Advancing the Education of our Workforce with XSEDE

Steven I. Gordon
sgordon@osc.edu

XSEDE
Extreme Science and Engineering
Discovery Environment

Slides are here

- http://hpcuniversity.org/trainingMaterials/222/

Opportunities and Challenges

- Workforce needs in computational science
- Changing how we teach
- Barriers to program implementation
- Competencies in computational science and data science
- Example Programs
- XSEDE Education Program services

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
  - Applications across a wide range of science, social science, and increasingly humanities

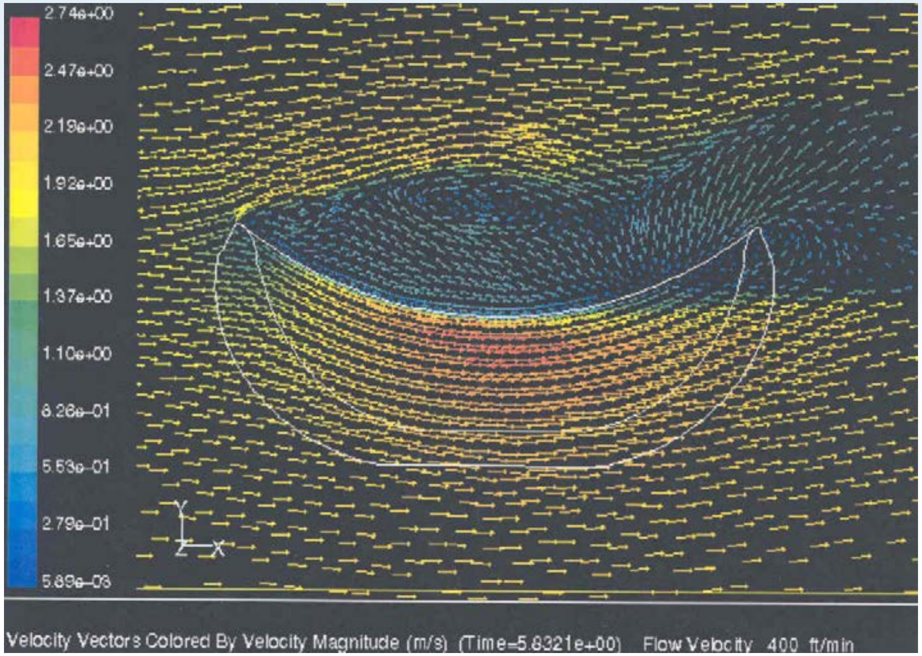
Crucial Tools for Manufacturing

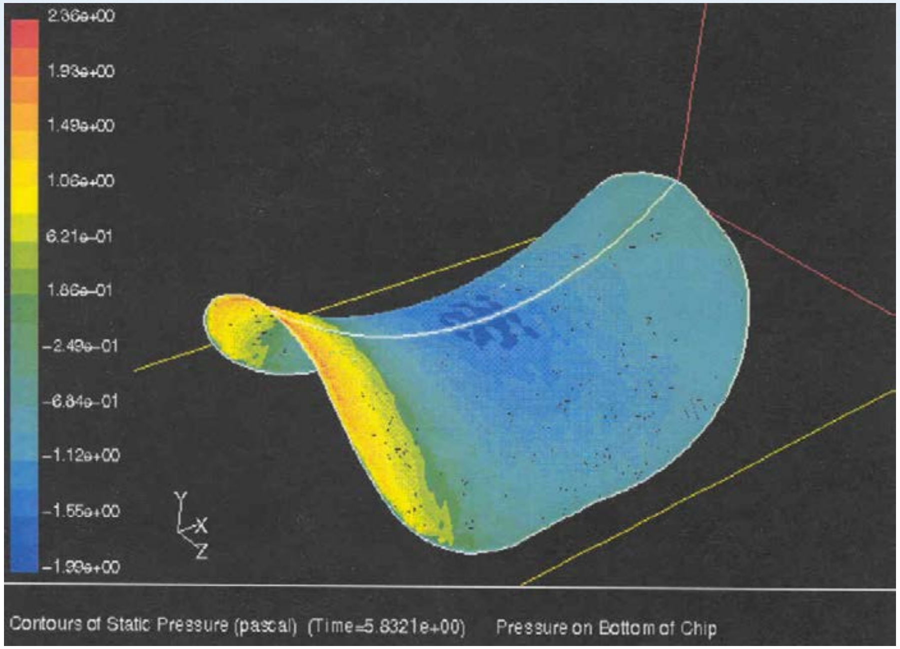
- At Ford, HPC …allows us to build an environment that continuously improves the product development process, speeds up time-to-market and lowers costs.
- The ongoing use of modeling and simulation resulted in new packaging and product design that propelled the brand to a leading market position over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

Ford EcoBoost Technology

Durable coffee package for P&G

Will Pringles Fly?





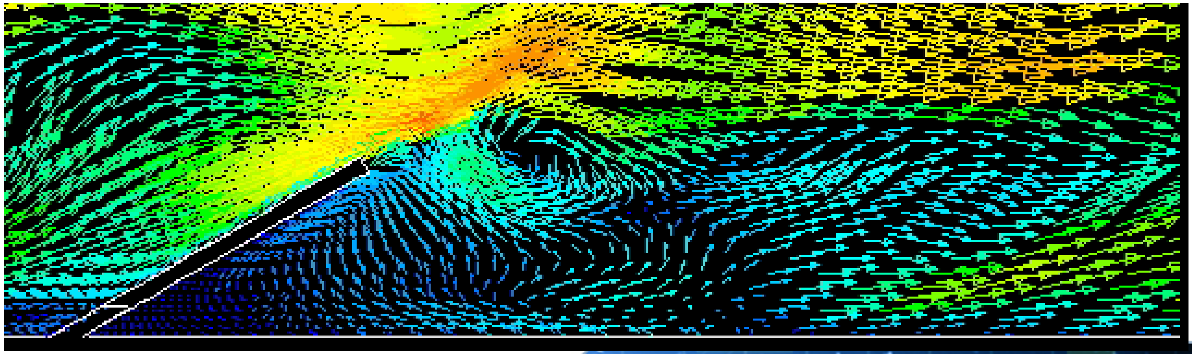
High Speed Conveying

Create Vortices

Shedding…

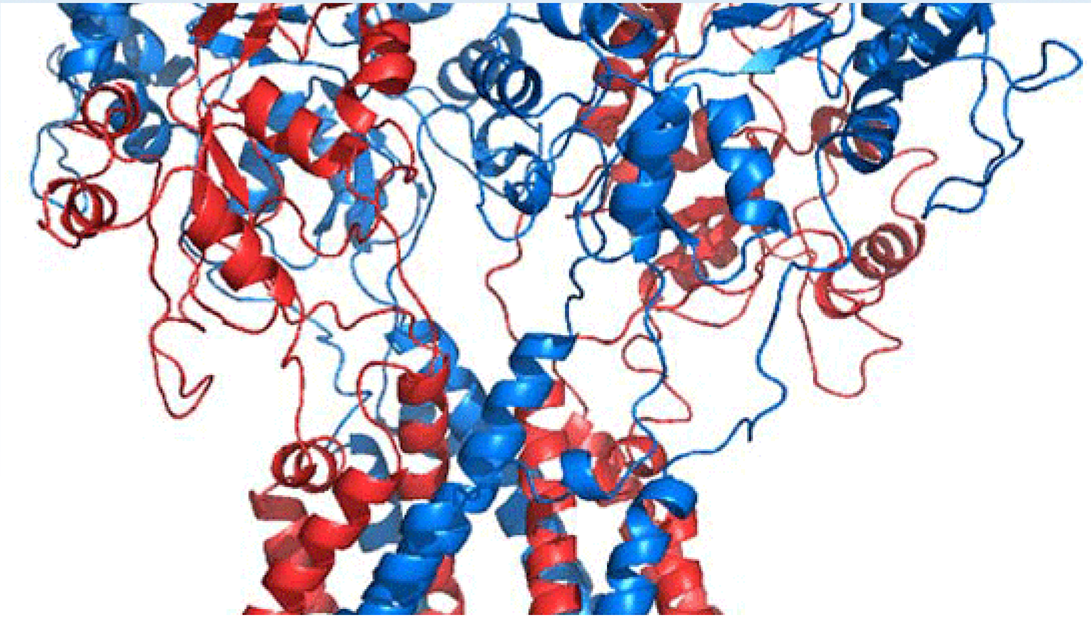
…'Rocking Chips'

NOT GOOD!



Brain Cell Linker Dependence Shown by XSEDE Supercomputer Simulations

- Neuroscientists at Stony Brook U. teamed with computational biophysicists at Florida State U. and found that the function of a key brain cell receptor depends on a short polypeptide segment, which they call a linker, to function.
  - Parkinson's disease, Alzheimer's disease, and a number of psychiatric disorders are associated with malfunctions of this brain receptor, called the NMDA (N-methyl-D-aspartate) receptor.
  - The researchers performed molecular dynamics simulations of the 300,000-atom NMDA receptor system on Stampede.
- Funded by the National Institutes of Health
- Published in *Nature Neuroscience*.



"The resources that are present in the Stampede and XSEDE facilities go far beyond what can be obtained in one single lab, or even an institution. It's a very important piece of the computational infrastructure that's going to be required to push the frontier of computational research."

Huan-Xiang Zhou,
Florida State University

This protein model represents an NMDA receptor, which juts halfway out of the surface of cells of the nervous system that include the brain and spinal cord. It relays signals between nerve cells. Researchers found that a mechanical coupling was needed between the clamshell-like region at the top of the protein that accepts a neurotransmitter and the channel in the middle that opens for electrical and chemical signals to flow in and out of the brain cell.

Image Credit: Lonnie Wollmuth, Stony Brook University

Myriad of Other Examples

- Behavior of new and existing materials at multiple scales
- Climate change and its potential social and economic impacts
- Concentration of environmental contaminants and their impacts on ecosystems and human health
- Genetic markers and disease
- Analysis of huge datasets
  - Market and customer behavior
  - Genomic data

Changing How We Teach

- Getting students actively involved in learning
  - Reducing traditional lectures
  - Increasing inquiry-based learning
- Ideally suited to instruction in computational science
  - Students need technical and analytical skills to create and test models and analyze data
  - Students enhance “soft” skills in teamwork and written and oral communication

Benefits to Students

- Inquiry-based learning is more effective than traditional lecture oriented instruction
  - Students are actively engaged in the learning process
  - Students gain deeper insights and have higher retention rates for the information
  - Facilitates the integration of information across academic disciplines – math, science, engineering, computer science

Challenges to Changing the Curriculum

- 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
  - 4-6 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

Adopting the Competencies

- Do not need to incorporate all possible competencies
  - Adjust based on target student population
  - Adjust based on available resources
- Does not mean new courses in all areas
  - Integrate materials in existing 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.)

	Topic	Course	Credit Hours	Terms offered	Required/Elective
Prerequisites	Calculus	MATH 1151.xx	5	Au, Sp	
		MATH 1152.xx or Math 1172	5	Au, Sp	
Core Courses	Simulation and Modeling (Choose one of these courses)	MATH 1157	3	Sp	Required
		CSE 2021	3	Sp	
		ISE 5100	3	Au, Sp	
		ME 5372	3	Au	
		MATSCEN 4321	3	Au	
	Programming and Algorithms (Choose one of these courses)	CSE 1222	3	Au, Sp	Required
		CSE 2221	4	Au, Sp, Su	
	Numerical Methods (Choose one of these courses)	AERO 3581	3	Au	Required
		CSE 5361	3	Au, Sp	
		ECE 5510	3	Au	
		MATH 3607	3	Sp	
		MATH 5401	3	Sp	
		MECHENG 2850	3	Au, Sp	

Discipline Specific Courses		CIVILEN 4000.01	2	Au, Sp	Required
	Capstone Research/Internship Experience (minimum 3 credits)	MATH 4998; CHEM 4998 or other approved individualized research credits **	3-5	Au, Sp, May, Su, May + Su/ Au, Sp/Au, Sp	Required
	Discipline-specific Computationally oriented Course	CSE 3521	3	Au, Sp	Required
		CSE 3341	3	Au, Sp	
		MICRBIO 5161H	3	N/A	
		BMI 5730	3	Sp	
		CHEM 5440	3	Au	
		MATH 5651	3	Sp	
		PHYS 6810	4	Sp	
		LING 5801	3	Au	
		LING 5802	3	Sp	
		ECON 4050	3	Au, Sp	
		ECON 5001	3	Au, Sp	
		GEOG 5221	3	Au	
		PSYCH 5608	3	Sp	
Elective: Choose at least one course from the following (3 credits total required)	Differential Equation and Discrete Dynamical Course	MATH 2255	3	Su, Au, Wi, Sp	Elective
		MATH 2415	3	Su, Au, Wi, Sp	
		MATH 2568	3	Su, Au, Wi, Sp	
	Parallel Programming	CSE 5441	3	Au	Elective
	Scientific Visualization	CSE 5544	1-5	Su, Au, Wi, Sp	Elective
		CEG (CIVILEN) 4760	3	Sp	E

Data Science Competencies

- Developed by multi-disciplinary group of researchers and practitioners
- Provided as guidance in the development of new programs
- Basic competencies
- Advanced competencies

Data Analytics Minor - University of Mary Washington		
Total credits: 23		
Required Courses	MATH 220	Introduction to Statistics
	MATH 200	Linear algebra
	CPSC220 Computer Science 1	Programming and Algorithms
	CPSC419	Data mining
	CPSC420	Modeling and Simulation
One of these electives	CPSC230 Computer Science II	Data structures
	BUAD 400	Analytics Application Development
One of these electives	BUAD 403	Foundations and Applications of Data Analytics
	CPSC 425	Parallel Processing

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

XSEDE Education Program

- Campus visits to discuss options
- Assistance in curriculum development
- Developing Faculty Expertise
- Sharing educational materials

Campus Visit

- Half-day to full day visit to campus
  - Meetings with faculty interested in curriculum changes
  - Meetings with administrators to explain the need for changes
  - Presentation to faculty, students, and administrators
  - Possible program review exercise
- Target outcome – local committee to work on curriculum change

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

XSEDE

Collaborative Online Courses

- Courses funded by XSEDE and Blue Waters Projects
- Prepared lectures, quizzes, and exercises online
- Collaborating faculty at local institutions create a local course number and supervise their students
- Use of XSEDE of Blue Waters education allocations

Collaborative Courses

- Applications of Parallel Computers led by University of California Berkeley
  - XSEDE funding for this year pending tentative spring 2017
- Introduction to HPC led by Kaust
  - Autumn 2016 sponsored by Blue Waters
- Algorithmic Techniques for Scalable Many-core Computing led by University of Illinois
  - Autumn 2016 sponsored by Blue Waters
- If interested, email me

Sources for Educational Materials

- Lists of reviewed training and education materials
  - http://hpcuniversity.org/resources/search/
  - http://sighpceducation.acm.org/resources.html
- List of materials and simple modeling tool examples
  - https://www.osc.edu/~sgordon/workshop/materials

Ties to Other Community Project

- SIGHPC Education Chapter
  - http://sighpceducation.acm.org
  - Webinars on education and training topics
  - Blog and forum to discuss related issues
- Journal of Computational Science Education
  - http://jocse.org
  - Peer reviewed articles on computational science education applications

How to Get Started

- Review the available materials with the faculty on your campus
- Request a campus visit
- Contacts
  - Steve Gordon – sgordon@osc.edu
  - Kate Cahill – kcahill@osc.edu

Questions?