XSEDE: An Advanced and Integrated Set of Digital Resources for Science and Engineering

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XSEDE Mission and Goals

Mission: Accelerate scientific discovery

Goals:

• **Deepen and Extend Use**
  • Raise the general awareness of the value
  • Deepen the use and extend use to new communities
  • *Contribute to the preparation of current and next generation scholars, researchers, and engineers*
• **Advance the Ecosystem**
• **Sustain the Ecosystem**
Total Research Funding Supported by XSEDE Through May 2016

$2.21 billion in research supported by XSEDE
July 2011-May 2016

Research funding only. XSEDE leverages and integrates additional infrastructure, some funded by NSF (e.g. Track 2 systems) and some not (e.g. Internet2).
Fields of Science Using XSEDE

XD SUs Charged: Total: by Field of Science

- Biophysics: 11,684,221.0
- Materials Research: 8,456,747.0
- Nuclear Physics: 6,560,216.0
- Astronomical Sciences: 5,981,755.0
- Physical Chemistry: 5,666,784.0
- Condensed Matter Physics: 3,487,664.0
- Physics: 3,253,272.0
- Chemistry: 3,351,788.0
- Fluid, Particulate, and Hydraulic Systems: 2,820,607.0
- Biochemistry and Molecular Structure and Function: 2,710,875.0
- All 69 others: 24,652,528.0

Legend:
- Biophysics
- Materials Research
- Nuclear Physics
- Astronomical Sciences
- Physical Chemistry
- Condensed Matter Physics
- Chemistry
- Physics
- Fluid, Particulate, and Hydraulic Systems
- Biochemistry and Molecular Structure and Function
- All 69 others
Broadening Participation

Bar chart showing the number of New URM, Women, or MSI PIs and Users from PY1 to PY5.
Community Engagement & Enrichment (CEE)

- Workforce Development (Education, Student Programs, & Training)
- User Engagement
- Broadening Participation
- User Interfaces & Online Information
- Campus Engagement
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
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!
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
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
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/](http://hpcuniversity.org/educators/competencies/)
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 the role of 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
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
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 or Blue Waters education allocations
<table>
<thead>
<tr>
<th>Course Title</th>
<th>Sponsor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Applications of Parallel Computers led by University of California Berkeley</td>
<td>XSEDE funding for this year pending tentative spring 2017</td>
</tr>
<tr>
<td>Introduction to HPC led by Kaust</td>
<td>Autumn 2016 sponsored by Blue Waters</td>
</tr>
<tr>
<td>Algorithmic Techniques for Scalable Many-core Computing led by University of Illinois</td>
<td>Autumn 2016 sponsored by Blue Waters</td>
</tr>
</tbody>
</table>

If interested, email me
Consortium for Computational and Data Science

CDS Curriculum Implementation Challenges:

- Resource Limitations

Consortium Benefits

- Minimizes faculty preparation time
- Increases number of courses serving non-majors
- Increases interdisciplinary course offerings
- Allows lower enrollment courses to be offered
- Coordinates access to resources for exercises
- Accommodates difference in academic calendars
Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.