# A Brief Tour of Computational Mathematics

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# Outline

- Computation and Science/Engineering
- Mathematical Models
- Computational Simulation
- Data Analysis
- Barriers to Efficiency
- Current Research

# What is Computational Math?

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- Need algorithms to perform more complicated math - differentiation, integration, root finding, etc.
- Research in Computational Math is focused on developing and improving these algorithms

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# Grand Challenges

- Grand Challenges are “fundamental problems in science and engineering, with potentially broad social, political, and scientific impact, that could be advanced by applying high performance computing resources.”
- Much of the effort in Computational Science is directed at these grand challenges, such as
  - electronic structure of materials
  - genome sequencing and structural biology
  - global climate modeling
  - pollution and dispersion

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- Common mathematical technologies are
  - MRI, ultrasound and CAT scan imaging
  - mp3 sound files
  - gif and jpeg image files
  - Nanotechnology

# Mathematical Modeling

- In order to use computers in science or engineering, we must be able to describe a problem in terms a computer can understand
- Typically, this is done by posing the problem as a mathematical one
- Mathematical models can be either continuous or discrete
- If the model is continuous, it must also be discretized before using a computer

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- To express these laws mathematically we can use either differential or integral equations

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  - Curls ($\nabla\times$) tell about rotations and circulations
  - Divergences ($\nabla\cdot$) tell about loss or gain of matter

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- To *discretize* a differential equation, we consider points of distance $h$ apart instead

# Finite Differences

- To discretize a differential equation, need to approximate derivatives
- Taylor Series give us a way:

$$u(x+h) = u(x) + hu'(x) + \frac{h^2}{2}u''(x) + \frac{h^3}{3}u'''(x) + O(h^4)$$
$$u(x-h) = u(x) - hu'(x) + \frac{h^2}{2}u''(x) - \frac{h^3}{3}u'''(x) + O(h^4)$$

# Finite Differences

- So

$$u'(x) = \frac{u(x+h) - u(x)}{h} + O(h)$$
$$= \frac{u(x) - u(x-h)}{h} + O(h)$$
$$u''(x) = \frac{u(x-h) - 2u(x) + u(x+h)}{h^2} + O(h^2)$$

- In a similar way, we can approximate higher order derivatives
- Also can do partial derivatives

# Finite Elements

- Redefine what it means for a function to solve the differential equation $Lu = f$:

$$Lu \cdot v = f \cdot v$$

$$\int_\Omega Lu \cdot v dx = \int_\Omega f \cdot v dx$$

- Now we can integrate by parts to come up with an equivalent statement of the PDE: Find $u$ such that for all $v$,

$$\int_\Omega L_1 u \cdot L_2 v dx = \int_\Omega f \cdot v dx$$

# Finite Elements

- Now ask that $u$ and $v$ belong to a finite-dimensional subspace
- Picking a basis for this space, we can express both $u$ and $v$ as linear combinations of the basis vectors.
- Then, problem becomes finding $u = \sum_{i=0}^{n} c_i \phi_i(x)$ such that for all $\phi_j(x)$,

$$\int_\Omega L_1 u \cdot L_2 \phi_j dx = \int_\Omega f \cdot \phi_j dx$$

- Allows theory for differential equations to be used in linear systems (e.g. existence and uniqueness)

# Computational Simulation

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- If an experimental apparatus is impossible to create (because of scale, cost, etc), computational simulation of a valid model can give information about the experiment considered

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  - Cannot easily image full flow
  - Cannot easily construct an equivalent apparatus

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- Want to predict behavior of systems that cannot be directly observed or tested

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- Must model complex geometries required by miniaturization

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- Data storage can be greatly reduced through efficient data compression

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- Mathematical models of behavior of waves in solids describes forward problem: Given a particular composition, how long would waves take to travel from a source to a receiver
- Inverse problem of determining composition from travel times is much more difficult, but also done mathematically

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- Information in medical situations often has interpretations related to frequencies from which we seek to recover spatial information

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- These compression schemes are *lossy* - Information is lost, but it is below the threshold of human observation

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- Many simulations require solution of large linear systems
- Many data processing applications require analysis of large quantities of data
- We’re interested in developing algorithms which are fast, efficient, and as accurate as necessary

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- We say an algorithm is *scalable* or *fast* if its runtime is proportional to the number of unknowns, $n$, or is bounded by $cn \log n$
- This says that if, for example, we double the number of unknowns in a problem, we at most double the total computation time.

# Efficiency

- The problems we consider are so large that optimal efficiency is necessary to have any hope of success
- Efficiency can be measured both in terms of time and storage
- Often need to trade-off one for the other
- Particular trade-off is determined by particular system requirements

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- When data is collected from an experiment, it has a certain level of noise
- There is no point in solving the problem to a finer accuracy than this, as you're just resolving the noise
- In practice, solve all problems to the level of measurement error or to the level of discretization error

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- The specialized hardware and software designed for these applications must be such that results are nearly instantaneous
- This requires fast algorithms specialized to a specific task - these are often the most efficient algorithms

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  - Truncation
  - Algorithmic improvements
  - Use of Cache

# Research Efforts - Accuracy

- As data-collection efforts improve, the allowable amount of error in calculation decreases
- This is most important in imaging, particularly diagnostic (medical) imaging
- Modern algorithms are designed with tunable accuracy - if given highly-accurate data, they can give highly-accurate answers

# Research Efforts - Robustness

- It is relatively easy to design an algorithm which solves one instance of a problem quickly
- More difficult is to create a method which can solve many problems, but is still efficient
- Look to generalize methods which work on “simple” problems so that they work on more difficult ones
- Goal is often to create a black box solution technique

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- Generalize/Specialize as needed