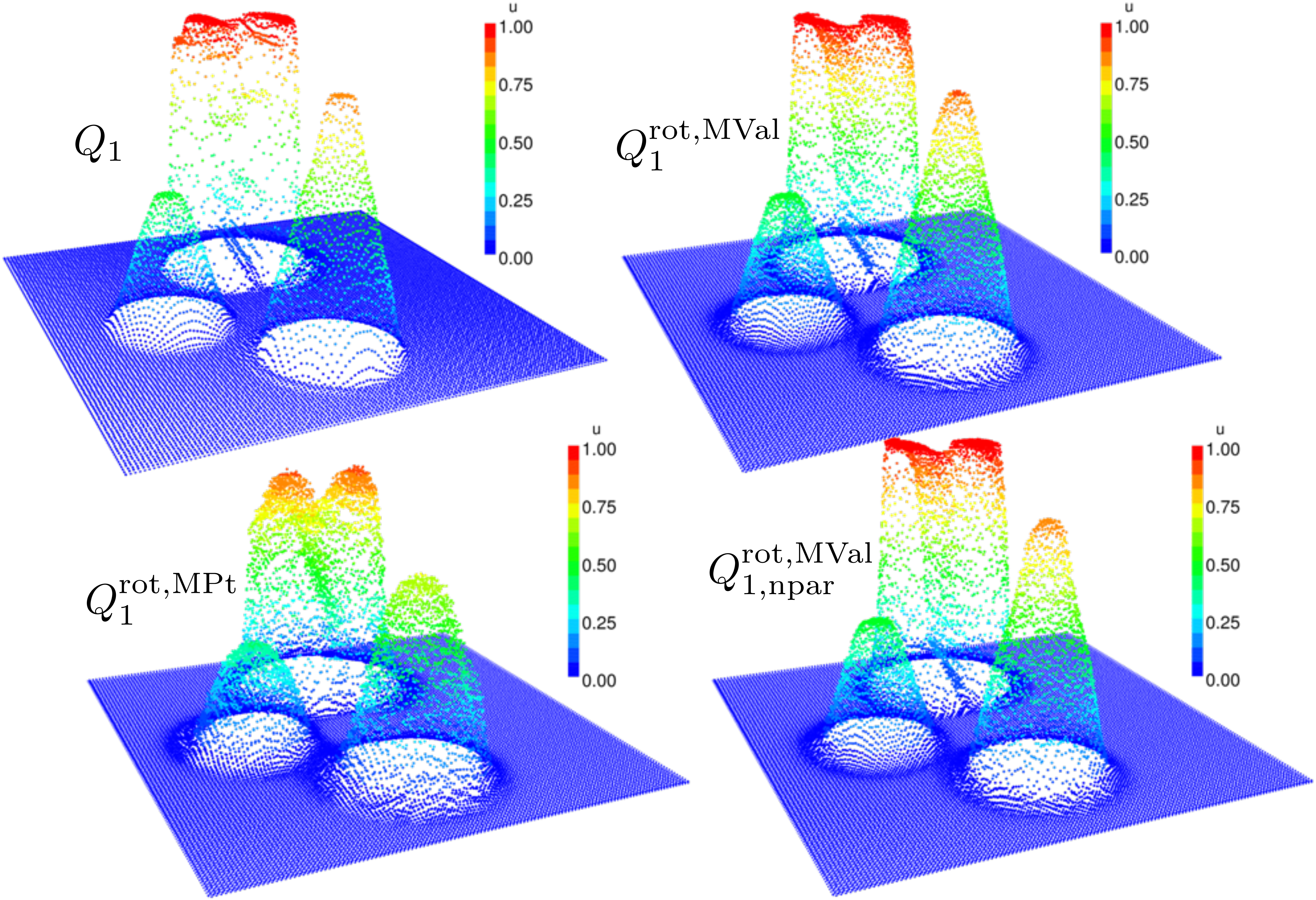
Q_1

$Q_1^{\mathrm{rot,MVal}}$

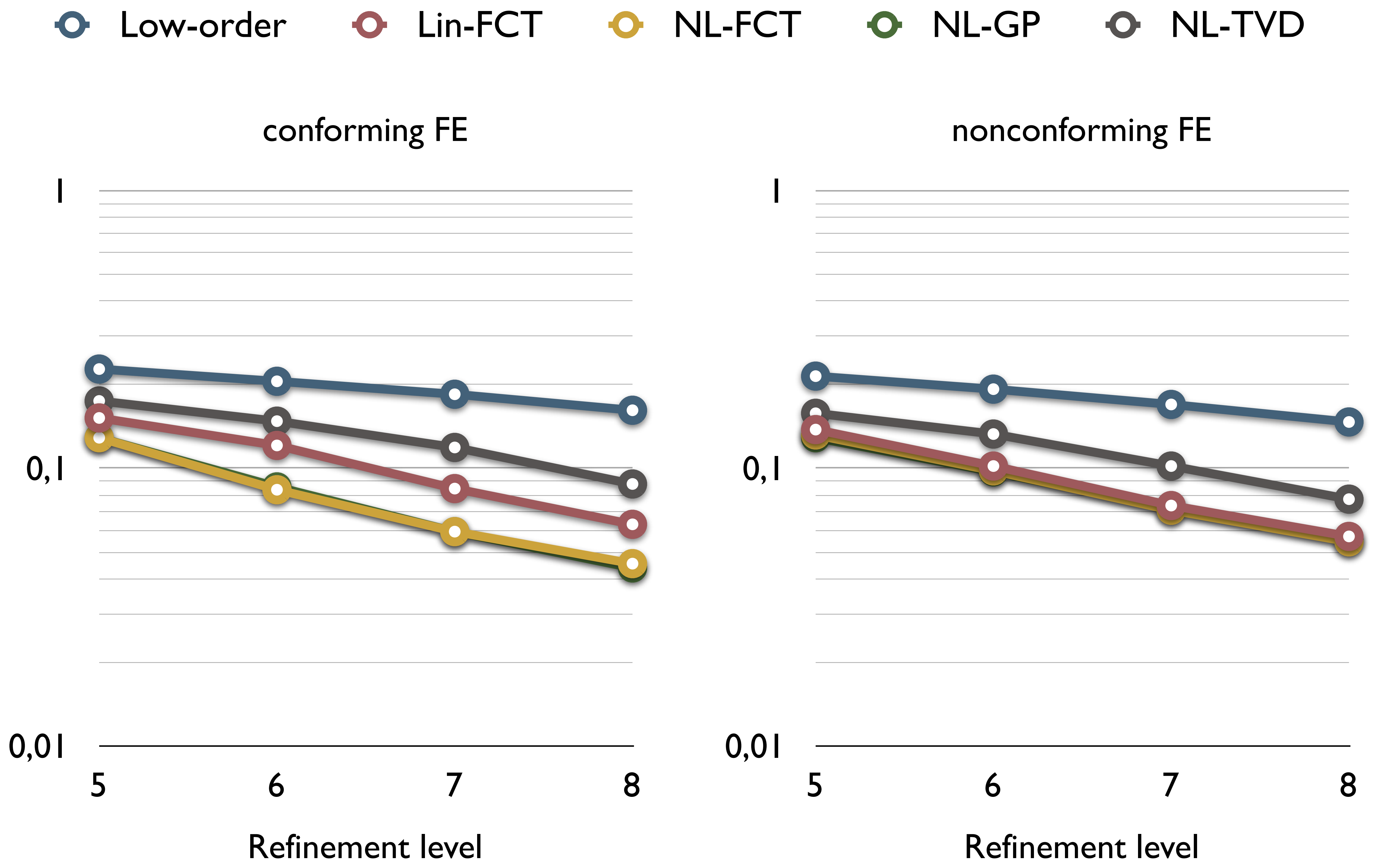
$Q_1^{\mathrm{rot,MPt}}$

$Q_{1,\mathrm{npar}}^{\mathrm{rot,MVal}}$

SBR: *NL-FCT solutions (5% mesh perturbation)*

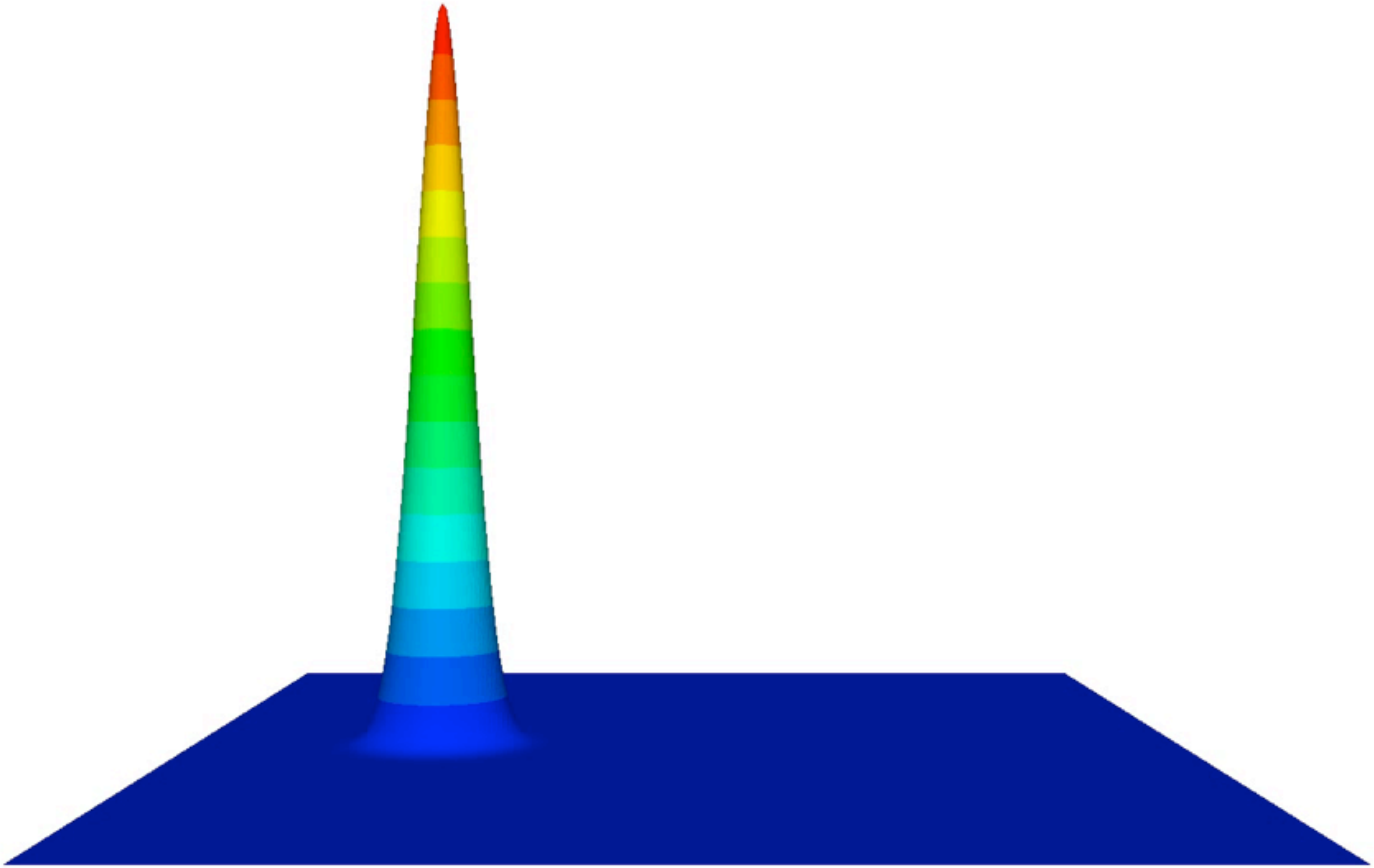


SBR: *L_2-error (5% mesh perturbation)*

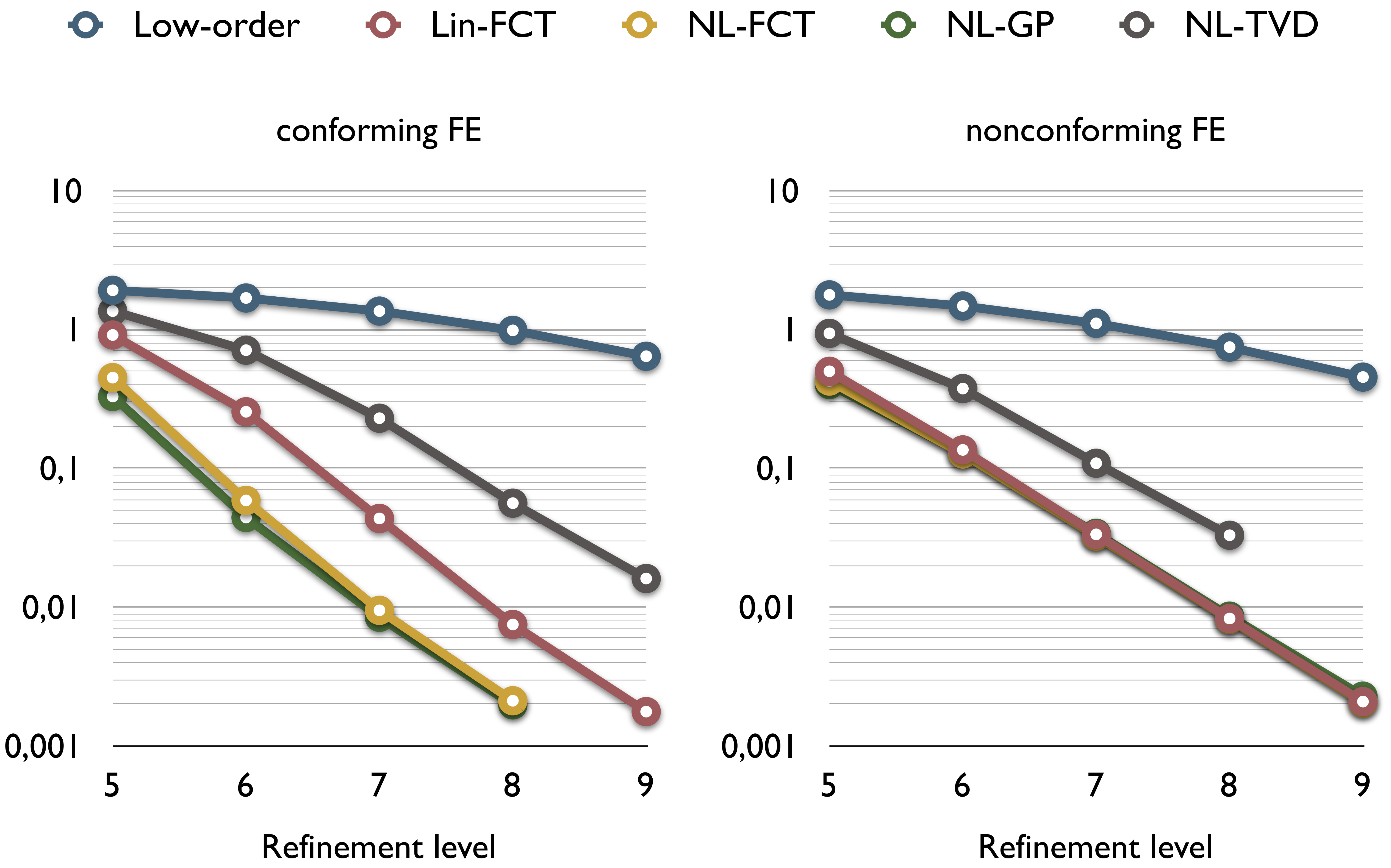


Rotation of a Gaussian hill

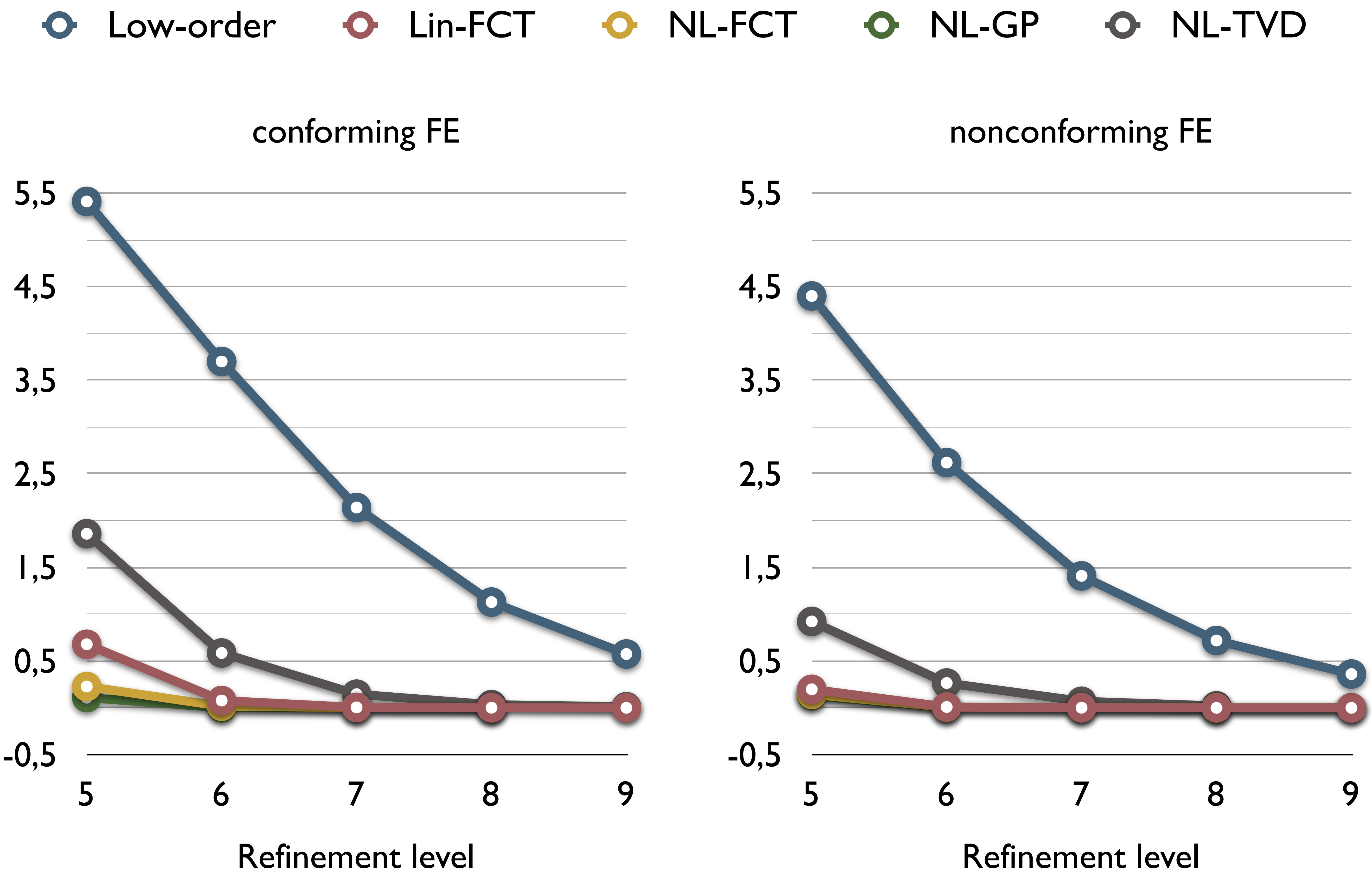
$$\dot{u} + \nabla \cdot (\mathbf{v}u - d\nabla u) = 0 \ \text{ in } (-1,1)^2, \ \mathbf{v}(x,y) = (-y,x), \ d = 0.001$$



RGH: L_2-error (5% mesh perturbation)



RGH: *dispersion-error (5% mesh perturbation)*



Taxonomy of finite elements

conforming FE		nonconforming FE
good	**accuracy**	good
small	**numerical diffusion**	small(er)
smaller	**#DOFs, #edges**	larger
irregular	**sparsity pattern**	regular

Boundary conditions

Convection-diffusion equation

$$\begin{aligned} \nabla \cdot (\mathbf{v}u - d\nabla u) &= f && \text{in } \Omega \\ u &= u_{\mathrm{D}} && \text{on } \Gamma_{\mathrm{D}} \\ (d\nabla u) \cdot \mathbf{n} &= g && \text{on } \Gamma_{\mathrm{N}} \end{aligned}$$

hyperbolic limit $d \to 0$

$$\begin{aligned} \nabla \cdot (\mathbf{v}u) &= f && \text{in } \Omega \\ (\mathbf{v}u) \cdot \mathbf{n} &= h && \text{on } \Gamma_{\mathrm{in}} \end{aligned}$$

- Y. Basilevs, T. Hughes, *Weak imposition of Dirichlet boundary conditions in fluid mechanics*, Computers & Fluids 32 (1) 2007, 12-26
  - $\gamma = 1$ consistent, adjoint-consistent
  - $\gamma = -1$ consistent, adjoint-inconsistent

$$\beta_b = \frac{Cd}{h_b}$$

- E. Burman, *A penalty free non-symmetric Nitsche type method for the weak imposition of boundary conditions*, eprint arXiv:1106.5612v2 (Nov 2011)

  $\gamma = -1, \ \beta \equiv 0$

Weak imposition of boundary conditions

$$
\begin{aligned}
&\int_\Omega -\nabla w_h \cdot (\mathbf{v} u_h - d \nabla u_h) \mathrm{d}\mathbf{x} + \int_\Gamma w_h (\mathbf{v} u_h) \cdot \mathbf{n} \mathrm{d}s \\
&- \int_{\Gamma_{\mathrm{D}}} w_h (d \nabla u_h) \cdot \mathbf{n} \mathrm{d}s - \int_{\Gamma_{\mathrm{D}}} (\gamma d \nabla w_h) \cdot \mathbf{n} u_h \mathrm{d}s \\
&- \int_{\Gamma_{\mathrm{D}} \cap \Gamma_{\mathrm{in}}} (\mathbf{v} w_h) \cdot \mathbf{n} u_h \mathrm{d}s + \sum_{b=1}^{N_{\mathrm{eb}}} \int_{\Gamma_{\mathrm{D}} \cap \Gamma_b} \beta_b w_h u_h \mathrm{d}s \\
&= \int_\Omega w_h f \mathrm{d}\mathbf{x} + \int_{\Gamma_{\mathrm{N}}} w_h g \mathrm{d}s - \int_{\Gamma_{\mathrm{D}}} \gamma (d \nabla w_h) \cdot \mathbf{n} u_{\mathrm{D}} \mathrm{d}s \\
&- \int_{\Gamma_{\mathrm{D}} \cap \Gamma_{\mathrm{in}}} (\mathbf{v} w_h) \cdot \mathbf{n} u_{\mathrm{D}} \mathrm{d}s + \sum_{b=1}^{N_{\mathrm{eb}}} \int_{\Gamma_{\mathrm{D}} \cap \Gamma_b} \beta_b w_h u_{\mathrm{D}} \mathrm{d}s
\end{aligned}
$$

$$\gamma = \pm 1, \quad \beta_b = \frac{Cd}{h_b}$$

Weak imposition of boundary conditions

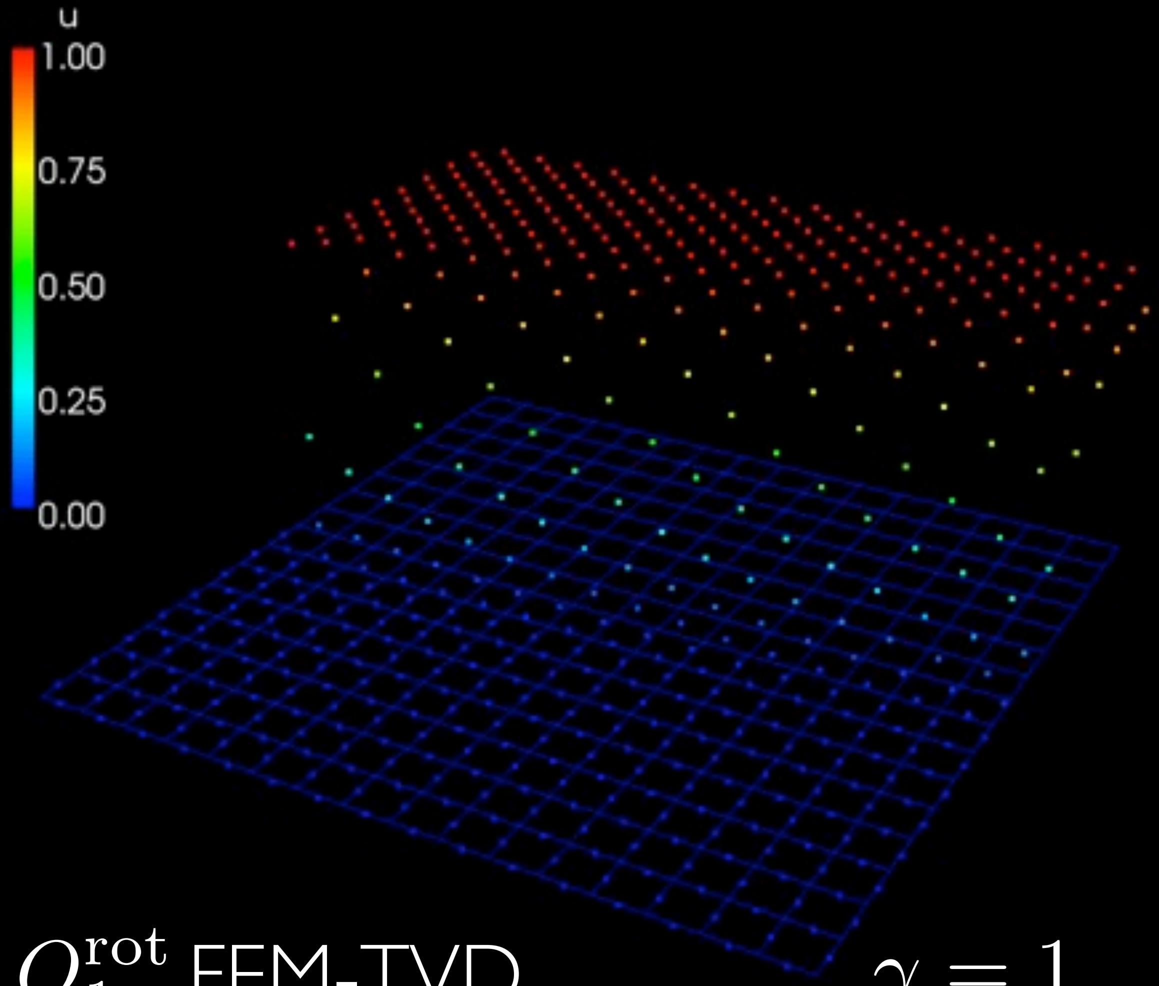
$$\int_\Omega -\nabla w_h \cdot (\mathbf{v}u_h - d\nabla u_h)\mathrm{d}\mathbf{x} + \int_\Gamma w_h(\mathbf{v}u_h)\cdot\mathbf{n}\mathrm{d}s$$

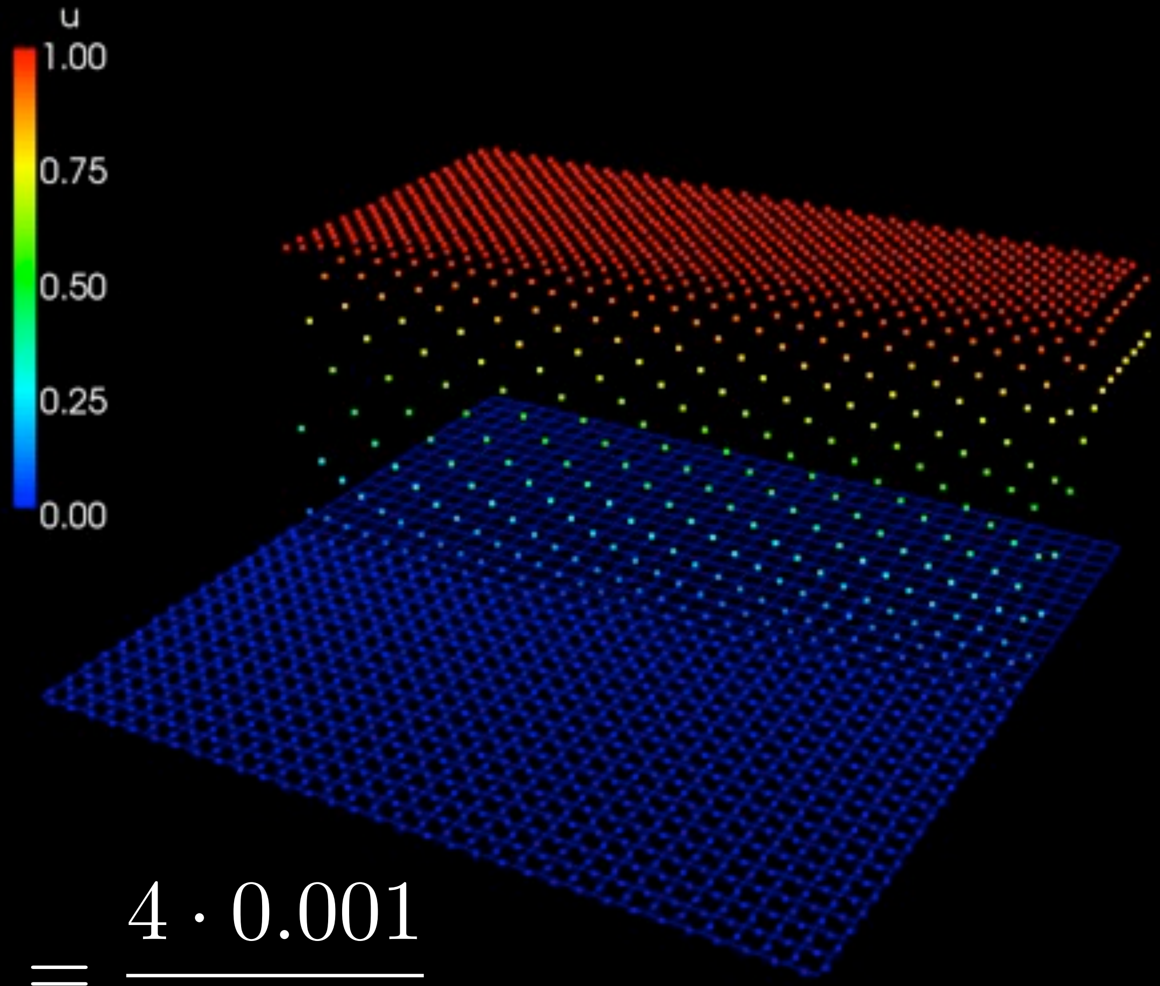
$$-\int_{\Gamma_\mathrm{D}\cap\Gamma_\mathrm{in}} (\mathbf{v}w_h)\cdot\mathbf{n}u_h\mathrm{d}s$$

$$\int_{\Gamma_\mathrm{out}} w_h\mathbf{v}\cdot\mathbf{n}u_h\mathrm{d}s$$

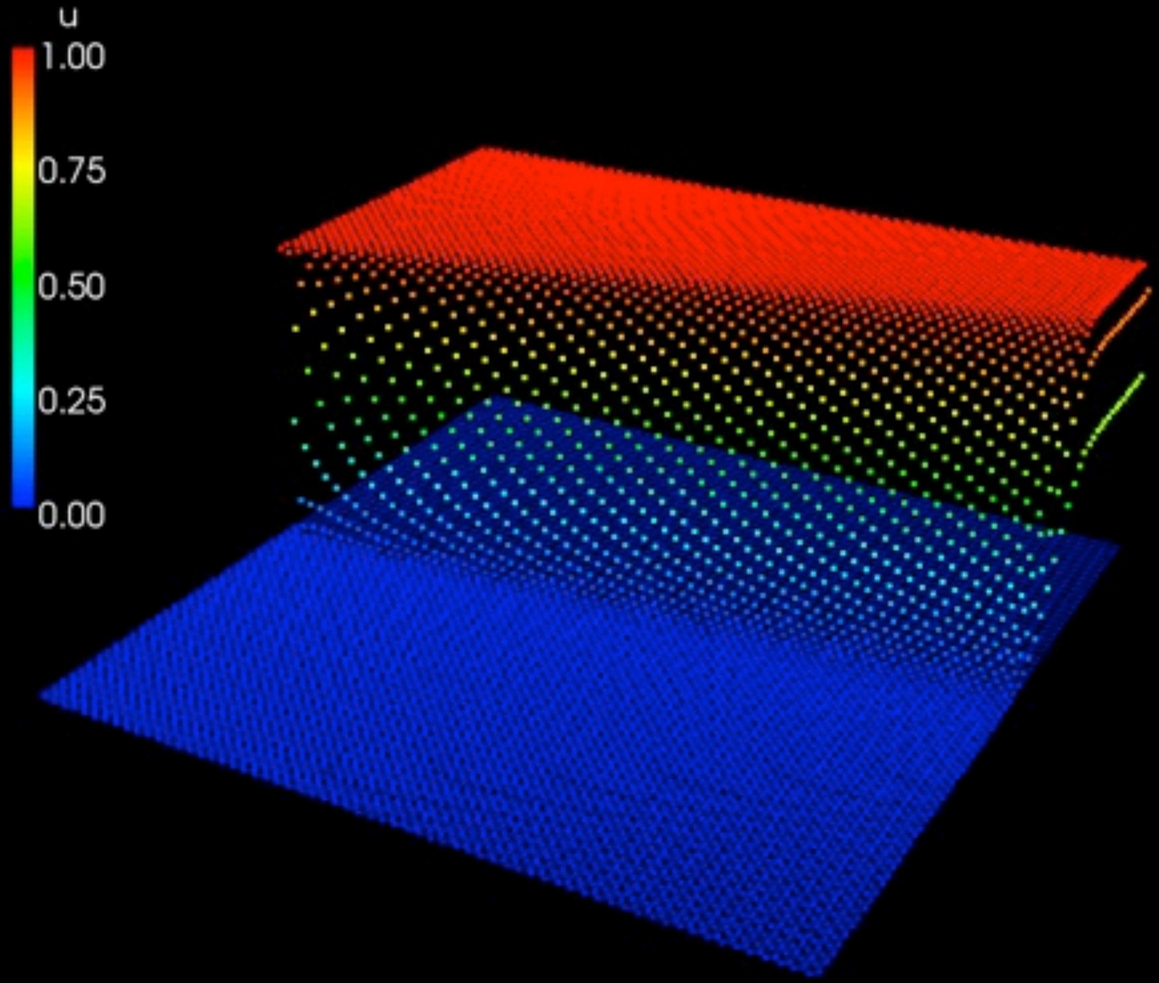
$$= \int_\Omega w_h f\mathrm{d}\mathbf{x}$$

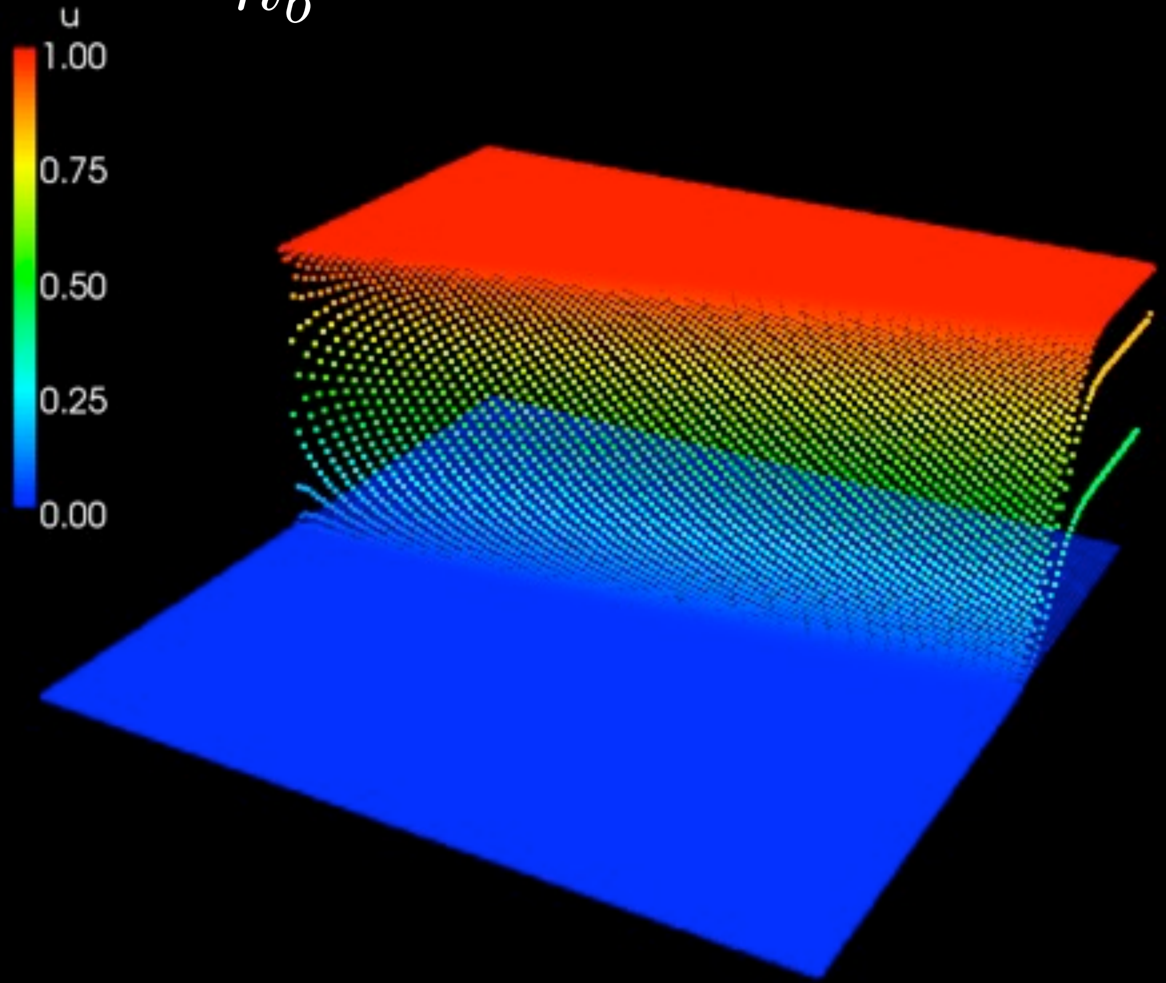
$$-\int_{\Gamma_\mathrm{D}\cap\Gamma_\mathrm{in}} (\mathbf{v}w_h)\cdot\mathbf{n}u_\mathrm{D}\mathrm{d}s$$

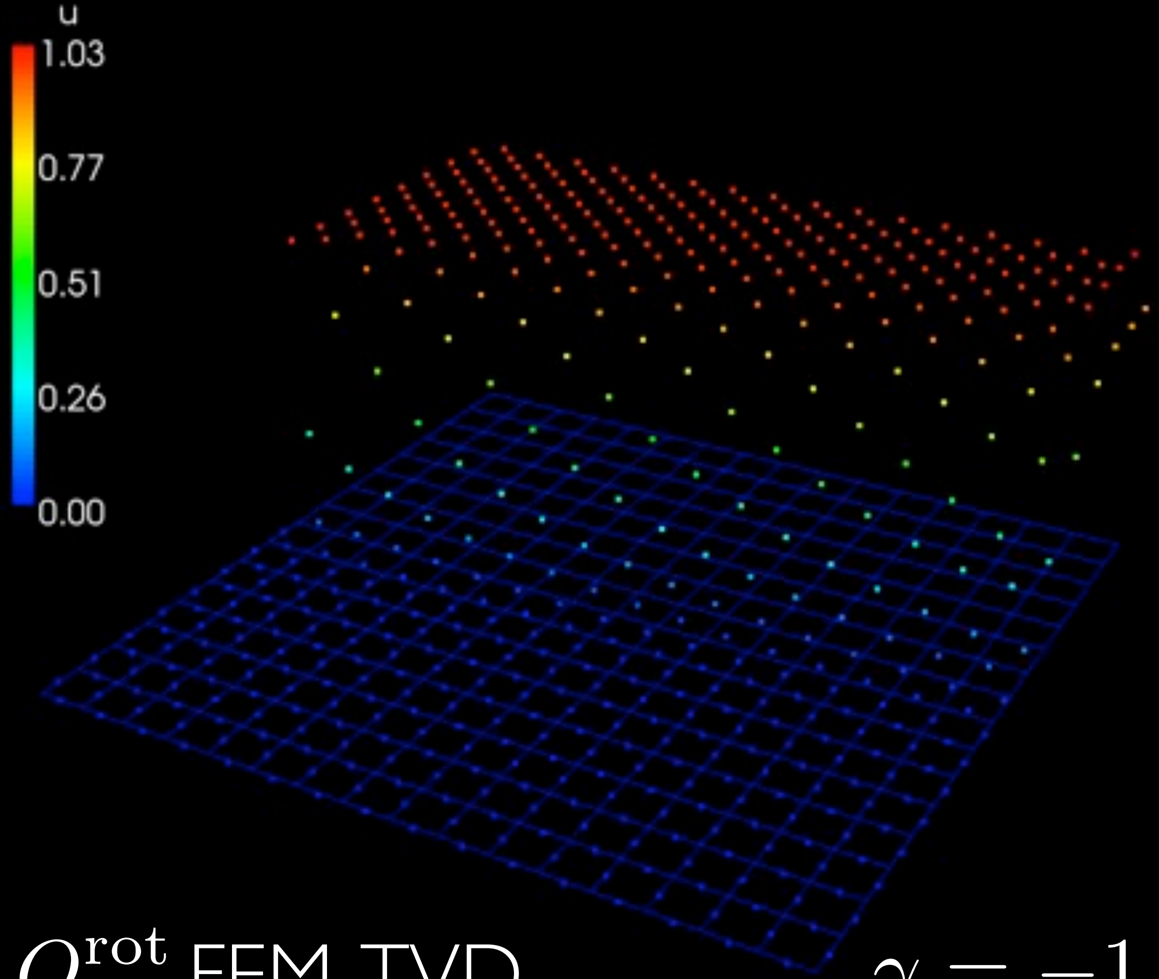


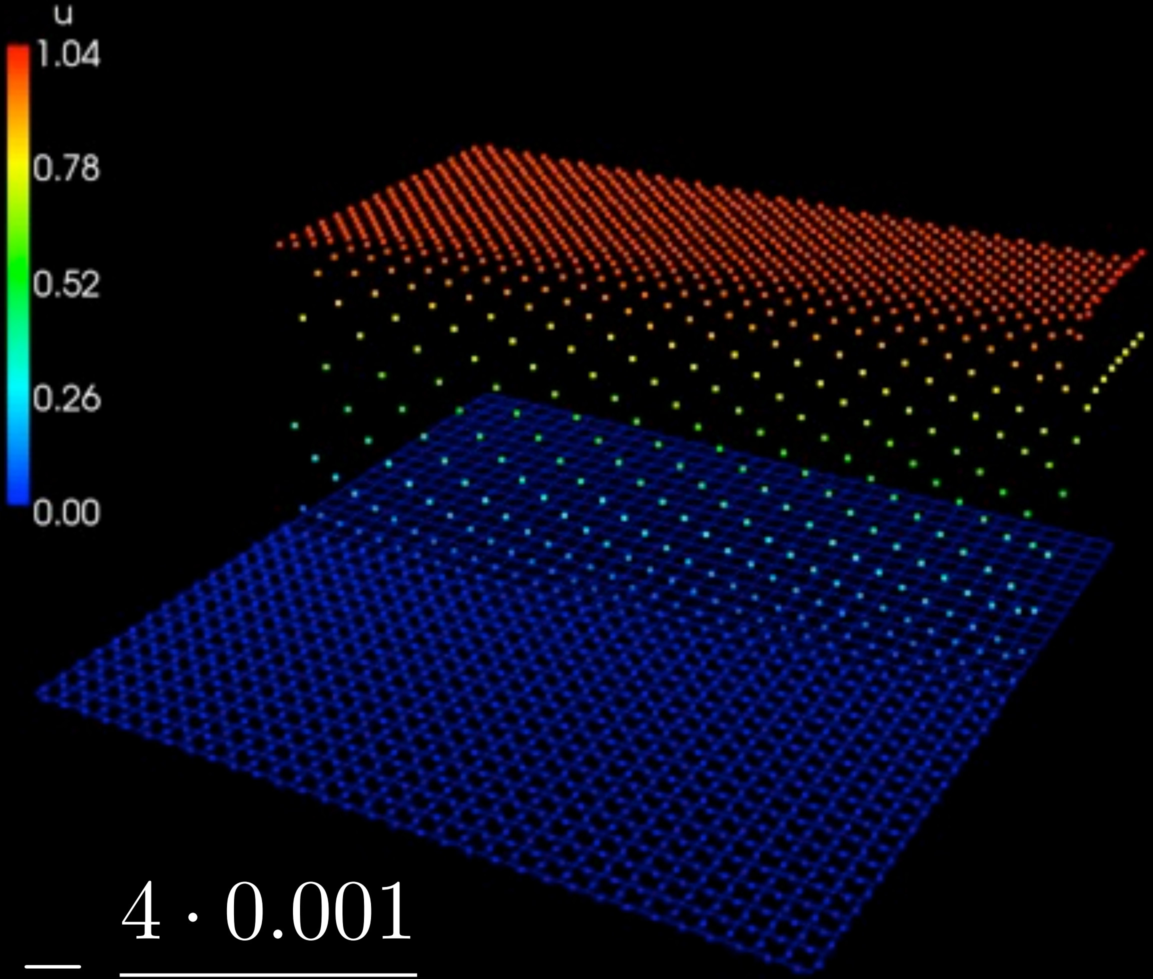


Q_1^{rot} FEM-TVD $\gamma = 1, \qquad \beta_b = \dfrac{4 \cdot 0.001}{h_b}$



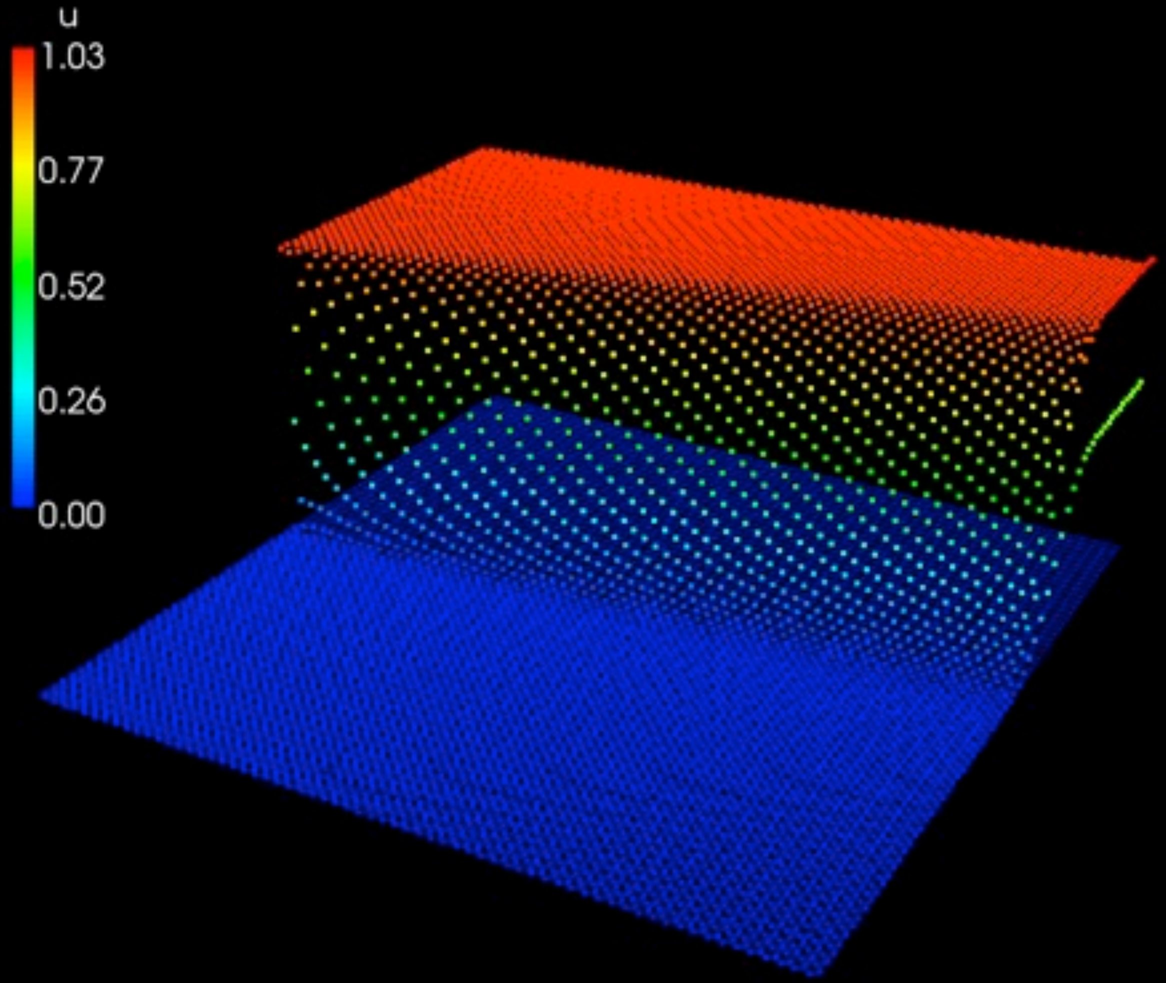


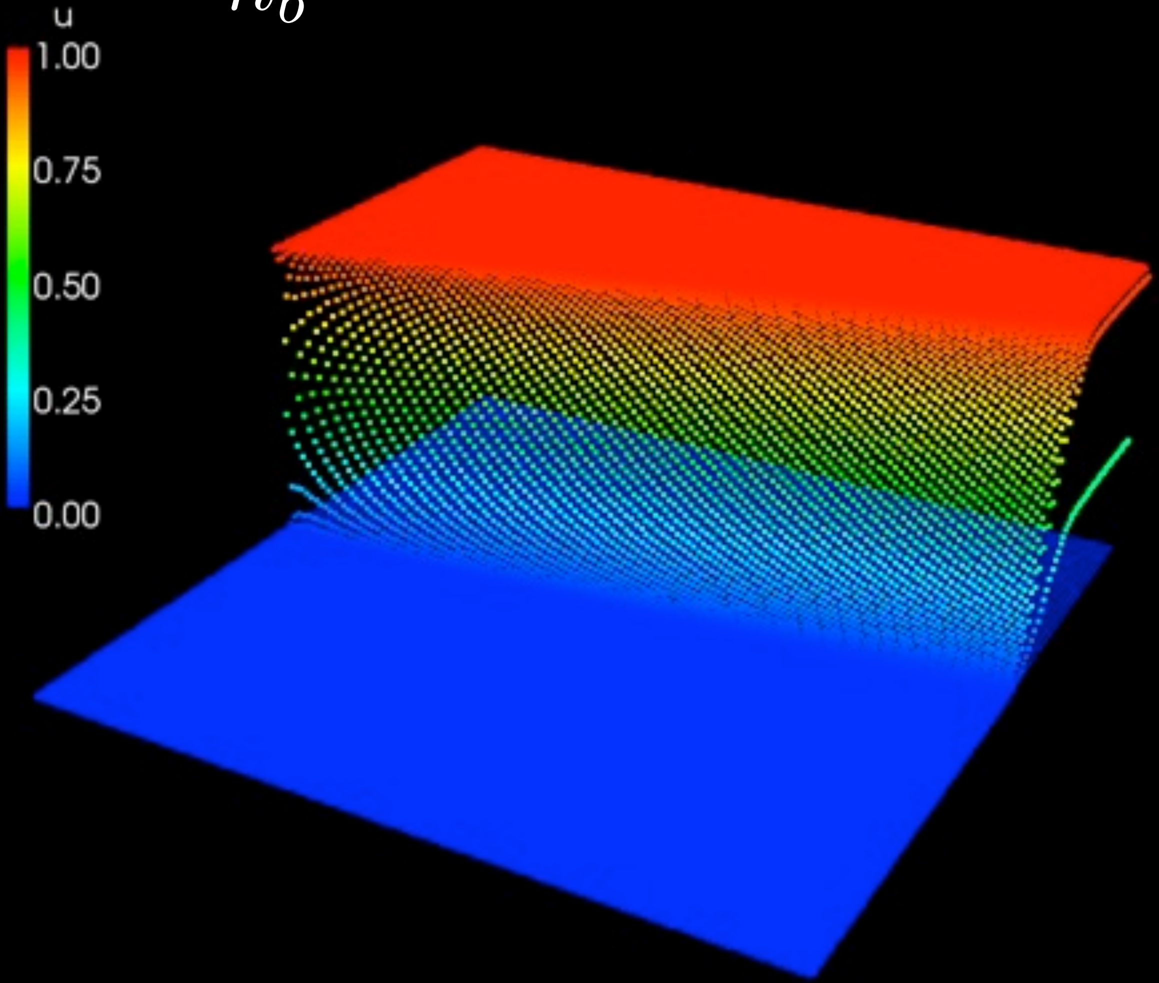


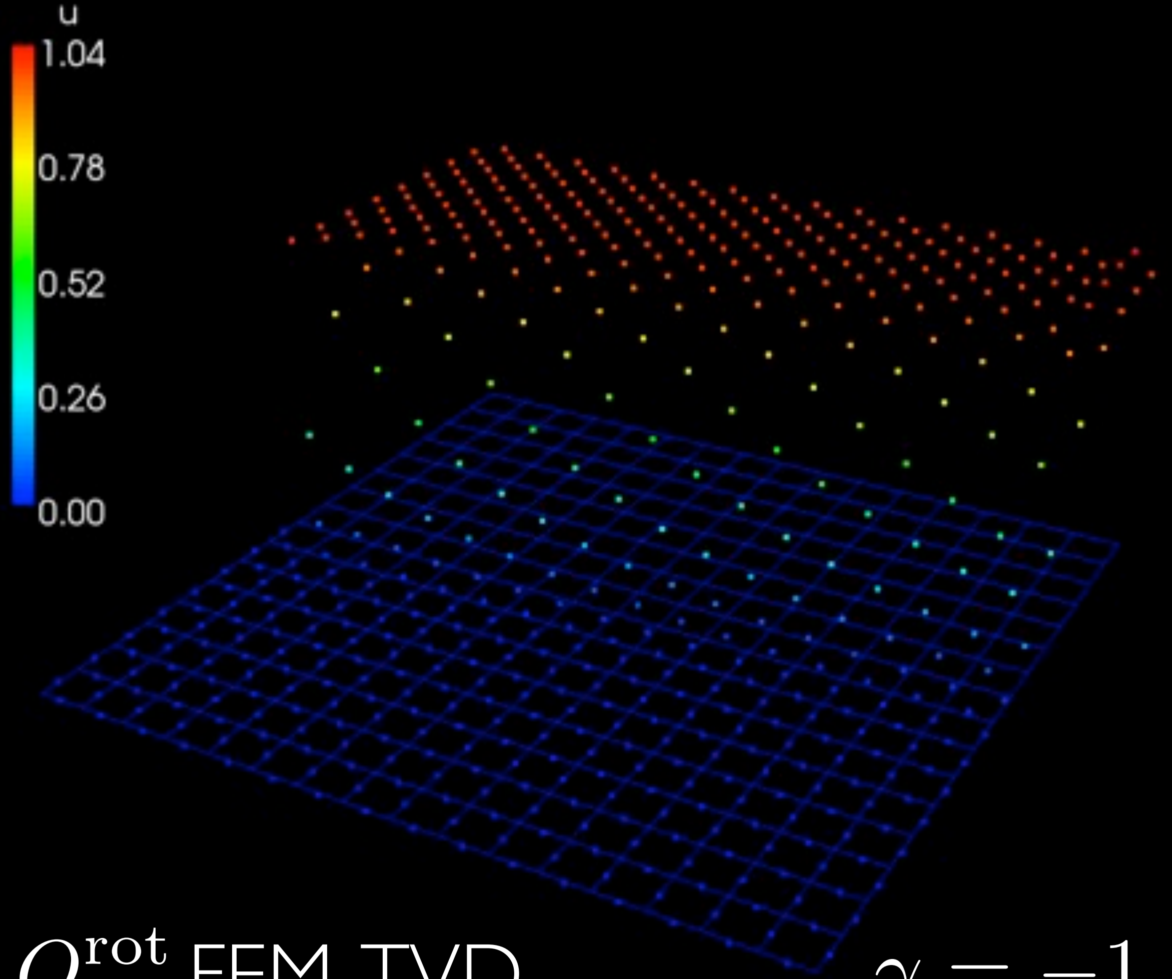


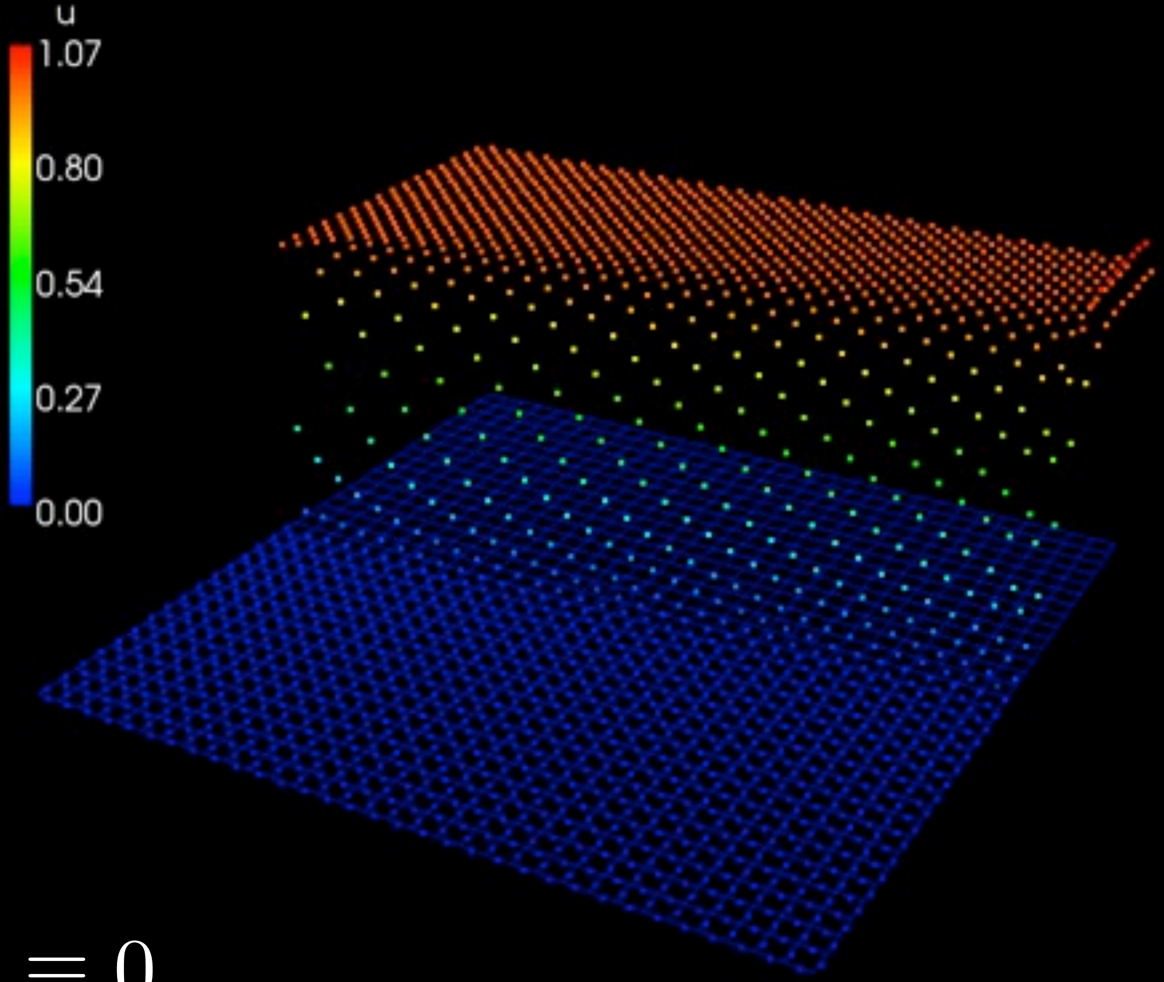
Q_1^{rot} FEM-TVD

$$\gamma = -1, \quad \beta_b = \frac{4 \cdot 0.001}{h_b}$$

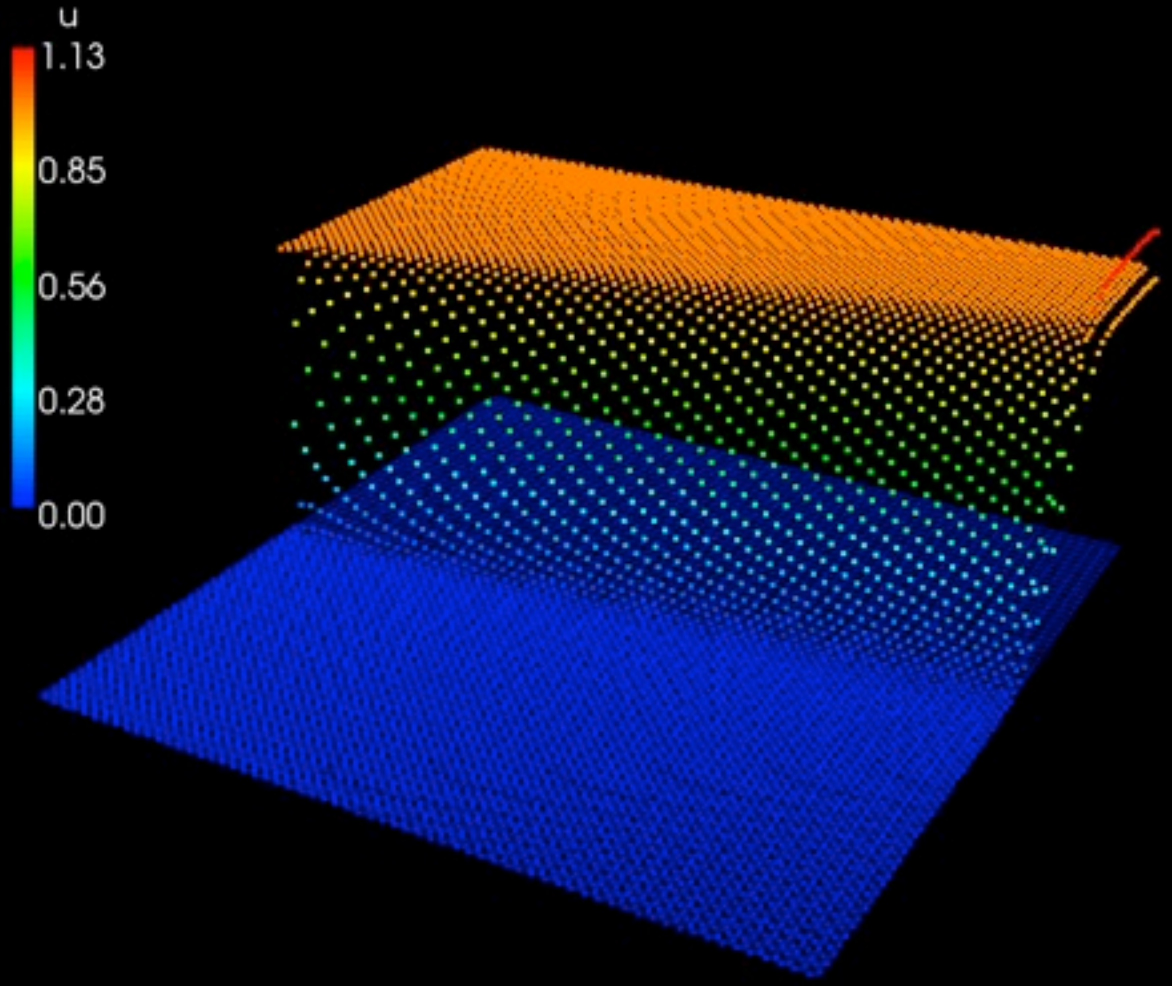


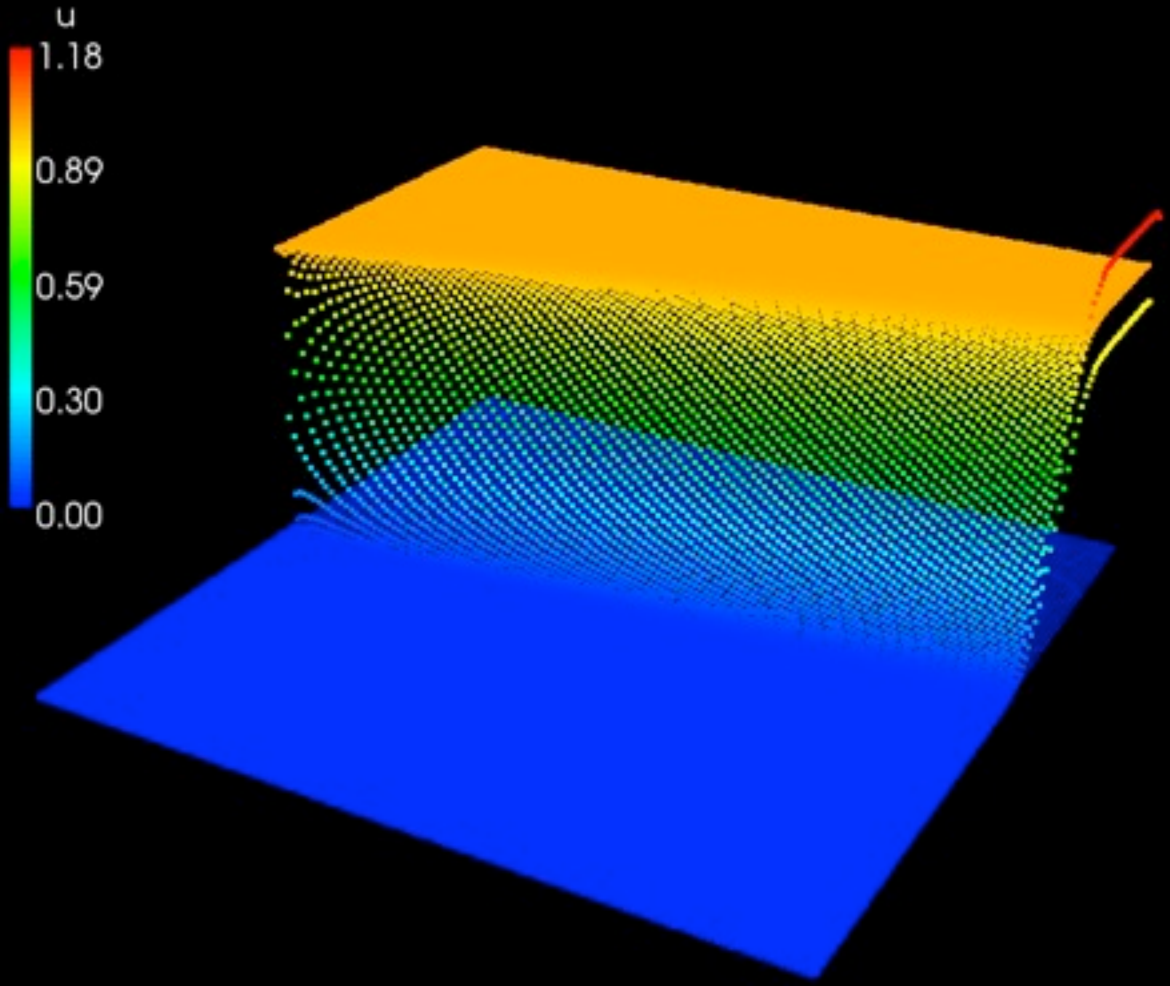






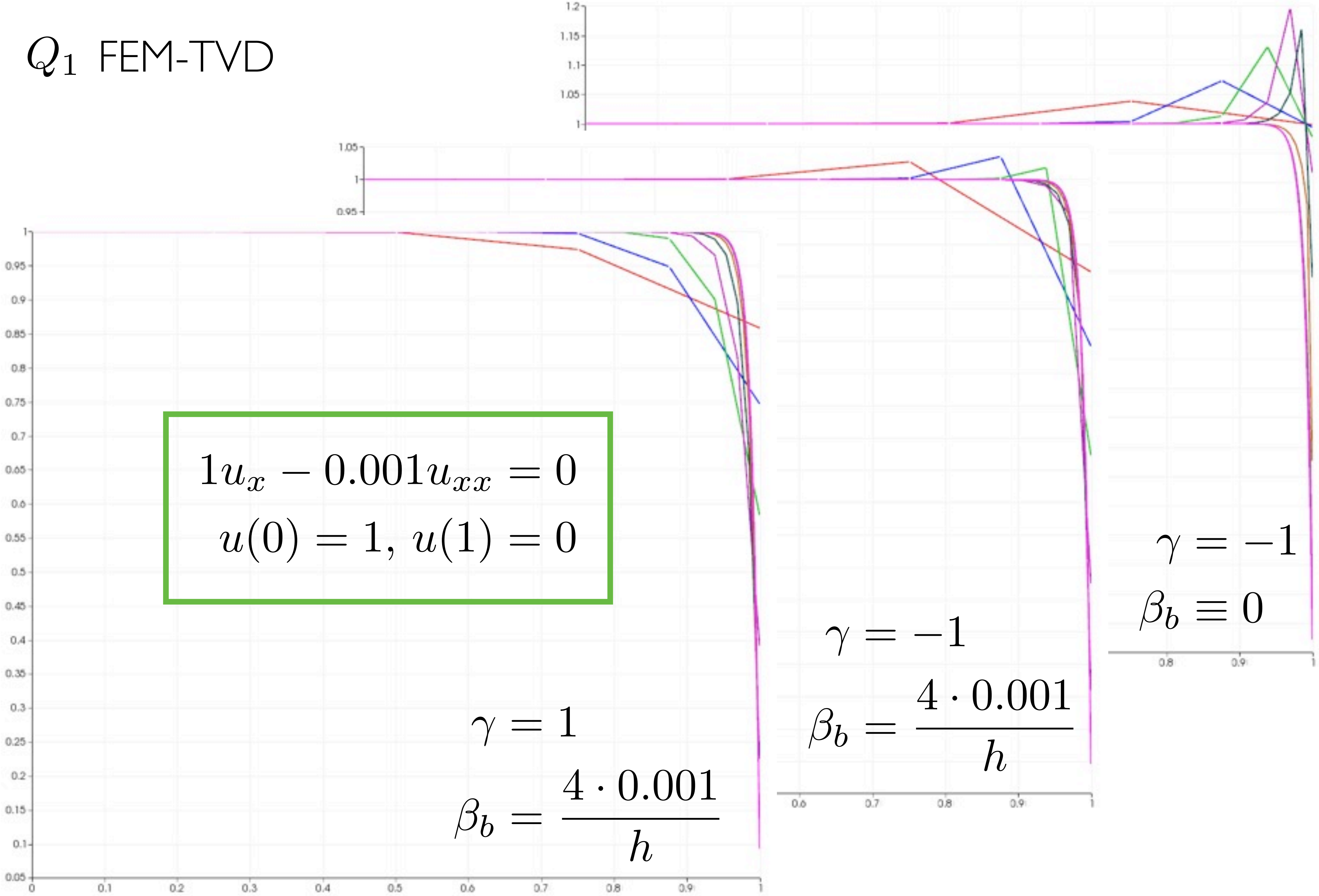
Q_1^{rot} FEM-TVD $\gamma = -1, \quad \beta_b \equiv 0$





1D convection-diffusion equation

Q_1 FEM-TVD



$$1u_x - 0.001u_{xx} = 0$$

$$u(0) = 1,\ u(1) = 0$$

$\gamma = 1$

$$\beta_b = \frac{4 \cdot 0.001}{h}$$

$\gamma = -1$

$$\beta_b = \frac{4 \cdot 0.001}{h}$$

$\gamma = -1$

$\beta_b \equiv 0$

Summary

- Do the algebraic design criteria apply to nonconforming elements?
  Yes, for the integral mean value based variant of nonconforming rotated bilinear finite elements.
- Is the accuracy of solutions comparable to P_1/Q_1 approximations?
  Yes, accuracy and numerical dissipation are comparable.
- How to implement essential boundary conditions?
  Apply consistent, adjoint-consistent Nitsche-type method.
- Is there any benefit from using nonconforming elements?
  Regular sparsity structure beneficial for parallel HPC.

Outlook

- Extend AFC schemes to other nonconforming finite elements
  - NC-Quad (Z. Cai, J. Douglas, Jr., X. Ye)
  - Composite Crouzeix-Raviart (F. Schieweck)
- Generalize consistent, adjoint-consistent approach towards the implementation of Dirichlet boundary conditions to periodic ones
- Improve (parallel) efficiency by exploring the regular sparsity structure
  - use variant of ELLPACK matrix storage format
  - reduce communication costs due to weaker coupling

Acknowledgment

AFC schemes

- D. Kuzmin (University of Erlangen-Nuremberg)

Featflow2

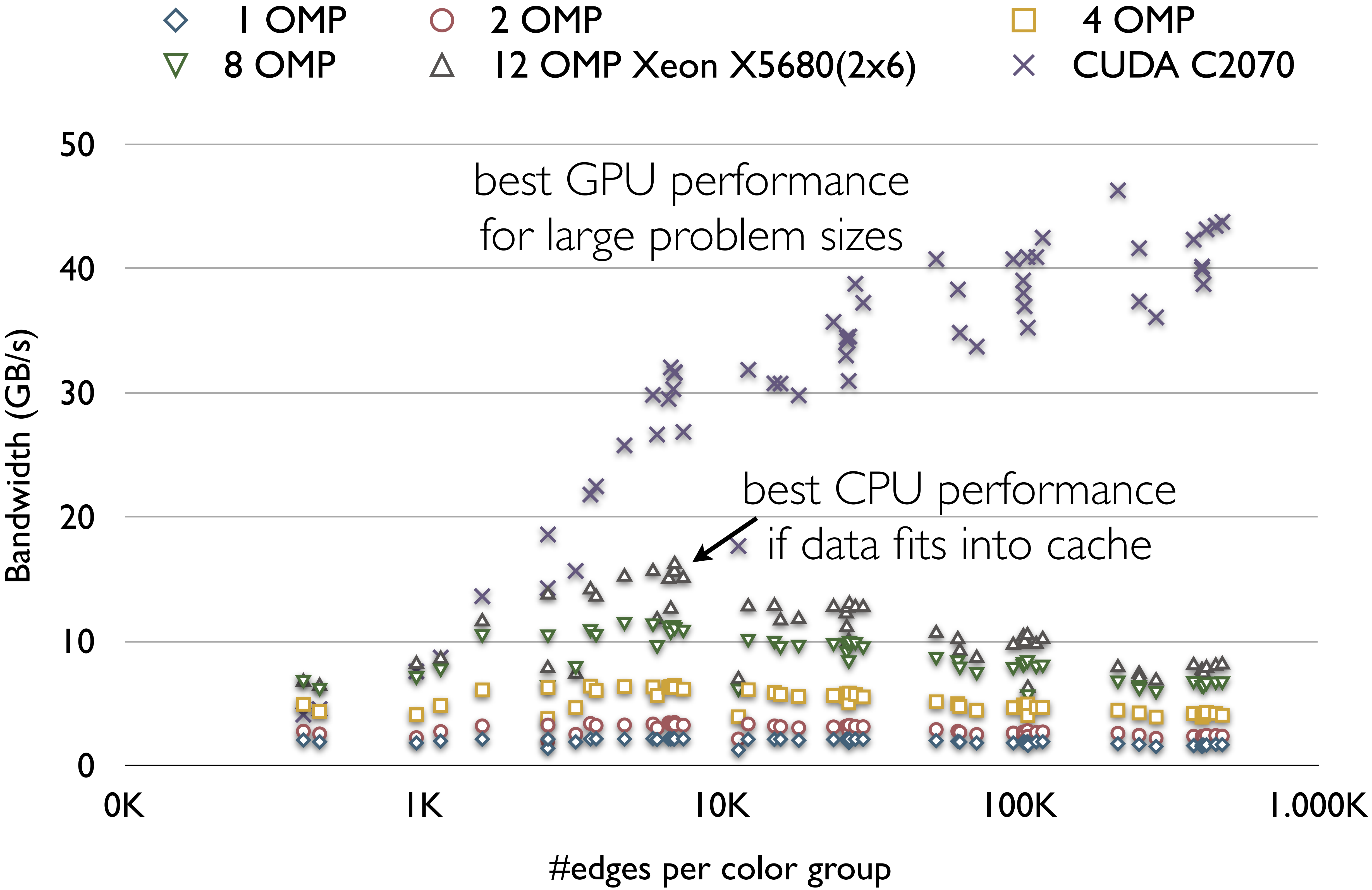
- M. Köster, P. Zajac (TU Dortmund)

Source code freely available at:

http://www.featflow.de/en/software/featflow2.html

Edge-based solvers for the compressible Euler equations on multicores and GPUs

Example: *edge-based flux-assembly with Q_1 FE*

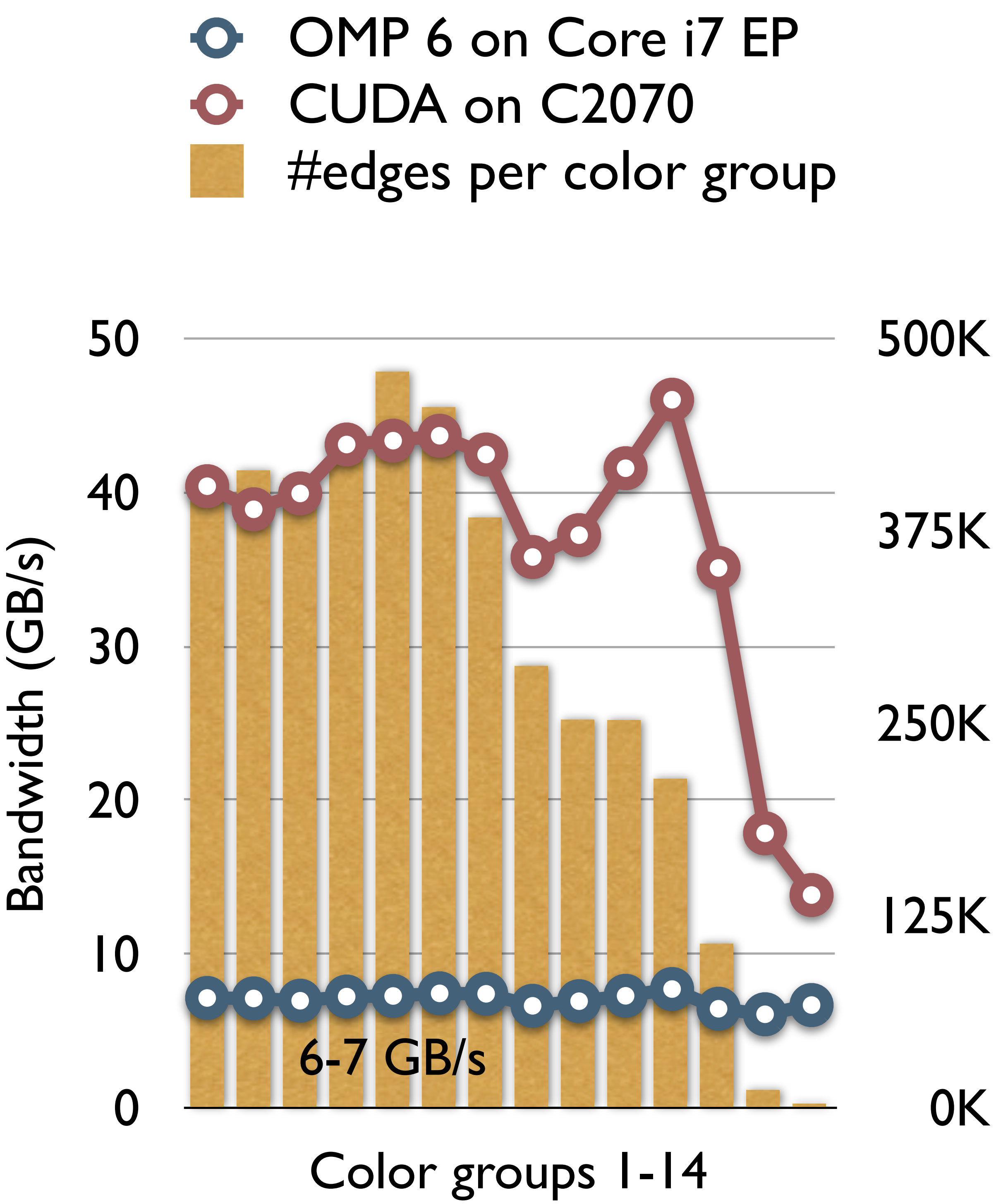


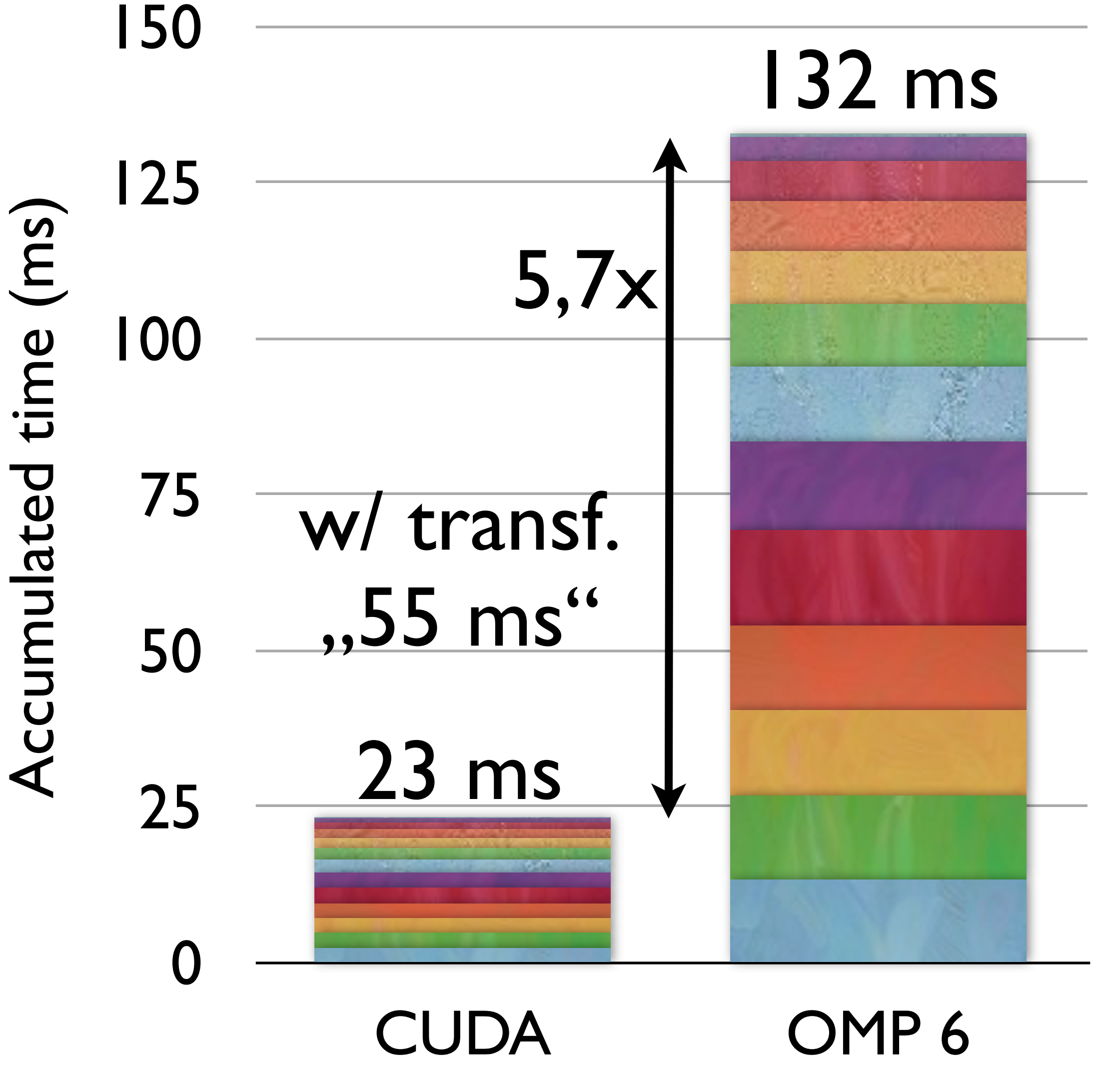
best GPU performance for large problem sizes

best CPU performance if data fits into cache

Example: *edge-based flux assembly with Q_1 FE*

$$F_i = \sum_{k=1}^{N_{\text{colors}}} \sum_{ij \in \text{CG}_k} \sigma_{ij}(U_j - U_i)$$





Example: *edge-based flux assembly with Q_1^{rot} FE*