

# Advancing Research and Education with XSEDE

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# XSEDE

Extreme Science and Engineering  
Discovery Environment



# Presentation slides

- <http://hpcuniversity.org/trainingMaterials/209/>



XSEDE



# XSEDE – *accelerating scientific discovery*

*XSEDE aspires to be **the** place to go to access digital research services.*

*Accelerate scientific discovery by enhancing the productivity of researchers, engineers, and scholars through the use of advanced digital services and infrastructure.*





# Motivation for XSEDE:

- Scientific advancement across multiple disciplines requires a *variety of resources and services*
- XSEDE is about increased productivity of the community and providing expanded capabilities
  - leads to more science
  - is sometimes the difference between a feasible project and an impractical one
  - lowers barriers to adoption
- XSEDE provides a *comprehensive eScience infrastructure* composed of expertly managed and evolving advanced *heterogeneous digital resources and services* integrated into a general-purpose infrastructure





# Why Would You Use XSEDE?

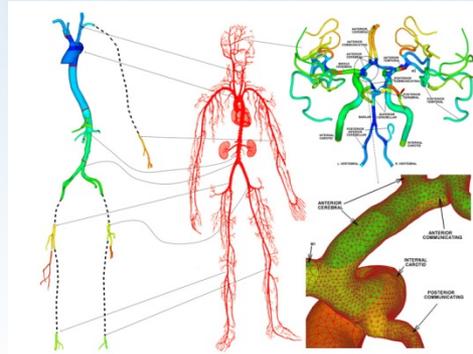
- Research codes that exceed the capacity of local computing resources (memory, processors, big data)
- Access to community codes that require large scale computing and data resources
- Science gateways that simplify research workflows
- Access to training and education resources



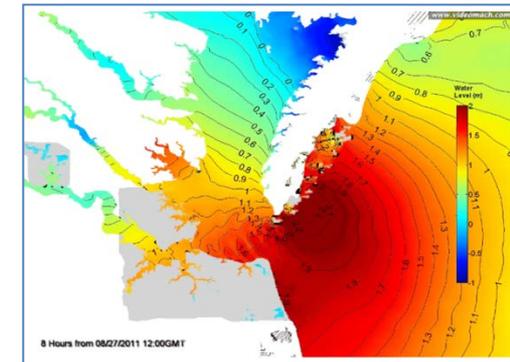
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# XSEDE Supports a Breadth of Research

- Earthquake Science
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm Modeling
- Epidemiology
- Particle Physics
- Economic Analysis of Phone Network Patterns
- Large Scale Video Analytics (LSVA)
- Decision Making Theory
- Library Collection Analysis



Three-dimensional model of major vessels and bifurcations of the human arterial tree reconstructed with gOREK from a set of computed tomography (CT), digital subtraction angiography CT and magnetic resonance angiography images.



A snapshot of an animation for water level prediction including the wind-wave signature.

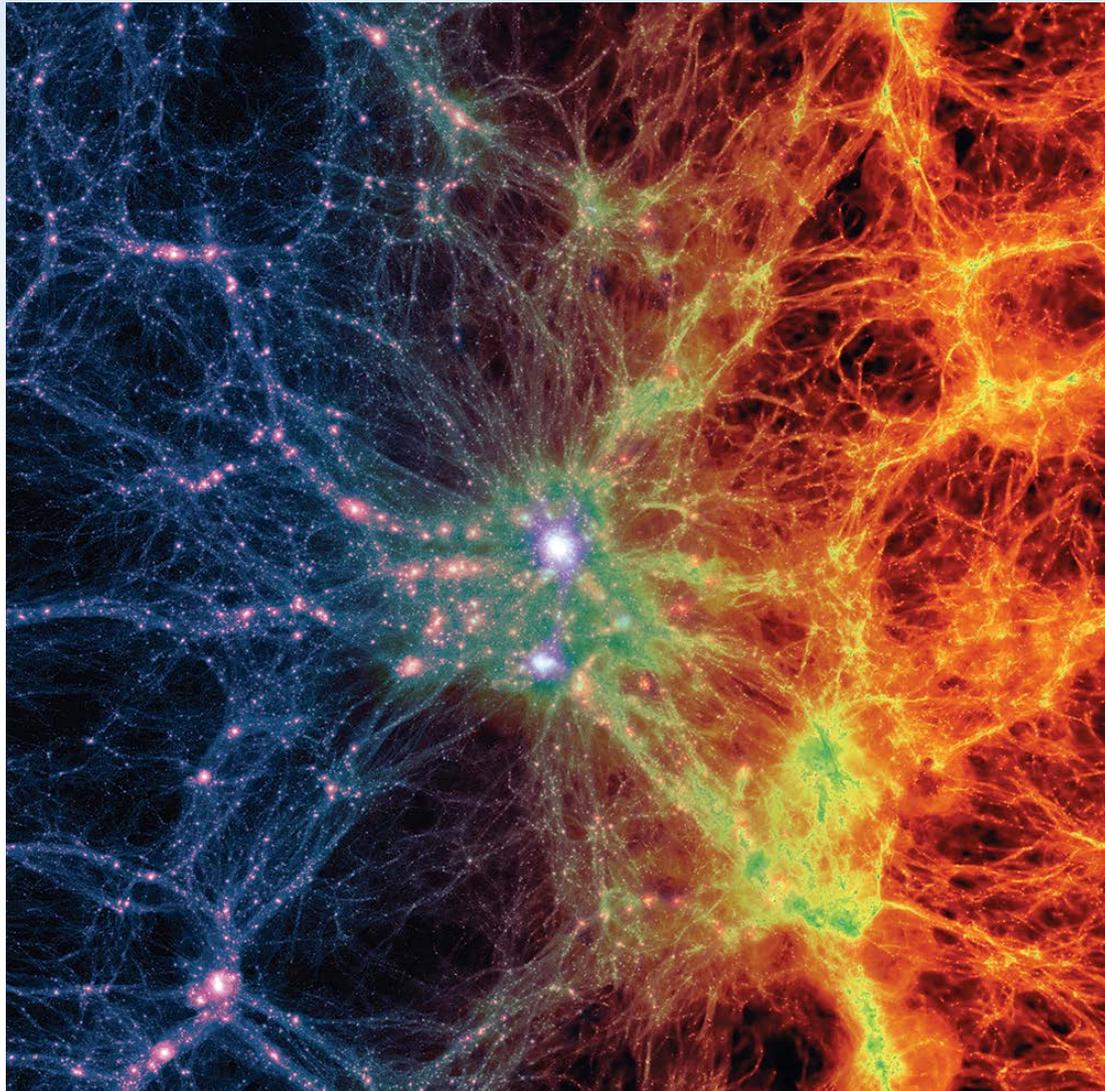


# Astrophysics: The Illustris Project

- Illustris, the most ambitious simulation of galaxy formation ever done, simulates the cosmos over 13.8 billion years. The simulated volume captures tens of thousands of galaxies with 12 billion resolution elements in a cube 350 million light-years across.
- An international team used XSEDE resources Kraken and Stampede to develop aspects of the Illustris project
  - Small-volume simulations run during development of the model
  - Coarser-resolution simulations otherwise identical to the flagship Illustris simulation, allowing the team to develop and test analysis tools
  - Simulations with less complete physics, providing insights into the effects of the components
- The project is described in a paper published in Nature, May 8, 2014.
- URL: <https://www.nics.tennessee.edu/illustris-project>

The logo for XSEDE (Extreme Scale Data Environment), consisting of the letters "XSEDE" in a bold, white, sans-serif font against a dark blue background with a grid pattern.

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The simulation volume at large scale, centered on the most massive galaxy cluster in the simulation at the present cosmic time. Dark matter density is shown on the left and normal matter (gas) density on the right

(Credit: Illustris Collaboration)



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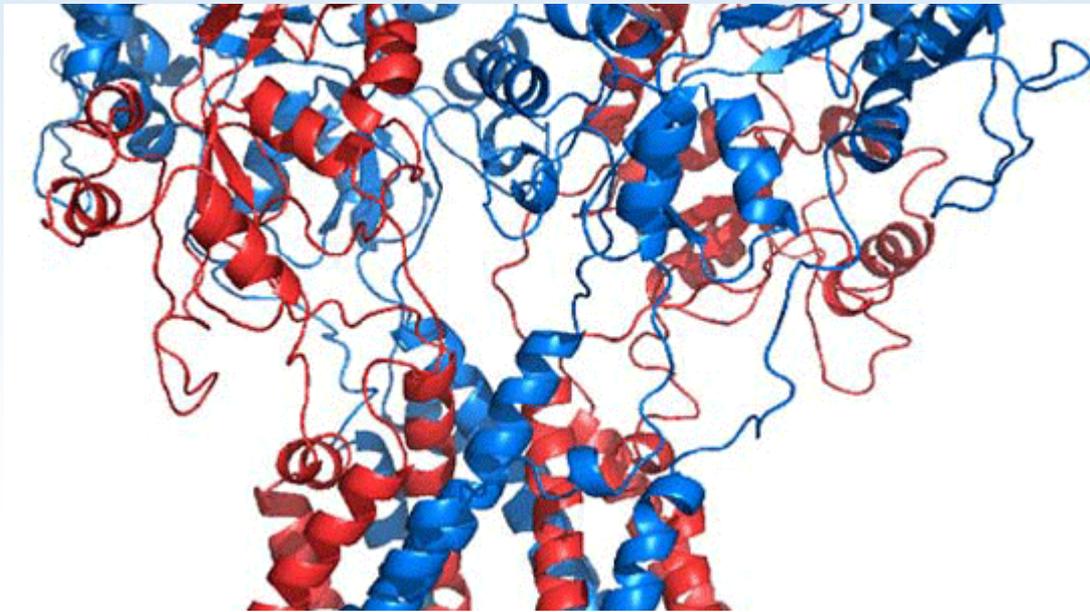


# Brain Cell Linker Dependence Shown by XSEDE Supercomputer Simulations

- 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*.

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"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.

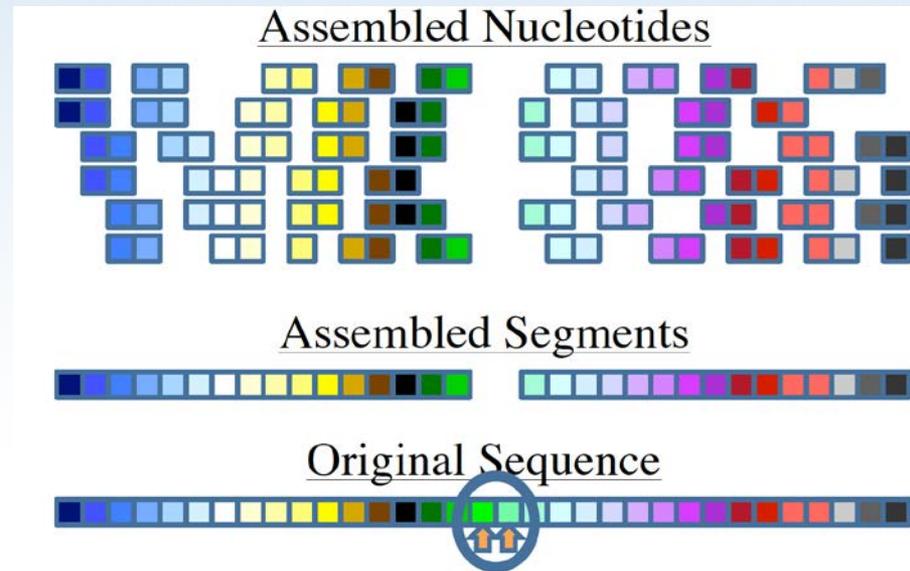
*Image Credit: Lonnie Wollmuth, Stony Brook University*



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# Improved Speed in Assembling Large Genome

- XSEDE Extended Collaborative Support staff modified ALLPATHS-LG to enable it to assemble very large genomes like that of *Ae. tauschii*
- The computation also required Blacklight's very large shared memory to enable the use of ALLPATHS-LG to create the best possible assembly of the new data
- Together with subsequent comparisons to related species, the new assembly allowed the group to identify at least 230 genes not present in the earlier assembly



The new assembly, together with comparisons to related species, allowed the group to identify genes missed in the previous assembly.

# 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

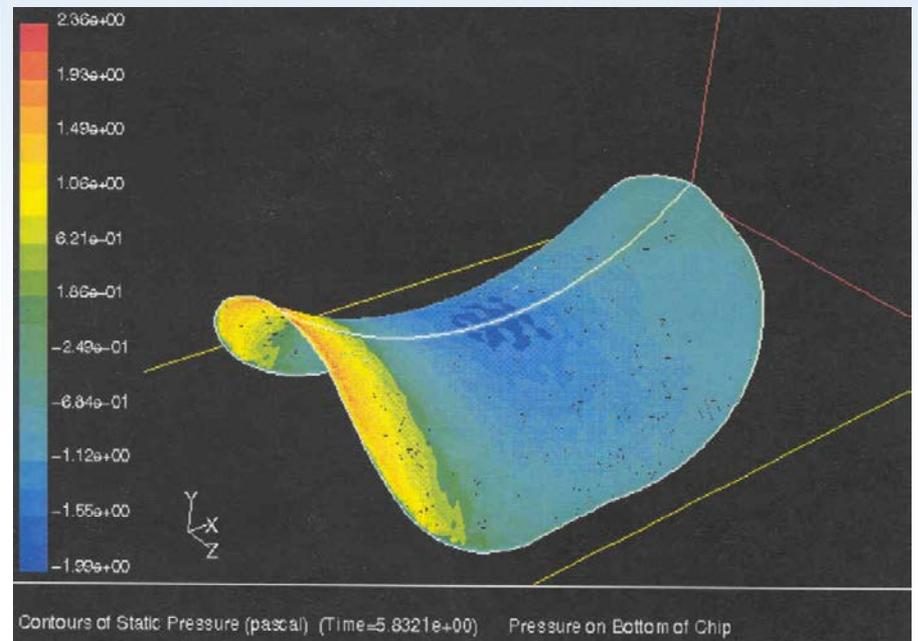
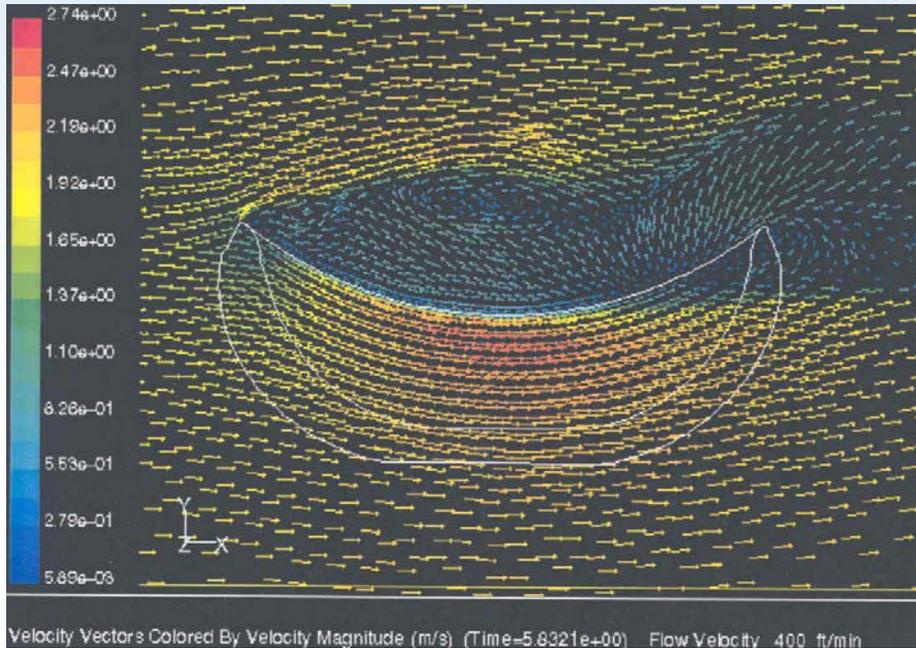


Durable  
coffee  
package  
for P&G

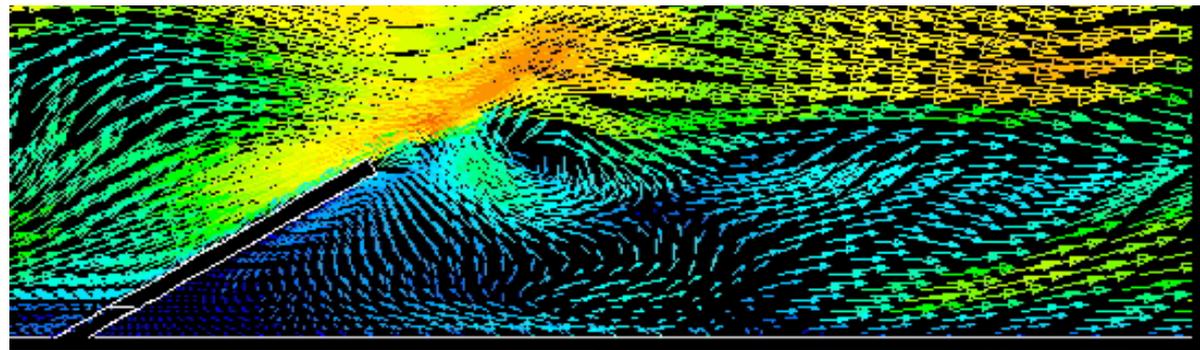


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# Will Pringles Fly?



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





# 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

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# Software and Community Codes

- Codes that have been optimized to run efficiently on XSEDE resources
- Loaded with appropriate computing environment using modules
- Wide range of open source software and some commercial software
- [XSEDE software](#)

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# Science Gateways:

Today, there are approximately 35 gateways using XSEDE



**NBCR** NATIONAL BIOMEDICAL COMPUTATION RESOURCE  
*Conduct, catalyze and enable multiscale biomedical research*



**SC/EC** Earthworks



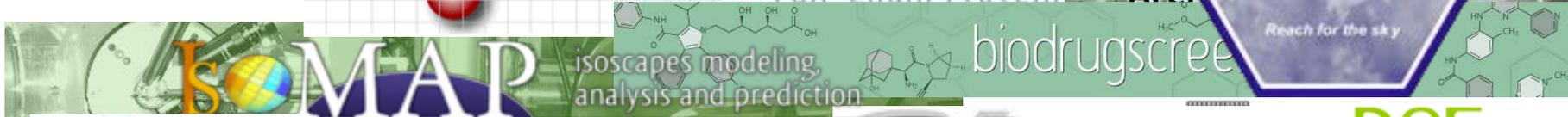
**UltraScan LIMS Portal**  
UNIVERSITY OF MINNESOTA  
for GEODYNAMICS  
portal Facilities Outreach Resources Publications



**Astero seismic Modeling Portal**



**CMMAP**  
Reach for the sky



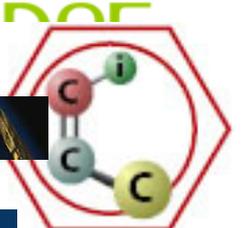
**biodrugscreen**  
isoscapes modeling, analysis and prediction



**X-ray Crystallography**  
Earth System Grid



**GI**



**CHEMBIOGRID**



**DARK ENERGY Survey**



Community Climate System Modeling Portal



**NEEShub**  
George E. Brown, Jr. Network for Earthquake Engineering Simulation



**CIPRES SCIENCE GATEWAY**



CyberInfrastructure for End-to-End Environmental Exploration

# XSEDE





# Science Gateways

- Access to XSEDE resources through web services focused on specific scientific domains
  - Managed by a research collaborative
  - Simplifies submission process
  - May limit options and extent of analysis
  - Excellent option for classroom use
- Gateways list
  - <https://portal.xsede.org/science-gateways>

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# 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

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# 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>
- Others expected next year
  - GPU programming
  - Parallel programming

# Getting Access to XSEDE Resources

- Start with your campus champion
  - Brian McDevitt -- [brianmcdevitt@boisestate.edu](mailto:brianmcdevitt@boisestate.edu)
  - Trial accounts on all machines
  - Experience with helping new users find the resources they need
- Create an XSEDE Portal Account
  - Access to training materials and allocation applications
- [Apply for an allocation](#)
  - Start-up
  - Research
  - Education
  - [Include help from Extended Collaborative Support Services](#)



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# Other Resources

- [HPCUniversity.org](http://HPCUniversity.org)
  - Index of training and education resources
  - Computational science education competencies
  - List of education programs
  - Opportunities for students
  - Calendar of events





# SIGHPC Education Chapter

- Virtual chapter of the ACM
  - <http://sighpceducation.acm.org/>
  - Inexpensive to join - \$10 professional, \$5 students
  - Webinars on education opportunities and programs
  - List of quality training and education materials

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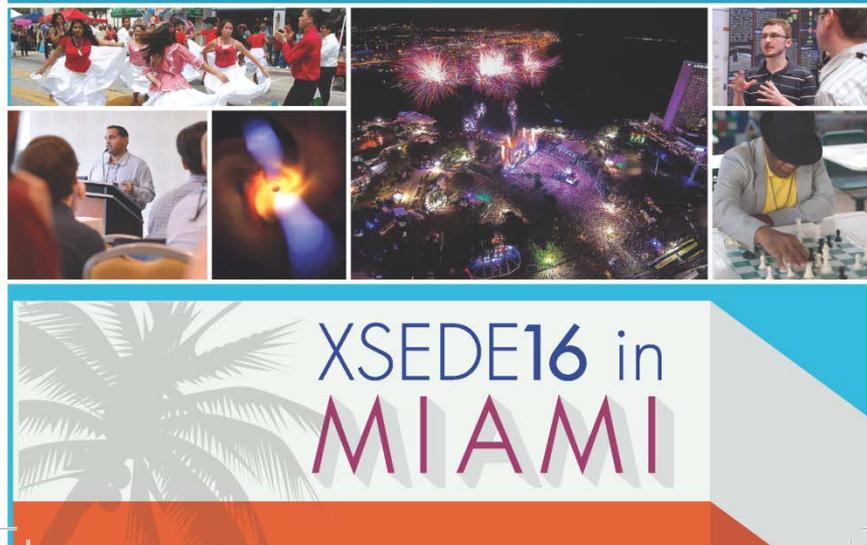
# Journal of Computational Science Education

- Online journal
- Refereed articles on a variety of education programs and experiences
- Student papers reflecting on internship experiences
- <http://www.jocse.org>



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# XSEDE16 Conference July 17 – 21, 2016



- Submissions will be accepted for papers, panels, tutorials, BOFs, student programs
- Topics span accelerating discovery, advanced technologies, software, science gateways and portals, and workforce development & diversity.
- Expect over 700 people from academia, industry, government, and other organizations
- Support for student participation

<https://www.xsede.org/web/xsede16/home>

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# Questions?



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