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Advancing Computational Science Education through Xsede

By Steven I. Gordon

There's a great need for computational science programs that prepare the current and next generation of researchers, educators, and practitioners to effectively utilize digital services in support of science, technology, engineering, and mathematics. Xsede helps facilitate the founding and expansion of such programs.

The Extreme Science and Engineering Discovery Environment (Xsede) is a five-year, $121-million project funded by the US National Science Foundation that replaces and expands the NSF TeraGrid. It's a collection of integrated advanced digital resources and services from several supercomputers and high-end visualization and data analysis resources across the country. Together they form a single virtual system that's robust, advanced, and powerful. The aim is to have scientists interactively share computing resources with no cost to the scientists. This was the model adopted by TeraGrid, which was used by more than 10,000 scientists.

Xsede's Education and Outreach service mission is driven by the critical need to advance computational science and engineering by recruiting, preparing, and sustaining a large and diverse scientific, academic, and industrial workforce. A number of national task forces and panels have highlighted the need to increase the number of scientists and engineers who have expertise in modeling and simulation.[1-3] In our view, computational science (that is, science in silico) involves expertise from computer science and mathematics, as well as science, engineering, art, or humanist domains. It involves the use of computer simulation, data management, data analysis, and visualization techniques to formulate new product designs, provide insights into the behavior of complex systems, and make new discoveries. Xsede's Education and Outreach services have three primary goals:

- prepare the current and next generation of researchers, educators, and practitioners to effectively utilize digital services in support of science, technology, engineering, and mathematics (STEM);
- create a significantly larger and more diverse workforce in STEM; and
- inculcate the use of digital services as part of the routine practice for advancing scientific discovery.

Although a number of academic programs in computational science have been created, starting and maintaining such programs is often difficult because of the interdisciplinary nature of the field. There's a need for new programs to fill the demand for skilled graduates that's complicated by the difficulties associated with starting new interdisciplinary programs at institutions of higher education. Although individual faculty might incorporate computational science materials in their classes, those activities are generally insufficient to provide students with all of the skills they need. They also lack the continuity of effort that comes with the creation of formal concentration, certificate, and degree programs. Faculty interested in creating such programs must take on the burden of defining program content, finding and organizing colleagues who might assist with the effort, providing evidence of the need for the program to administrators, and shepherding program proposals through departmental, college, university, and sometimes university system committees.

Designing Programs

In recognition of these constraints, Xsede has initiated a program to assist two- and four-year colleges and universities, minority-serving institutions, campuses in the Experimental Program to Stimulate Competitive Research (Epscor) jurisdictions, and PhD-granting universities with the design and implementation of formal computational science programs at the undergraduate and graduate levels. The project is working to reduce the barriers to program creation by

- providing program models,
- working with the community to define student competencies for both undergraduate and graduate programs,
- visiting campuses to meet with faculty and administrators to discuss

the needs and possible approaches for starting new programs,
- creating professional development workshops for faculty, and
- building a virtual community to share instructional materials.

One of the major barriers to building an interdisciplinary program is defining the program requirements and target student outcomes given the diversity of interests across the participating disciplines. Xsede assists institutions who are considering formal programs by providing both program models and a set of student competencies that can expedite program formation. The competencies for undergraduates are based on those created for an interinstitutional program in Ohio called the Ralph Regula School of Computational Science (www.rrscs.org), updated to reflect recent changes in technology. A draft set of graduate-level competencies also has been formulated for computer science and mathematics skills. With the assistance of a broad cross-section of scientists, Xsede staff will revise and update those competencies with competencies that span several science and engineering domains. The competencies and a form for comments are available at www.rrscs.org/competencies.

Implementation

Along with the competencies and examples of existing programs, Xsede also assists campuses in starting formal computational science programs. Following the initial expression of interest, Xsede facilitates discussions with the interested faculty and administrators, visits the campus to present information on the need for computational science programs, guides discussions regarding current faculty experience and interests, and begins the process of formulating a program suited to the interests and expertise on that campus. In addition, Xsede shares materials used in other programs, program proposals, and sample course syllabi. To date, a dozen institutions are actively working on programs at both the undergraduate and graduate levels. Campuses interested in engaging with the Xsede staff can do so by contacting me (sgordon@osc.edu) at the Ohio Supercomputer Center.

Although participating campuses already have faculty actively engaged in computational science research or education, interested faculty can benefit from professional development workshops focused on recent computational science tools and instructional materials in their domain. Xsede collaborates with a number of other projects to offer such workshops. Workshops vary in length from one day through a full week and can include topics such as an overview of computational science and computational thinking, parallel computing, scientific visualization, or in-depth foci on typical domains in biology, chemistry, physics, and so on. Over the past year, Xsede has offered more than two dozen workshops for faculty on campuses across the country.

Finally, Xsede is building a virtual community of computational science educators who are sharing educational materials and experiences. A comprehensive index of education and training materials that will reference and review available educational materials is being developed (see http://hpcuniversity.org). When completed, the metadata will allow faculty to find materials referenced by computational science competency, subject area, or keywords. The site also will provide reviews of materials and a mechanism to submit new items for review and inclusion.

These efforts are being enhanced through several other campus programs. Xsede is working with campuses to identify local campus champions to raise the level of awareness, understanding, and access to high-performance computing resources and services available for research and education. Xsede also is working to address campus-bridging capabilities that fit the needs of researchers and faculty to exchange information across campuses and easily access national resources. Please contact me if you're interested in becoming a campus champion or if you're interested in developing standards for computational science education.

One of the primary goals of the Xsede project is to broaden the community by applying computational science within education and research. Xsede is actively seeking collaborations with related projects and programs, university educators and researchers, and professional organizations to help meet this goal and provide a future work force with a working knowledge of computational science.

References

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