Preparing the Workforce for the Future of Science and Engineering

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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/218/

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

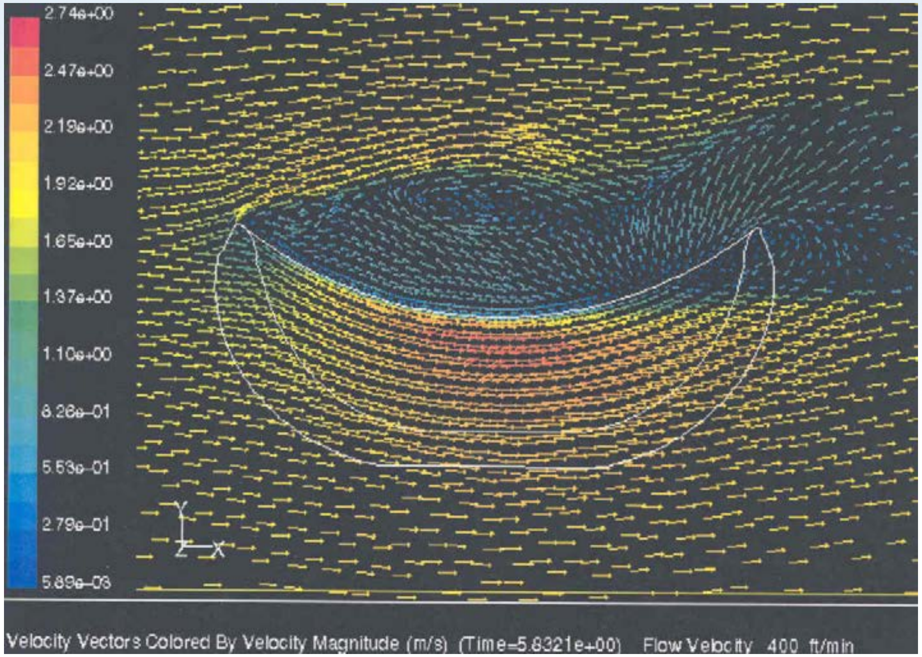
Crucial Tools for Manufacturing

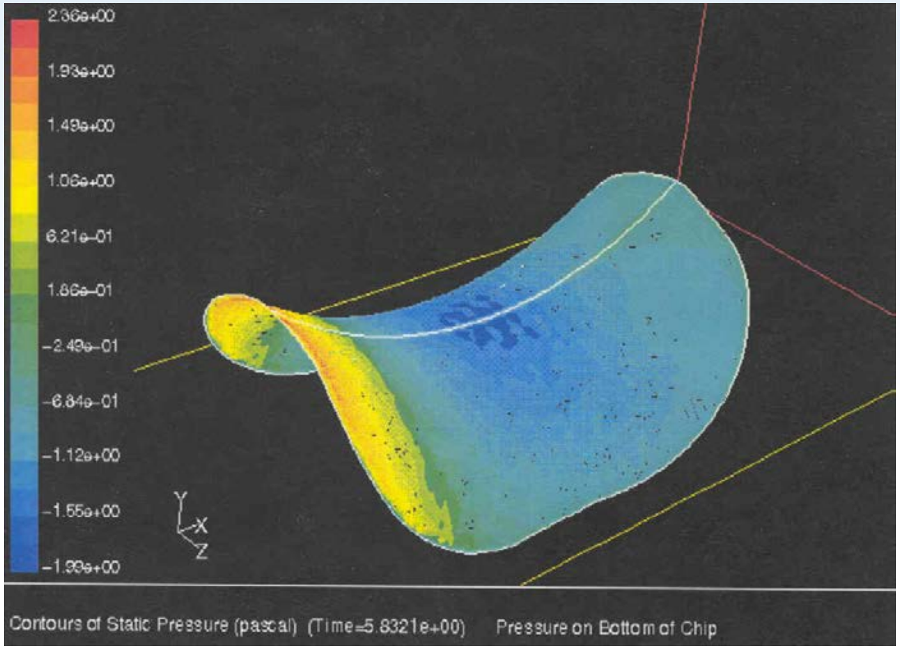
- At Ford, HPC …allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.
- The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over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

Ford EcoBoost Technology

Durable coffee package for P&G

Will Pringles Fly?





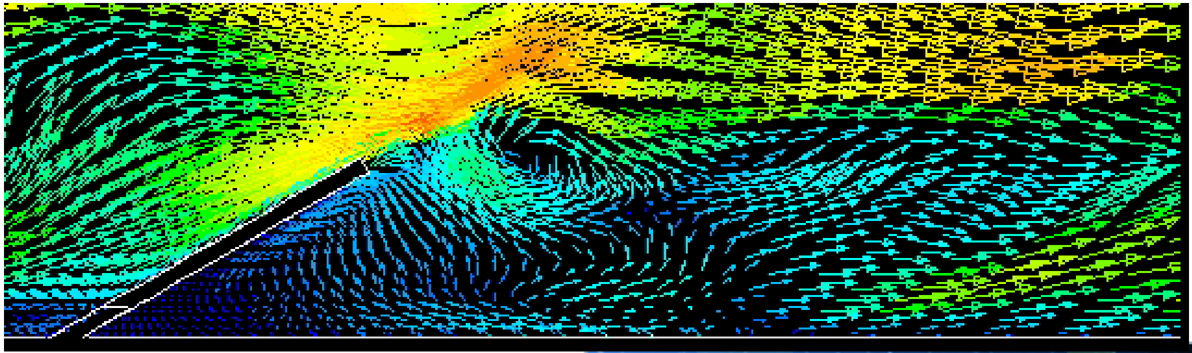
High Speed Conveying

Create Vortices

Shedding…

…'Rocking Chips'

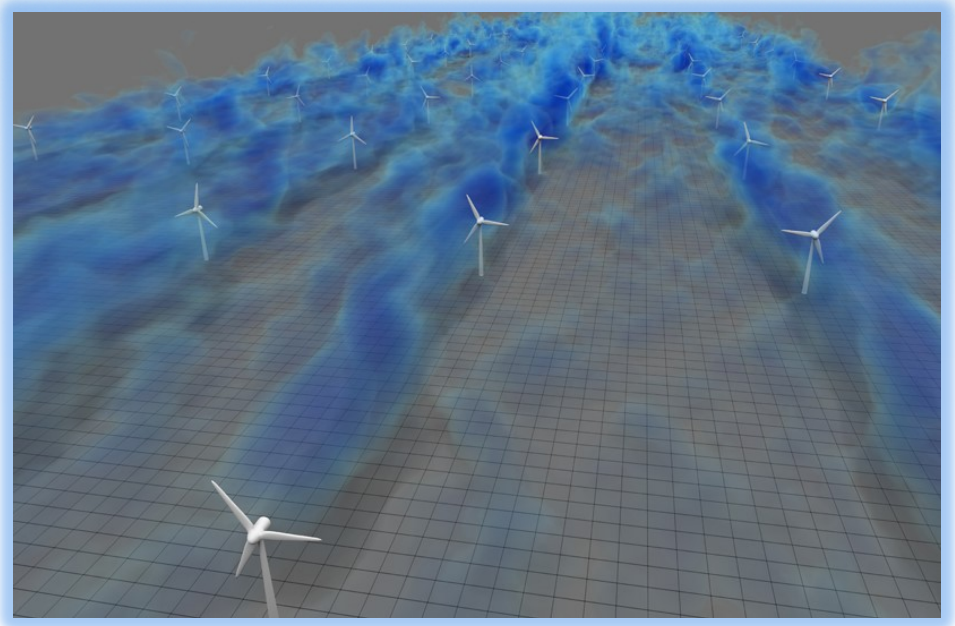
NOT GOOD!



XSEDE Supercomputer Simulations Used to Model Optimum Turbine Placement for Large Wind-Farms

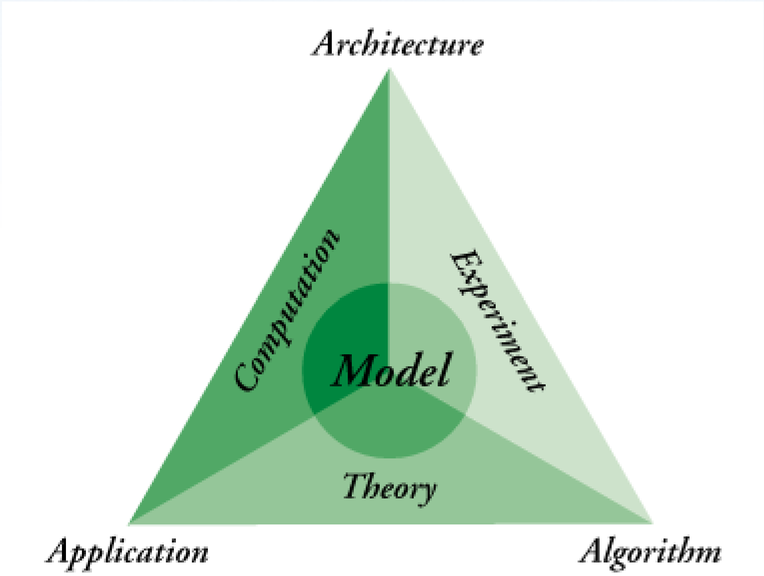
- Published in the *Journal of Renewable and Sustainable Energy*, this study challenges conventional wisdom that the highest power output results when turbines are arranged in a checkerboard pattern.
- Using SDSC's Trestles supercomputer, these simulations show the highest output results when the lateral offset of turbines is such that they are just outside each other's wakes.
- As wind energy becomes more important globally as a source for clean, renewable power, understanding the effect of spacing and relative positioning of turbines crucial for good wind-farm design.

XSEDE Supercomputer Simulations Used to Model Optimum Turbine Placement for Large Wind-Farms



Detailed computer simulations such as this one using SDSC's Trestles system allow researchers to study the flow in wind-farms in great detail. This image shows a visualization of the flow in a very large wind-farm. The blue regions indicate the low velocity wind-speed regions (wakes) formed behind the turbines. *Visualization by David Bock (NCSA) as part of XSEDE's Extended Collaborative Support Services.*

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.

Expertise Required

- Need skills in several areas to effectively use computation at these scales
  - Modeling and simulation
    - How to create a model and know whether it is “right”
  - Mathematics
    - Representing system behavior with the appropriate mathematical representation
  - Computer science
    - Technical skills in programming and data management
  - Domain knowledge
    - Expertise in the subject area being studied

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

Minor Program in Computational Science and Engineering

- Core courses
  - Simulation and Modeling
  - Numerical methods
  - Discipline specific course
  - One elective
  - Capstone research or internship experience

Minor in Computational Science and Engineering

<u>Prerequisites</u>

Programming and Algorithms (choose one of the following)

- CSE/ENGR 1221: Intro to Comp. Pgming in MATLAB (2 credit hours)
- CSE 1222: Intro to Computer Programming in C++ (3 credit hours)
- CSE 1223: Intro to Computer Programming in Java (3 credit hours)

<u>Core Courses</u>

Simulation and Modeling (choose at least 3 credit hours)

- BIOMEDE 5430: Finite element applications in BIOMEDE (3 credit hours)
- CBE 5790: Modeling and simulation (3 credit hours)
- ISE 4100: Stochastic Modeling and Simulation (4 credit hours)
- MECHENG 5139: Applied finite element method(3 credit hours)
- MATSCEN 2321: Modeling and simulation Lab I (3 credit hours)

Minor Program Example (continued)

Numerical Methods (choose at least 3 credit hours)

- AEROENG 3581: Numerical methods in Aerospace Engineering (3 credit hours)
- CIVILEN 2060: Numerical analysis methods for Civil/Env. Eng. Applns (3 cr hrs)
- CSE 5361: Numerical methods (3 credit hours)
- ECE 5510: Intro to computational electromagnetics (3 credit hours)
- MATH 3607: Beginning scientific computing (3 credit hours)
- MECHENG 2850: Intro to numerical methods (3 credit hours)

Minor Program Example (continued)

Discipline-Specific Computational Study (choose at least 3 credit hours)

- AEROENG 5615: Intro to computational aerodyn. (3 credit hours)
- CBE 5734: Molecular Informatics (3 credit hours)
- CHEM 5440: Computational chemistry (3 credit hours)
- CSE 2331: Foundations II: Data structures and alg. (3 credit hours)
- CSE 2431: Systems II: Intro to Operating Systems (3 credit hours)
- CSE 3241: Intro to database systems (3 credit hours)
- CSE 3341: Prin. of prog. langs. (3 credit hours)
- CSE 3421: Intro to computer architecture (3 credit hours)
- CSE 3461: Computer networking and internet technologies (3 credit hours)
- CSE 3521: Survey of AI I (3 credit hours)
- CSE 3541: Computer game and animation tech. (3 credit hours)
- ECE 5510: Intro to Computational Electromagnetics (3 credit hours)
- MATSCEN 6756: Computational Materials Modeling (3 credit hours)

Minor Program Example (continued)

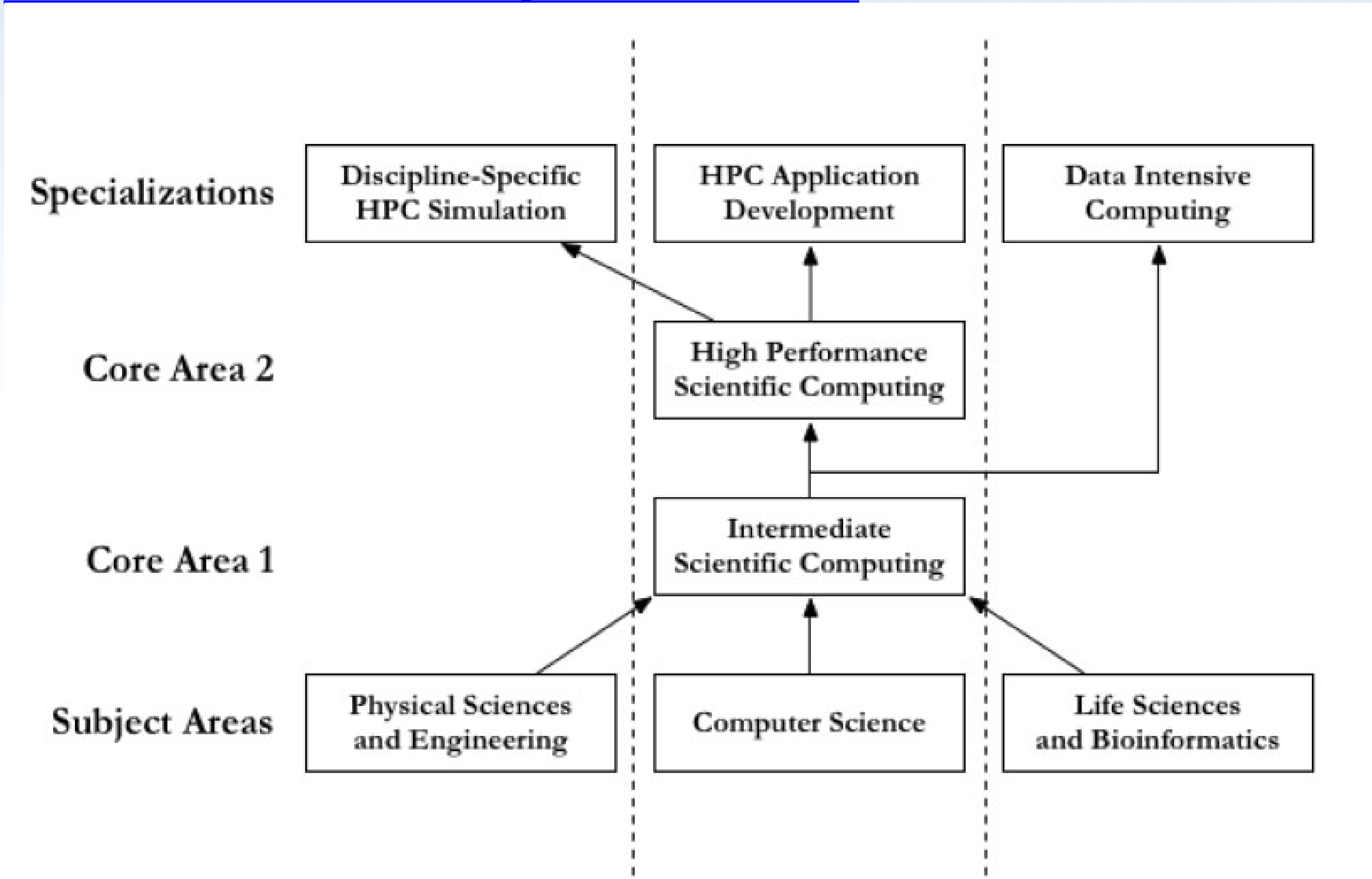
Electives (choose at least 3 credit hours)

- CIVILEN 3080: Econ. evaluation and optimization in Civ/Env. engr. (3 cr hrs)
- CSE 5441: Intro to parallel computing (3 cr hrs)
- CSE 5544: Intro to scientific visualization (3 cr hrs)
- ECE 5759: Optimization for static and dyn. systems (3 cr hrs)
- ISE 3200: Optimization for enterprise systems (3 cr hrs)
- ISE 3210: Optimization for system design (3 cr hrs)
- ISE 3990: Engineering optimization (3 cr hrs)
- ISE 5200: Linear optimization (3 cr hrs)
- MATSCEN 4181: Materials Selection (3 cr hrs)
- MATH 2255: Diff. equations and their applications (3 cr hrs)
- MATH 2415: Ordinary and partial diff. equations (3 cr hrs)

Discipline-specific capstone research/internship (at least 2 cr-hrs)

- Computationally oriented capstone course(s) or individual research

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 Training

- Live workshops webcast or hosted at multiple sites
- Online self-paced tutorials on a variety of technical topics
- New digital badges attached to workshops and related post-workshop assessments

Full Courses Taught Collaboratively

- Applications of Parallel Computers
  - https://cvw.cac.cornell.edu/apc/default)
- Blue Waters courses
  - Designing and Building Applications for Extreme Scale Systems
    - http://wgropp.cs.illinois.edu/courses/cs598-s15/index.htm
  - Next fall
    - Introduction to High Performance Computing
    - Algorithmic Techniques for Scalable Many-core Computing

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/

Other Student Opportunities

- Blue Waters undergraduate internships
  - Year-long program for undergraduates
- Blue Waters Graduate Fellowship
  - One year fellowship for PhD students
- Both have deadlines in February 2016.

New Chapter of the ACM

- SIGHPC Education Chapter
  - http://sighpceducation.acm.org/
  - Inexpensive to join - $10 professional, $5 students
  - Webinars on education opportunities and programs
  - Reviewing training and education materials to create a list of high quality materials

Access to XSEDE Resources

- Accounts to XSEDE User portal are free and provide access to training materials
- Science gateways providing access to specific applications
- Allocations to use computing resources
  - Trial accounts through your campus champion (Don McLaughlin and Nathan Gregg)
  - Start up allocations
  - Education allocations
  - Research allocations

More than Computational Resources

- Extended collaborative support service
  - Access to expertise to work with research groups on a variety of issues
    - Porting and optimization of codes to XSEDE resources
    - Data analytics
    - Visualization
    - Workflows
    - New science gateways

Summary

- Market for computational science skills is expected to grow rapidly
- Opportunity for careers across a wide range of science and engineering applications
- Multiple opportunities for students to gain the requisite skills through their academic programs and projects such as XSEDE and Blue Waters