



# **NCSA Update for Joint Laboratory on Petascale Computing**

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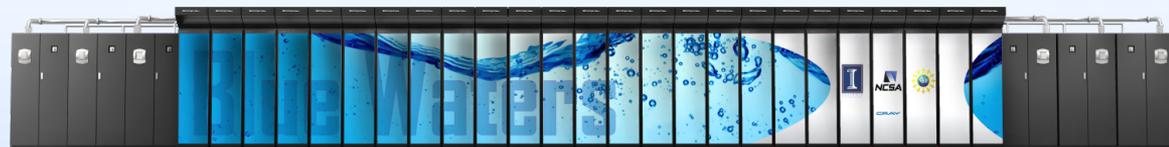


# NCSA Focus

- **Developing and supporting powerful, reliable computing, data, and networking resources that enable researchers to solve demanding science and engineering problems.**
- **Developing and exploring innovative architectures and techniques to accelerate scientific computing.**
- **Working with research communities to help them fully exploit the extraordinary resources available on the Internet (computing systems, data sources and stores, and tools) with cyberenvironments.**
- **Developing software, techniques, and tools to improve national cybersecurity and to help law enforcement better respond to cyberattacks.**
- **Providing insights into complex systems and sharing the thrill of scientific discovery with the broadest possible audience through artful visualizations of scientific phenomena.**
- **Helping to improve economic development**
- **Preparing the next generation of scientists and engineers to effectively use computational tools and techniques.**

## XSEDE

Extreme Science and Engineering  
Discovery Environment

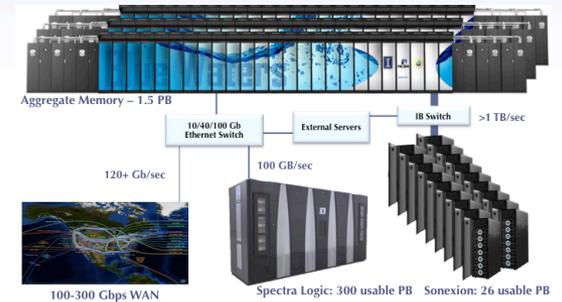


# NCSA Strategic Areas

- **@Scale Computing Science and Technologies**
  - Blue Waters, JLPC, *Exascale* Software and Hardware, ...
- **Data Focused Science and Technologies**
  - Astronomy, medical records, genomics, ....
- **e-Science Science and Technologies**
  - XSEDE, environments, frameworks, education, ....
- **Industrial Engagement and Support**
  - Private Sector Partners, National Manufacturing Initiative, ....
- **Other areas**
  - Cyber Protection
  - Education for all levels
  - Partners with other organizations
    - International - INRIA, KISTI, Jurlich, Cypress, Riken, ...
    - Within Illinois – PCI, CESC, IACAT...

# NCSA Accomplishments in the past year

- **@Scale**
  - Blue Waters in Full Service – more later
- **E-Science**
  - XSEDE Successes
- **Data**
  - Dark Energy Survey, LSST
  - Genomics and Medical Information
- **Industry**
  - Manufacturing Pipeline, “UI Labs”



# XSEDE – Led by NCSA

- *Mission - XSEDE accelerates open scientific discovery by enhancing the productivity of researchers, engineers, and scholars and making advanced digital resources easier to use.*
- *Activities - XSEDE is a virtual organization that provides a dynamic distributed infrastructure, support services, and technical expertise that enable researchers, engineers, and scholars to address the most important and challenging problems facing the nation and world. XSEDE supports a growing collection of advanced computing, high-end visualization, data analysis, and other resources and services. XSEDE is funded by the National Science Foundation.*

# XSEDE Accelerating Scientific Discovery

- **Over the past year, XSEDE supported:**
  - 2,237 projects with 9,483 users across 33 NSF divisions
  - 521 institutions w/20% international that accounts for 3.3% of usage
  - Science Gateways users average 1,594/quarter, 42% of XSEDE users

# Computational and Genomic Medicine @ NCSA

- Program Leader: Victor Jongeneel
- Achievements
- The iForge machine, which provides resources to the partners in NCSA's Private Sector Program (PSP), was selected as the most suitable environment for the task of processing raw human genome sequence reads at the Urbana campus using workflows developed at Mayo Clinic.
- Mayo became a formal partner in NCSA's PSP program
  - performance testing has indicated that iForge would indeed be a cost-effective platform for processing Mayo data, with an estimated charge of \$20 per exome and \$1000 per full genome at 50x read coverage
  - A common software repository was put in place, which allows a systematic comparison between the Mayo and UI versions to keep them up-to-date at both institutions.
- We managed to substantially optimize the Mayo workflows to run on iForge, in three different ways: (1) by adapting the syntax to the PBS/Torque job manager; (2) by simplifying the logic of the workflows and reducing the number of job submissions and (3) by introducing a coarse

# Thoughts on the Joint Lab Future

- **The real charter of a Joint Lab can be summarized as “Enabling scientists and engineers to solve their most challenging computational problems”**
  - Does not focus on any particular technological scale – just the most challenging
  - Scientists and engineers need more computing power to improve the fidelity of their computational simulations—the goal being predictive simulations and data analysis
  - NCSA is committed to working closely with the science and engineering community to provide the resources that enable them to reach these goals.
- **The original Joint Lab is successful because of the sustained and equitable contributions of all parties and the balance of interests between INRIA and NCSA.**
  - Inria's interests and UIUC interests are overlapping and mutual strengthening
  - The focus around one large system was very helpful to give concrete projects
  - The onsite presence of Franck at UIUC made it easy to do coordination and sponsor visits
- **A uniqueness of the joint lab is fostering the impact and engagement with researchers who are early in the careers. Other efforts only engage senior people**  
**The Joint Lab is a fertile environment to try many ideas. It also is helping some ideas evolve to have broader and sustaining impacts.**
- **Illinois would like to foster limited expansion that is manageable and the follow the general principles and goals of the original joint lab**

# Summary of NSF SAVI Proposal

- **NCSA is submitting an proposal for additional funding for coordinating international activities.**
- **NSF early reaction is positive**
- **Goals**
  - Provide support for the presence of a technical facilitator (at NCSA) with significant commitment to and responsibility for the success of the collaboration.
  - Replace the need for physical presence with a virtual organization (VO) methodology.
  - Maintain a high standard for entry into the collaboration, such that any new partners are willing and able (and expected) to commit sufficient energy, staff, and resources to ensure the success of the project.
  - Ensure that the quality of the partnership is consistently excellent.
  - Ensure that technical facilitators and other researchers are able to travel to partner sites periodically for face-to-face meetings with collaborators at those institutions.
  - Provide a strong accountability mechanism.
  - Always be conscious of building and maintaining a professional and trust-worthy relationship between the key partners.

# Thoughts on the Joint Lab Future

- **Sites having their own systems could either dilute the interest and efforts, create other complications such as equitable exchange of resources or greatly enhance the usefulness of the Joint Labs activities**
  - Opportunity for joint projects across systems may not require mutual access - just collaborators who can run on their own systems
  - Can be very helpful, particularly for algorithm and library development.
  - Creating algorithms and tools of demonstrated value to the broader extreme scale community
- **Sites may not (or may not plan to) equally contribute to the expand joint lab.**
  - Cause issues of equity and also be a governance challenge.
- **Some issues the governance need to be resolved**
- **What the role of the Joint Lab is relative to developing high level agreements between governments**
  - Be a easily accessible expertise repository for international efforts?
  - Be at the individual institutional level