

Preparing the Future Workforce for Careers in Science and Engineering

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XSEDE

Extreme Science and Engineering
Discovery Environment



Resources for Computational Science Education

- XSEDE resources for training and education
- Workforce needs in computational science
- How science and engineering (and social science and humanities) research is done
- What should our students know?
- Implementing changes to the curriculum
- Other opportunities



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XSEDE Vision/Mission/Goals

- **Tag line:**
 - *XSEDE – accelerating scientific discovery*
- **Vision:**
 - XSEDE aspires to be **the** place to go to access digital research services.
- **Mission:**
 - Accelerate scientific discovery by enhancing the productivity of researchers, engineers, and scholars by deepening and extending the use of XSEDE's ecosystem of advanced digital, services and by advancing and sustaining the XSEDE advanced digital infrastructure.
- **Goals:**
 - *Deepen and extend* the use of the XSEDE ecosystem.
 - *Advance* the XSEDE infrastructure.
 - *Sustain* the XSEDE infrastructure.

XSEDE Resources Summary

- Main access through XSEDE user website and portal:
 - <https://www.xsede.org/>
 - <https://portal.xsede.org/>
 - Portal accounts are free and allow access to sign-up for training events
- Training materials available
 - Live, webcast, and online training
 - More about full shared courses later



More XSEDE Resources

- Gateways
 - Web or light client access to domain analysis programs that run on supercomputers
 - Maintained by separate research groups
 - Good for light use and educational introductions
 - Examples
- Campus Bridging
 - Tools to make local clusters look more like XSEDE
 - Reduce systems management
 - Make transition to XSEDE easier



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XSEDE offers a variety of resources

- Leading-edge distributed memory systems
- Very large shared memory systems
- High throughput systems, e.g. OSG
- Visualization servers
- Accelerators and co-processors including NVIDIA GPUs and XEON Phi (MICs)

Many scientific problems have components that call for use of more than one architecture.



XSEDE Allocations

- XSEDE allocates access/time on powerful, valuable systems providing different capabilities at NO COST TO YOU
 - HPC
 - High throughput computing
 - Remote visualization
 - Data storage
 - Etc.
- Users may request XSEDE staff support to assist with optimization of research codes, visualization, workflows, novel projects, and science gateways
- Single Sign-On allows you to use just one username and password (your User Portal one). You will be recognized by all XSEDE services on which you have an account, without having to enter your login information again for each resource.



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XSEDE Allocations (2)

- Request allocations through the XSEDE User Portal
- It's **easy** to get a 'Startup allocation' —best way to get started
- Education allocations for classroom use via XSEDE and Blue Waters
- Larger year-long 'research' allocations can be requested 4 times/year, are peer reviewed, and have a longer lead-time
- Quarterly webinars on writing allocations



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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



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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

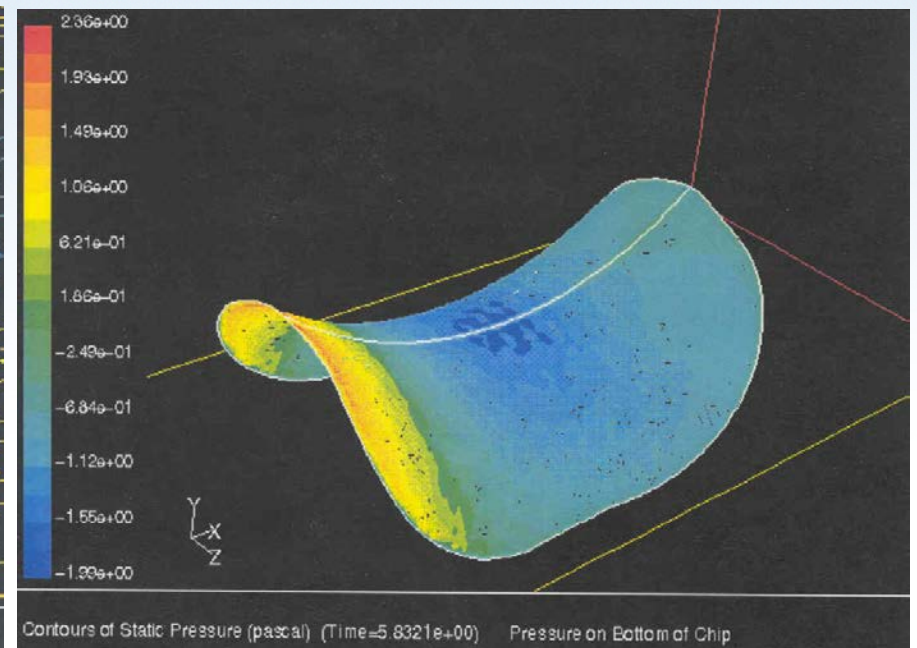
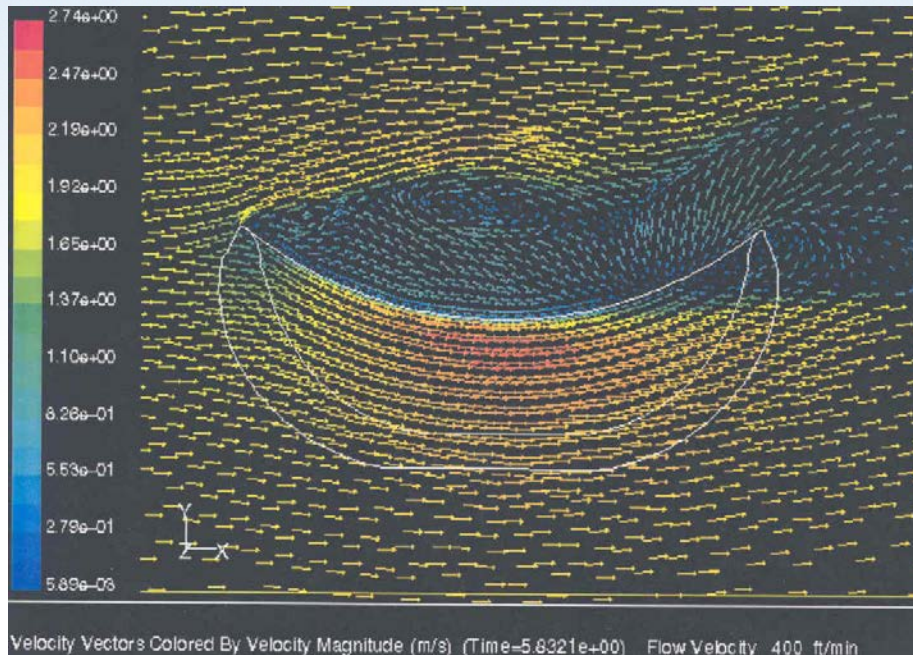


Durable
coffee
package
for P&G

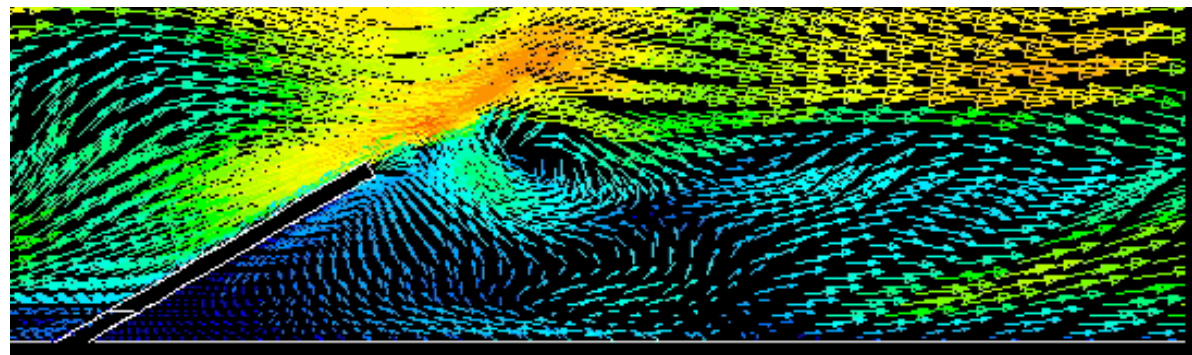


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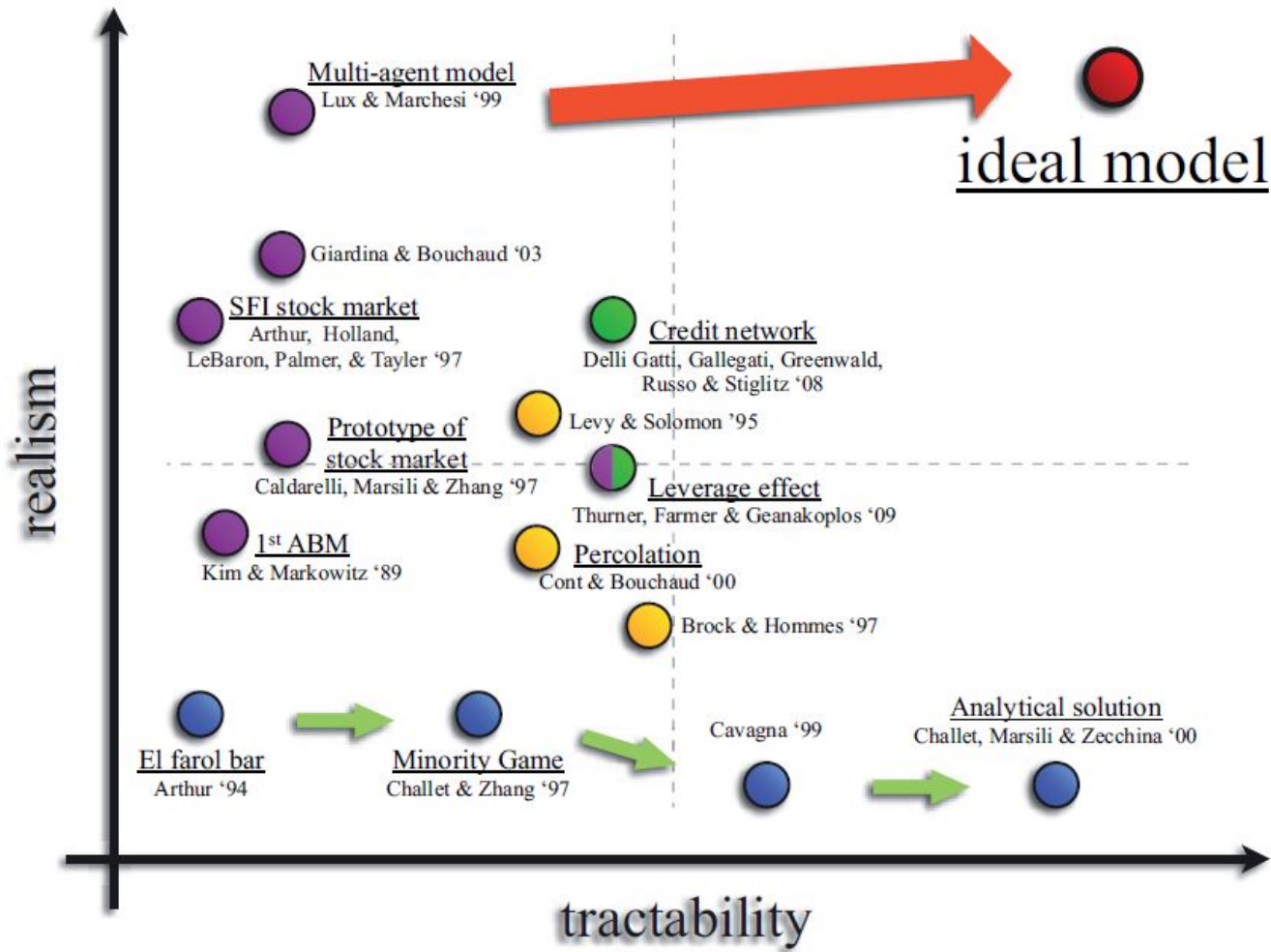
Will Pringles Fly?



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



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Adapted from a picture by M. Marsili

M. CRISTELLI, L. PIETRONERO, and A. ZACCARIA



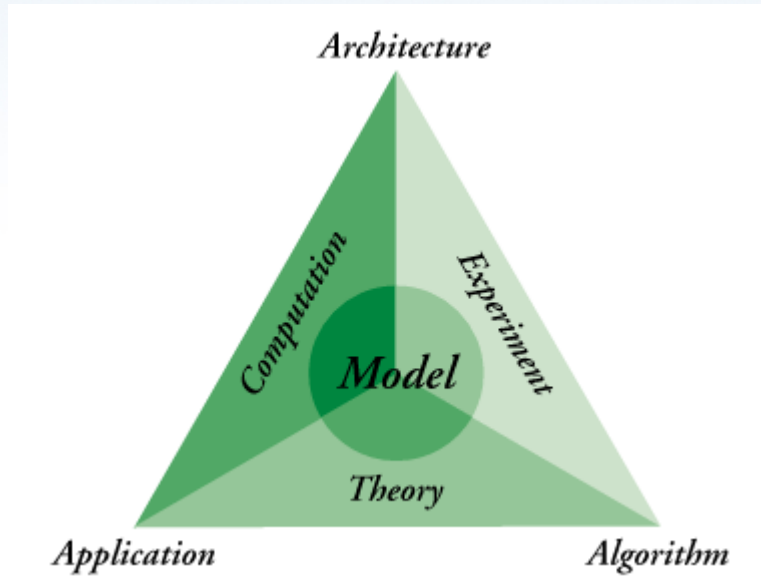
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Marketing Computational Science



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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.)

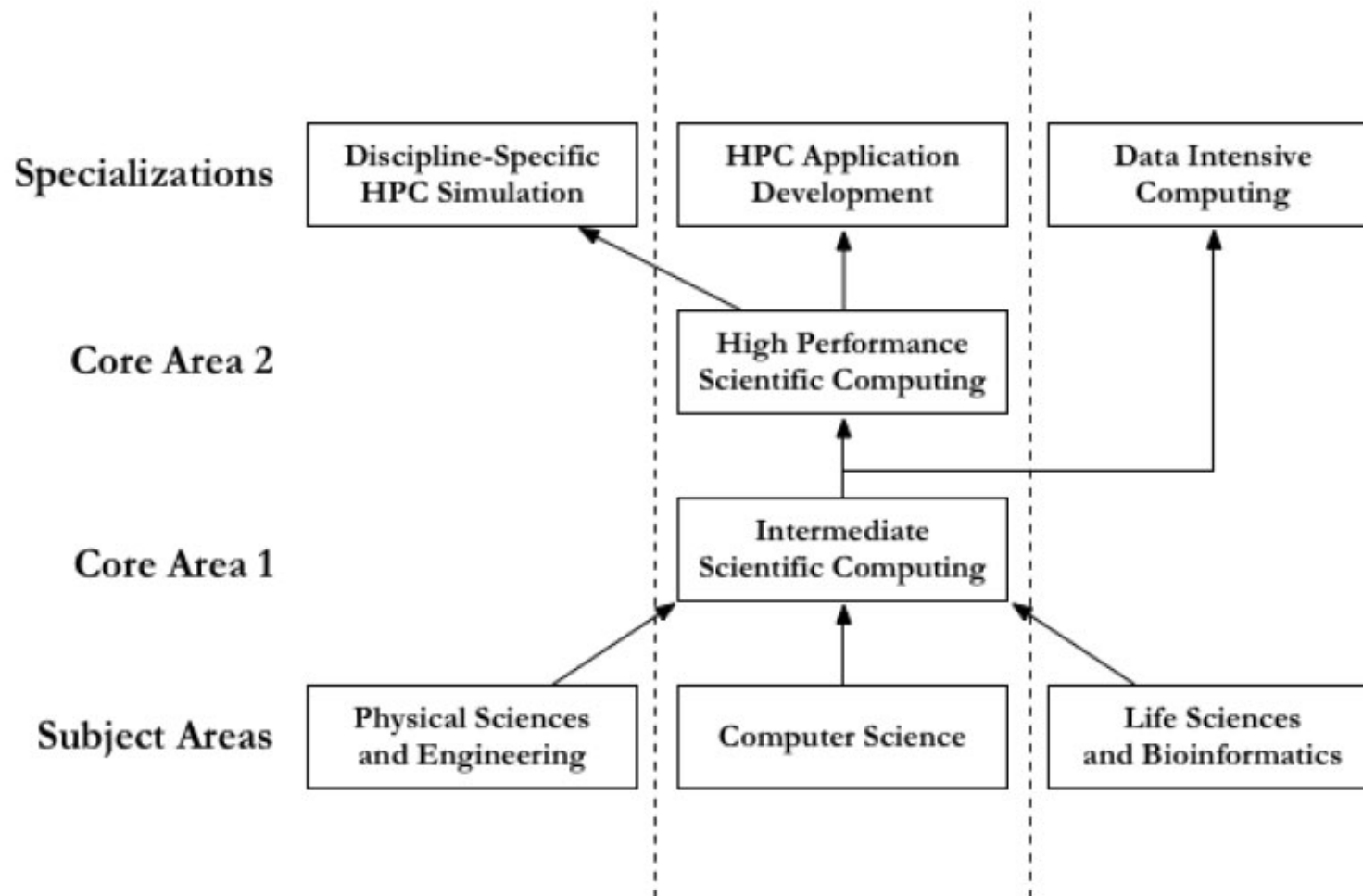
Discuss application across various industries (e.g., economics, health, etc.)



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 some of the background of an undergraduate
- Focus more on research skills across several disciplines
- Core areas focus on the computer science and related modeling skills
- Need to branch into a wider array of specializations based on the nature of the graduate program
- Needs the participation of multiple disciplines to be successful

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.



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Assistance with Program Development

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



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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://www.xsede.org/xsede-offers-free-online-parallel-computing-course>)

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/>

Some Other Opportunities

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



Opportunities for Students and Faculty

- Internships
 - Within XSEDE
 - List of opportunities on HPCU site
- Fellowships
 - [Blue Waters Graduate Fellowship](#)
- [XSEDE Scholars Program](#)
- [Faculty workshops](#)



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Question and Discussion



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