A XSEDE: eXtreme Science and Engineering Discovery Environment

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B Project Summary

The eXtreme Science and Engineering Discovery Environment (XSEDE) will enhance the productivity of scientists and engineers and provide them with new capabilities, facilitating scientific discovery and enabling transformational science and engineering and innovative educational programs. XSEDE’s integrated, comprehensive suite of advanced digital services will federate with other high-end facilities and with campus-based resources, serving as the foundation for a national cyberinfrastructure ecosystem. XSEDE’s innovative, open standards-based architecture will facilitate an unparalleled level of integration, making possible the continuous addition of new technology capabilities. Enabling this architecture are XSEDE’s professional systems engineering approach and technology insertion efforts, which will ensure robustness and security while continuously strengthening XSEDE by incorporating new and improved technologies and services driven by the evolving needs of existing, emerging, and new communities. The XSEDE partnership will be led by NCSA, NICS, PSC, and TACC—world-class cyberinfrastructure centers with vast experience—and includes technology and education partners who strongly complement their expertise. The architecture, engineering, operations, support, and education activities are co-designed by this team to ensure that XSEDE ‘exceeds’ TeraGrid in usability, reliability, capability, performance, and security—and ultimately, in user productivity and science impact.

Researchers will use XSEDE directly, from campus and personal systems, from other high-end centers and cyberinfrastructure resources, and via science gateways and discovery environments. XSEDE users will be backed by an integrated national user support program offering an array of services from experts in the application of technology to advance science and engineering, including extensive training and advanced user support and collaboration. XSEDE’s governance model will include participation by these users as stakeholders, while providing centralized management to ensure robustness and to facilitate rapid responses to new issues and opportunities.

Thus, XSEDE will enable scientists, engineers, and educators to exploit powerful digital services and social networking environments to support knowledge exchange and advance understanding across domains. Just a few examples of the advances to science and society include: accurately predicting earthquake damage to urban structures; modeling of protein and nucleic acid folding and structure prediction to understand how drugs interact with target macromolecules to improve health care; developing novel designs for nanoscale microprocessors; advancing scientific understanding of plants to provide a safe and sustainable food supply, as well as benefits in renewable energy; and simulating pandemic spread to create a virtual laboratory where policy decisions such as school closure, vaccine deployment, and quarantine can be explored.

Intellectual Merit: XSEDE will develop a cyberinfrastructure that is unique in scale and diversity designed to enhance user productivity, interface with other CI resources, and evolve in capabilities over its lifetime. This project will evaluate and integrate the latest CI technologies, develop missing CI functionalities as needed, document and publish experiences and results, and provide requirements that drive future CI R&D. XSEDE will also work directly with leading researchers to apply XSEDE to groundbreaking science. The resulting architecture, engineering, operations, and support activities will advance distributed systems, high-end computing, data-intensive computing, and other technologies.

Broader Impacts: XSEDE will be the framework for a national CI ecosystem, serving as a stimulus and platform for multiscale CI integration and transforming the conduct—and sociology—of scientific collaboration. Working with applications teams and tool developers, XSEDE will adapt best practices from utilizing digital services into professional and curriculum development programs to prepare current and future science, technology, engineering, and mathematics (STEM) researchers, educators, and practitioners. XSEDE constituencies will develop the U.S. workforce in collaboration with educational institutions across the nation by establishing certificate programs to prepare researchers, educators, and practitioners in the effective use of advanced digital technologies with programs designed to engage under-represented groups to expand this workforce and improve digital science literacy.