Computational Science
An Engineering Perspective

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Outline

- **General Observations**
- **"Continuum Level or Macroscopic" Simulation**
- **"Atomistic Level" Simulation**
- **Curriculum Issues**

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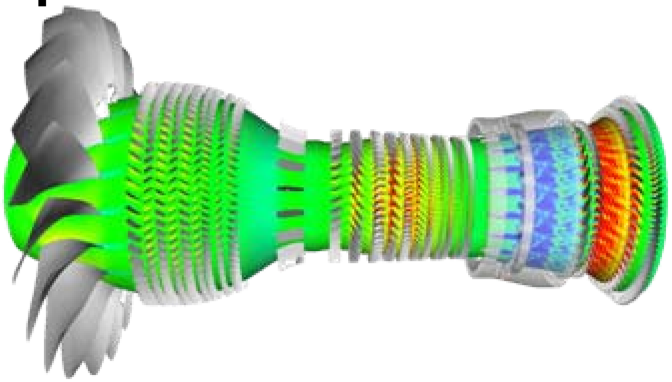
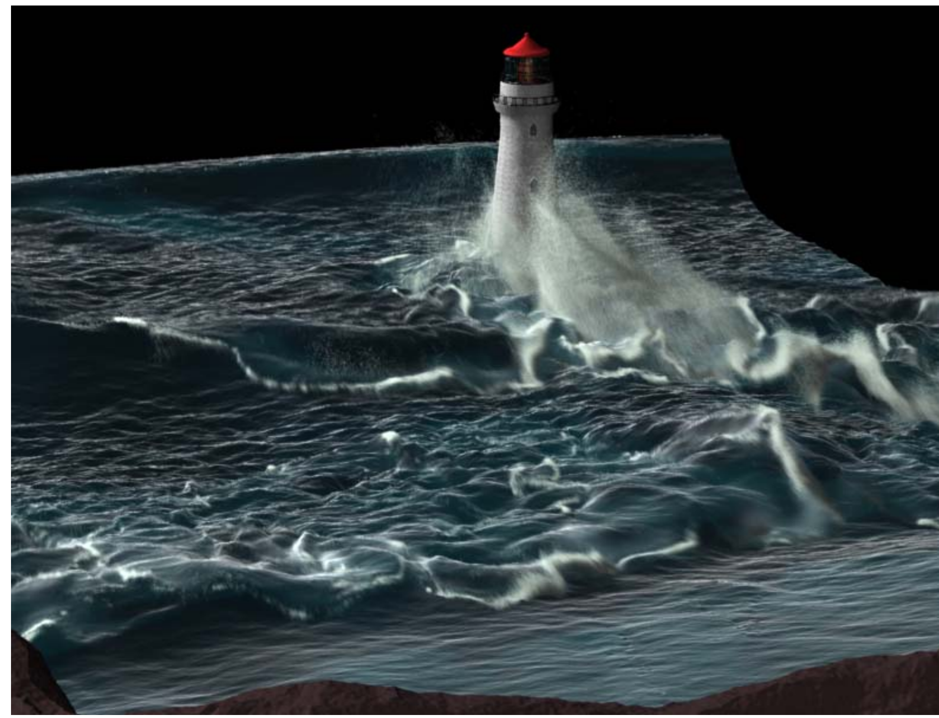
General Observations

- Computational science is now foundational to engineering. It is pervasive in academia and in industry.



QuickTime™ and a
BMP decompressor
are needed to see this picture.



Movies
(Ron Fedkiw)

Jet Engine
(Parviz Moin)

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General Observations

- Engineers take basic discoveries from science and apply them to solve problems that improve our lives.

- Every engineering student needs to develop expertise with computational tools.

- They are as useful as teaching aids as they are in research.
  - Students today are completely comfortable with computer simulations.
  - But they do not in general appreciate nor understand the scientific bases for these tools.
  - And they do not understand the limitations.

- In research (and in teaching), the most important issue is often access to adequate computational resources in a cost effective way.
  - Every faculty member wants his/her machine.
  - The hardware is only a fraction of the cost.
  - Power, cooling and system administration are often neglected.
  - New models for shared resources are needed.

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“Continuum Level or Macroscopic” Simulation

- Most engineering systems can be described by PDEs at the continuum level. Simulators based on solving PDEs are pervasive in engineering.
- Research issues here seem to be modeling more complex systems (planetary weather prediction etc), with more powerful machines, and incorporating more physics in the simulations (chemistry and combustion in jet engine simulations etc.)
- Teaching issues include setting up coherent courses to educate students about how these simulators work, what their limitations are, and providing supported computing systems for HW, in-class demonstrations etc.
- Most engineering research groups in universities are quite familiar with these tools, at least in their research domain.
- Increasingly experimentalists use these tools and there are

“Atomistic Level” Simulation

- Much less commonly used in engineering applications, probably because engineers “build things” that are generally well described by continuum approaches.
- But we are reaching the time when this will change.
    - Nanoscale semiconductor devices, surface catalysis, energy conversion pathways, protein folding . . . .
- Simulation capability generally limited by machine capability.
- Simulation results have not reached the point where engineers believe and trust them.
- Many engineering schools have few faculty who are knowledgeable and comfortable with these methods.
- Issues with how to hire faculty and successfully tenure them in engineering schools.
- Issues with how to integrate faculty who do this kind of work with experimentalists.

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Curriculum Issues

- Since computational engineering is foundational to essentially all engineering disciplines, we need to educate our students in this area
- Arguably the courses that need to be taught transcend specific departments (like basic math, physics, chemistry,bio courses).
- So how should engineering schools do this?
  - Convince math departments to teach these courses?
  - Form "Applied Math" departments in engineering school?
  - Some other approach?

Stanford's ICME in the School of Engineering

The Institute for Computational and Mathematical Engineering (iCME) has its own M.S. and Ph.D. programs. Both programs have a strong foundation in mathematics, but are interdisciplinary and students are give a wide choice of disciplines to pursue both within the School of Engineering and elsewhere in the University. The strength of the program lies within both its core faculty and courses coupled with the opportunities at Stanford to study classical areas of the physical sciences and the new emerging areas of business, biology, informatic and medicine.

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Curriculum Issues

ICME:

- **Does not appoint faculty, but does have a faculty director chosen by the Dean of Engineering**
- **Funded by the school of engineering (≈ $500K per year)**
- **Admits MS and PhD students and grants degrees**
- **Organizes school-wide UG and graduate curricula**
- **Teaching is done by faculty from a variety of departments**
- **Organizes workshops, seminars and school-wide research proposals (recent Army center good example).**
- **Research mission is to develop new numerical methods, algorithms, and computer codes for many disciplines**

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ICME Courses

Service Undergraduate Courses

CME 100	Vector Calculus for Engineers
CME 102	Ordinary Differential Equations for Engineers
CME 104	Linear Algebra and Partial Differential Equations for Engineers
CME 106	Introduction to Probability and Statistics for Engineers
CME 108	Introduction to Scientific Computing
CME 110	Matrix Computations with Applications to Data Mining and IT

Service Graduate Courses

CME 200	Linear Algebra with Application to Engineering Computations
CME 204	Partial Differential Equations in Engineering
CME 206	Introduction to Numerical Methods for Engineering
CME 208	Mathematical Programming and Combinatorial Optimizatio
CME 211	Computer Programming in C++ for Earth Scientists and Engineers
CME 212	Introduction to Large-Scale Computing in Engineering

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ICME Courses

Graduate Core Courses

CME 200 Linear Algebra with Application to Engineering Computation
CME 204 Partial Differential Equations in Engineering
CME 206 Introduction to Numerical Methods for Engineering

CME 208 Mathematical Programming and Combinatorial Optimization
CME 211 Computer Programming in C++ for Earth Scientists and Engineers
CME 212 Introduction to Large-Scale Computing in Engineering

Graduate Specialty Courses

CME 303 Partial Differential Equations of Applied Mathematic
CME 324 Advanced Methods in Matrix Computation: Iterative Methods
CME 326 Numerical Methods for Initial Boundary Value Problems
CME 330 Applied Mathematics in the Chemical and Biological Sciences
CME 332 Computational Methods for Scientific Reasoning and Discovery
CME 334 Advanced Methods in Numerical Optimization
CME 336 Linear and Conic Optimization with Applications
CME 337 Information Networks
CME 338 Large-Scale Numerical Optimization
CME 340 Computational Methods in Data Mining
CME 342 Parallel Methods in Numerical Analysis
CME 346A Introduction to Molecular Simulations
CME 352 Molecular Algorithms
CME 380 Constructing Scientific Simulation Codes

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http://icme.stanford.edu/

Conclusions

- **Computational engineering really has become the third foundation of engineering (along with theory and experiment).**

- **All engineering disciplines use these tools and all engineering students need to be exposed to them as part of their education.**

- **Biggest issues for engineers are:**
  - **How to integrate these tools in engineering education.**
  - **How to begin to incorporate atomistic simulation methods and tools in teaching and research.**

- **It's important in engineering that computational engineering not be regarded as a "separate" branch of engineering but rather as an equal partner to experiment and theory. Engineers build things and simulations by themselves build nothing.**

- **Infrastructure issues are key - how do we support research computing facilities and teaching facilities?**

Question 1

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Question 2

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Question 3

Question 4