Preparing the Future Workforce for Careers in Science and Engineering

Steven I. Gordon
sgordon@osc.edu

XSEDE

Extreme Science and Engineering Discovery Environment

NSF

Preparing Students

- Need for a workforce which understands both modeling and simulation principles and applications of models and data analysis at large scale
  - Requirements for high fidelity models of complex systems
  - Managing and understand large datasets – data science

Presentation slides

- http://hpcuniversity.org/trainingMaterials/201

Making Progress in Science

- A number of studies document the need for computational scientists
  - …" computer modeling and simulation are the key elements for achieving progress in engineering and science." NSF Blue Ribbon Panel on Simulation-Based Engineering Science
  - "Unfortunately, the translation of systems biology into a broader approach is complicated by the innumeracy of many biologists" Cassman et al. Barriers to Progress in Systems Biology, Nature Vol. 438|22/29 December 2005
  - Nearly 100% of the respondents indicated that HPC tools are indispensable, stating that they would not exist as a viable business without them or that they simply could not compete effectively. IDC Study for Council on Competitiveness of Chief Technology Officers of 33 Major Industrial Firms

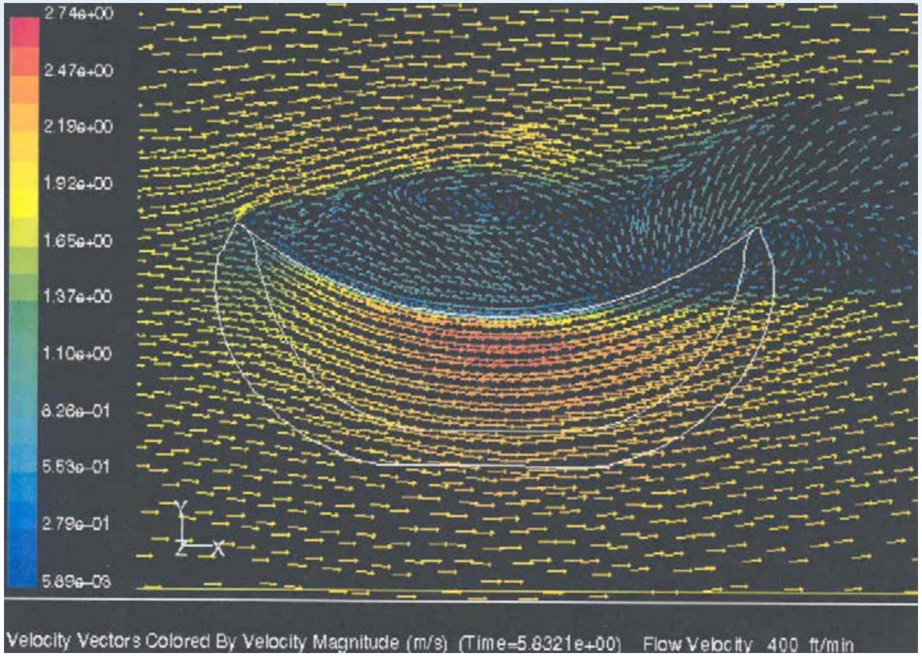
Crucial Tools for Manufacturing

- At Ford, HPC …allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.
- The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over a several-year period.

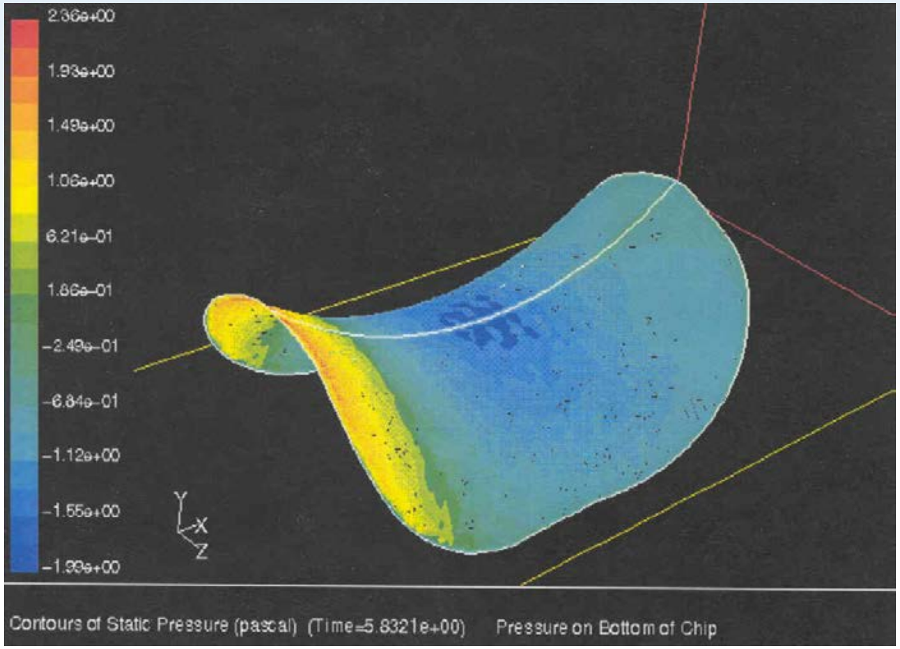
Ford EcoBoost Technology

Durable coffee package for P&G

Will Pringles Fly?

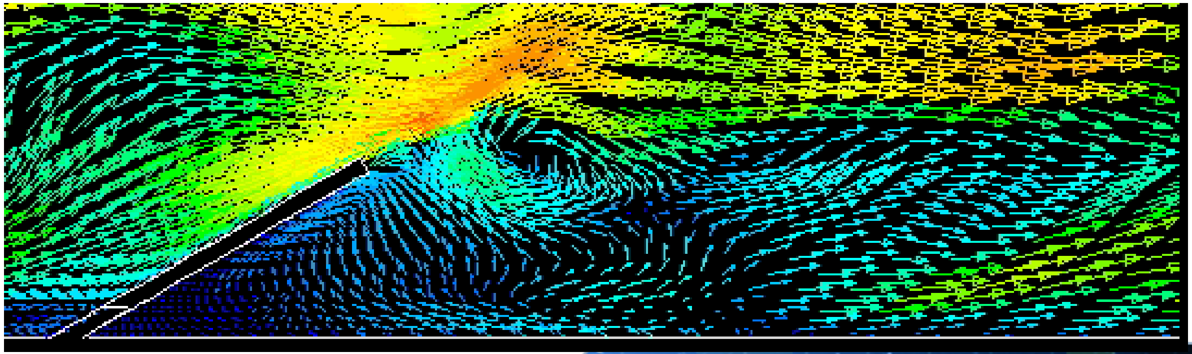


Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=5.8321e+00) Flow Velocity 400 ft/min

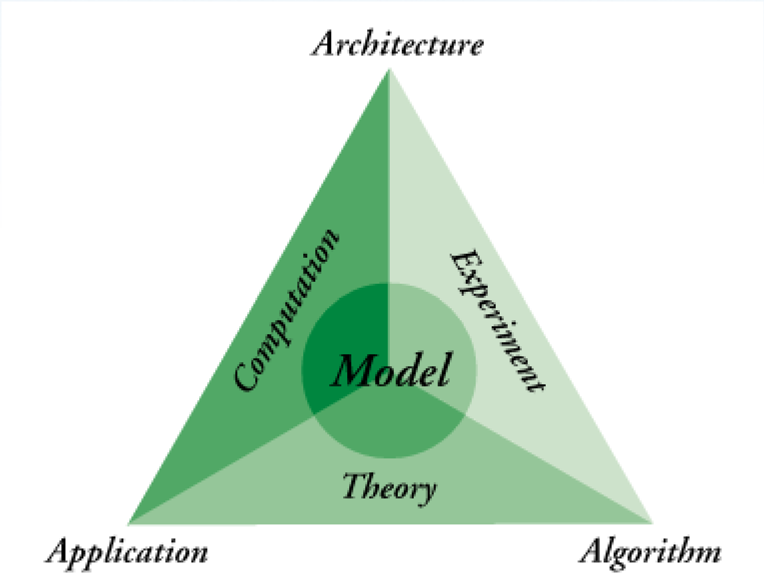


Contours of Static Pressure (pascal) (Time=5.8321e+00) Pressure on Bottom of Chip

High Speed Conveying
Create Vortices
Shedding…
…'Rocking Chips'
NOT GOOD!



Computation is Central to How Science is Done



- Computation lets us explore phenomena that are too big or complex to experiment, too small, or changes too fast or too slowly.
- Computation allows us to explore more options more quickly.

Challenges to Changing How and What We Teach

- We tend to teach in the way we were taught
- Computational science is interdisciplinary
  - Faculty workloads fixed on disciplinary responsibilities
  - Coordination across departments is superficial
  - Expertise at universities is spotty
- Major time commitments are required to negotiate new programs and develop materials
- Curriculum requirements for related fields leave little room for new electives
- Change is hard

Pathways to Reform

- Integrate computational examples into basic science and math courses
- Create general education courses that introduce simulation and modeling concepts and applications
- Combine those efforts to create formal concentrations, minors, or certificates in computational science
- XSEDE is working with institutions to assist with those activities

What Do Students Need to Know?

- Considerable discussion across many disciplines
- Difficulty working from general conceptual ideas to specific skills and knowledge
- Several efforts focused on a competency based model to arrive at consensus of the essential knowledge base
- Competencies reviewed by both academic and non-academic experts
- See http://hpcuniversity.org/educators/competencies/

Ohio Minor Program Example

- Undergraduate minor program
  - 6-8 courses
  - Varies based on major
- Faculty defined competencies for all students
- Reviewed by business advisory committee
- Program started in Autumn 2007
- Agreements to share students at distance, instructional modules, revenues, and teaching responsibilities

Competencies for Undergraduate Minor
Simulation and Modeling
Programming and Algorithms
Differential Equations and Discrete Dynamical Systems
Numerical Methods
Optimization
Parallel Programming
Scientific Visualization
One discipline specific course
Capstone Research/Internship Experience
Discipline Oriented Courses

Example Competencies Simulation and Modeling

- Explain the role of modeling in science and engineering
- Analyze modeling and simulation in computational science
- Create a conceptual model
- Examine various mathematical representations of functions
- Analyze issues in accuracy and precision
- Understand discrete and difference-based computer models
- Demonstrate computational programming utilizing a higher level language or modeling tool (e.g. Maple, MATLAB, Mathematica, Python, other)
- Assess computational models
- Build event-based models
- Complete a team-based, real-world model project
- Demonstrate technical communication skills

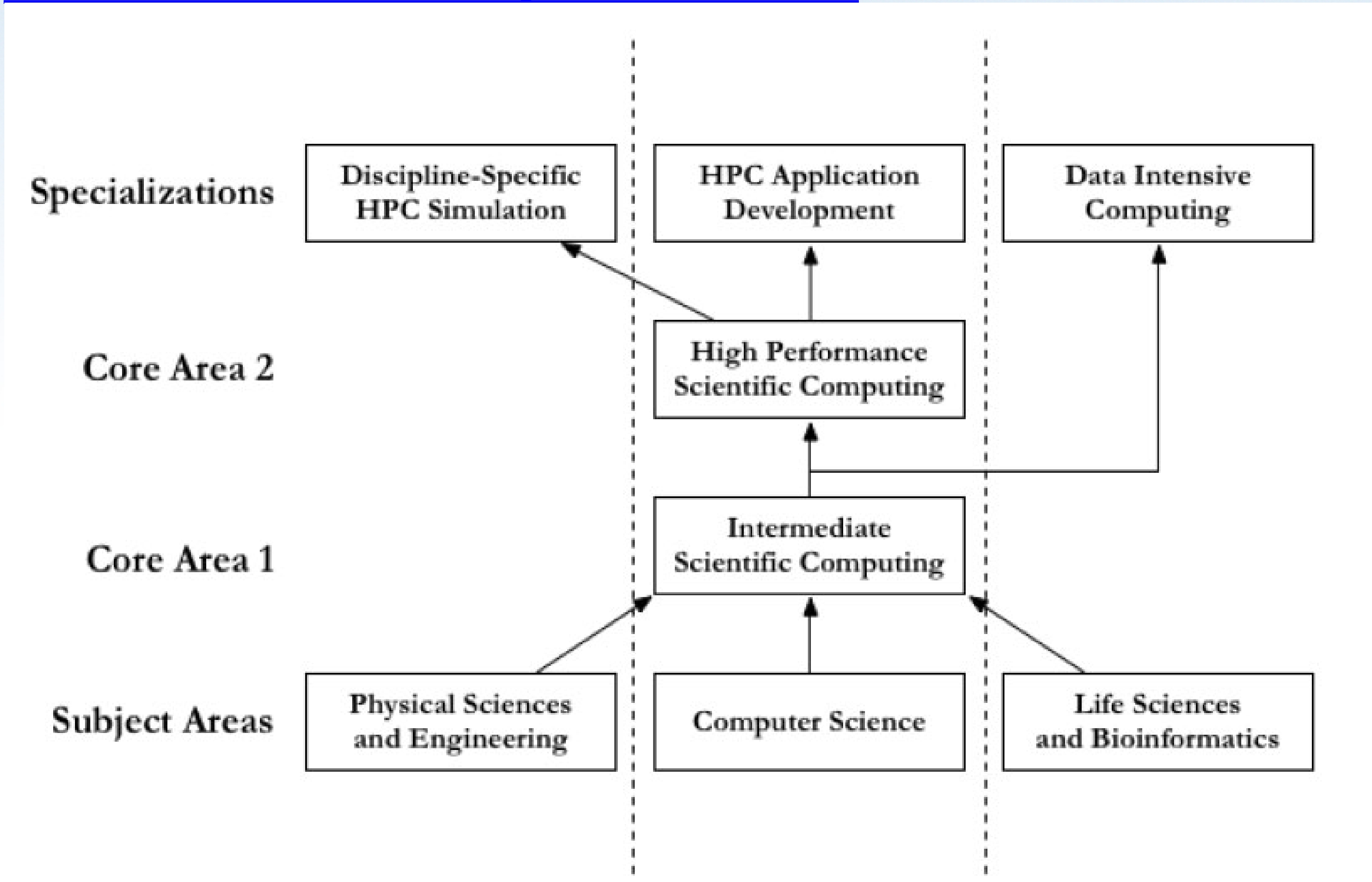
Detailed Descriptors

Explain the role of modeling in science and engineering
Descriptors:
Discuss the importance of modeling to science and engineering
Discuss the history and need for modeling
Discuss the cost effectiveness of modeling
Discuss the time-effect of modeling (e.g. the ability to predict the weather)
Define the terms associated with modeling to science and engineering
List questions that would check/validate model results
Describe future trends and issues in science and engineering
Identify specific industry related examples of modeling in engineering (e.g., Battelle; P&G, material science, manufacturing, bioscience, etc.)
Discuss application across various industries (e.g., economics, health, etc.)

Flexibility in Implementation

- Adapt existing courses by adding computationally oriented modules
- Discipline oriented courses dependent on existing faculty expertise and interests
- Different subsets of required and optional competencies tied to major, required math, and example projects

Graduate Competencies



Graduate Program Development

- Assumes or provides some of the background of an undergraduate
- Focus more on research skills across several disciplines
  - Dependent on expertise of current faculty

Computational Science Throughout the Curriculum

- Should be preparing all students to understand computation
  - "Computational thinking"
  - Building analytical skills
  - Basic understanding of modeling principles and computing skills (beyond spreadsheets)
  - Linking problem solving, mathematics, and computational methods
- XSEDE education program works with campuses to make this happen

What is XSEDE?

- Comprehensive program of digital services sponsored by the National Science Foundation
- Unprecedented integration of diverse digital resources
  - innovative, open architecture making possible the continuous addition of new technology capabilities and services
- Focus on building a workforce capable of using these services and techniques

XSEDE Education Program Goals

- Prepare the current and next generation of researchers, educators and practitioners.
- Create a significantly larger and more diverse workforce in computational sciences
- Inculcate the use of digital services as part of their routine practice for advancing discovery.

Assistance with Program Development

- Campus visits
- Model programs and competencies to shorten the time to implementation
- Assistance with program proposals

NSF

XSEDE

Developing Faculty Expertise

- Faculty professional development workshops
  - Two to six day workshops on a variety of topics
    - Computational thinking
    - Computational science education in science and engineering domains
  - Focus on local/regional audiences to reduce travel costs
  - Subsidies for faculty to travel to workshops at other sites

Special Workshops for Faculty and Students

- Development of synchronous and asynchronous education and training sessions
  - Multi-site broadcasts of workshops
  - Online training and education modules
  - Experimenting with full courses that can be widely shared for credit and non-credit inclusion in curricula (e.g. https://cvw.cac.cornell.edu/apc/default)

Blue Waters Online Courses

- Similar in format but focused on more advanced topics
- Topic for Spring 2016
  - Designing and Building Applications for Extreme Scale Systems
  - Taught by William Gropp, University of Illinois
- Possible second course
- Watch for formal announcements soon

Other XSEDE Online Materials

- https://portal.xsede.org/web/xup/online-training
- Materials on a wide range of technical topics
- Free self-paced tutorials
- Could be embedded in a class or used to help students advance their skills

XSEDE Badging Program

- Beginning to add assessments to both live and online training events
- Assessments used to earn a badge on that topic
- Should be added to a number of materials in the near future
- Provides a way to measure expertise for both academic and non-academic learners

Repository of Shared Materials

- Developing a repository of computational science education materials
  - Reviewed by professional staff and faculty
  - Indexed by subject and a detailed competency-based ontology
  - Goal: trusted, comprehensive source of information for computational science educators
  - http://hpcuniversity.org/resources/search/

Student Opportunities

- Blue Waters undergraduate internships
  - Year-long program for undergraduates
  - Two-week intensive training on parallel computing techniques
  - Work with a mentor on a project for the rest of the year
  - Need both applicants and mentors with projects

Some Other Opportunities

- Journal of Computational Science Education
  - www.jocse.org
  - Peer reviewed articles on computational science education experiences
- Become a reviewer for JOCSE or reviewer and contributor to the online repository

Opportunities for Students and Faculty

- Internships
  - Within XSEDE
  - List of opportunities on HPCU site
- XSEDE Scholars Program
- Faculty workshops

New Chapter of the ACM

- SIGHPC Education Chapter
  - http://sighpceducation.acm.org/
  - Inexpensive to join
  - Webinars on education opportunities and programs
  - Reviewing training and education materials to create a list of high quality materials

Question and Discussion