Great Lakes Consortium for Petascale Computation
Virtual School of Computational Science and Engineering
Educating a New Generation of Computational Scientists and Engineers for
Discovery and Innovation in the 21st Century

Background

Computer modeling and simulation were among the most significant developments in the practice of scientific inquiry in the 20th Century. Scientific research has been extraordinarily successful in identifying the fundamental physical and mathematical laws that govern our world. Computer-based modeling and simulation provide the means of understanding and predicting the behavior of real-world natural and engineered systems based on a knowledge of these fundamentals laws. Computational science is now considered to be one of the three pillars of science, complementing theory and experimentation/observation.

Computer simulation can be as simple as solving the mathematical equations that describe the motion of a projectile under the influence of gravity and buffeted by winds—a major driver for the development of the first electronic computer. It can be as complex as simulating the evolution of the earth’s climate as the gaseous composition of the atmosphere changes, which requires the fluid dynamics of atmospheric motion to be coupled to models that describe the interaction of the land, oceans, and ice packs with the atmosphere as well as the chemical and biological processes occurring therein. Computational modeling and simulation are rooted in the scientific and engineering disciplines, but build on fundamental contributions from applied mathematics and computer science. Computational modeling and simulation are inherently interdisciplinary, and are being used by researchers across the US to design new materials for solar cells, fuel cells, and batteries; invent new approaches to treat cancer and Alzheimer’s disease; predict the paths of hurricane and the impact of storm surges; prepare for earthquakes; design new automobiles, aircraft and bridges; design the next generation of integrated circuits and microelectronics; understand the spread of infectious diseases, and so on.

American economic and societal competitiveness requires continuing innovation in computational modeling and simulation. In industry, computational modeling and simulation reduces product development cycles and improves the design and reduces the cost of producing new products. Breakthroughs in computer speeds, data densities, and networking bandwidth have paved the way for a revolution in science and engineering that is enabled by unprecedented capabilities in computational modeling and simulation. The ability of the coming generation of computers to attain petaflops speeds will transform our ability to attack complex scientific and engineering problems, but only if we are prepared to utilize the full power of these new computers. Today’s students, whose careers will extend to the middle of the 21st century, must understand the foundations, advantages, and limitations of computational modeling and simulation; must be able to use these techniques to help solve the scientific and engineering problems they will encounter; and must be prepared to utilize petascale computing to solve the most important problems facing our world. Meeting these goals will require a transformation in
the graduate and undergraduate curriculum in science and engineering. Ongoing advances in
cyberinfrastructure will support this transformation in ways not possible a decade ago.

Virtual School of Computational Science and Engineering

We propose to establish a Virtual School of Computational Science and Engineering that brings
together the faculty at each of the universities in the Committee on Institutional Cooperation
(CIC\(^1\)) under the Great Lakes Consortium for Petascale Computation (GLCPC\(^2\)) to address the
unique opportunities and challenges associated with petascale computing and petascale-enabled
science and engineering. The Virtual School will explore new instructional technologies and
sponsor the creation of courses, curricula and certificate programs that are tailored to the
educational needs of 21\(^{st}\) Century scientists and engineers. The Virtual School will further
facilitate the education of students in computational science and engineering through workshops,
conferences, summer schools, and seminars. The National Center for Supercomputing
Applications (NCSA) and other computing centers at the CIC universities and GLCPC research
laboratories will jointly provide resources and expertise to the students of the Virtual School and
of partner schools within GLCPC. Funding agencies will be approached and an industrial
consortium will be formed for long term support of a national effort for which the CIC schools
and selected partners will serve as a testbed. International partners have also been identified.

The Virtual School will be the first of its kind within the US in the field of computational
science and engineering to bring together faculty, programs, and expertise across multiple states.
The Virtual School will leverage the experience of the State of Ohio’s Ralph Regula School of
Computational Science, a virtual school recently established across multiple universities within
the State of Ohio and targeted at “blue-collar” computing. In contrast, the Virtual School will
target the next generation of computational scientists and engineers to prepare them to harness
petascale computing for scientific discovery and engineering innovation. The Virtual School will
leverage major investments in cyberinfrastructure taking place on the CIC university campuses
and enable unprecedented access to cutting-edge curricula, and drive the development of new
instructional technologies for teaching computational modeling and simulation. It will bring a

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\(^1\) The CIC is a consortium of 12 research universities, including the 11 members of the Big Ten Athletic Conference
(Northwestern University, University of Illinois, Indiana University, University of Iowa, University of Michigan,
Michigan State University, University of Minnesota, The Ohio State University, Pennsylvania State University,
Purdue University, and University of Wisconsin) and the University of Chicago. With campuses in 8 states, CIC
universities enroll more than 300,000 undergraduates and 76,000 graduate students, and employ some 33,000 full-
time faculty. The CIC is guided by the provosts of the member universities and collaborate in such activities as
sharing access to specialized courses and study abroad offerings, coordinating large scale purchases and electronic
licenses, creating programs for professional development, coordinating access to library materials, and building
shared data networks.

\(^2\) In addition to the CIC universities, members of the GLCPC include Iowa State University, Louisiana State
University, University of North Carolina, Argonne National Laboratory, Fermi National Accelerator Laboratory, and
Los Alamos National Laboratory as well as the Southeastern Universities Research Association, several
predominately undergraduate universities and colleges, two educational institutes, and two high schools.
Virtual School of Computational Science and Engineering

competitive advantage to the Great Lakes region, and eventually the nation, by providing a unique and powerful educational experience in computational science and engineering to students and others within the Consortium that will provide them with the tools and expertise they need to help solve the outstanding scientific and technological problems of the 21st century.

Graduate Education in Computational Modeling and Simulation

To ensure that the nation reaps the full benefits of the advances being made in computational modeling and simulation, we will educate a new generation of computational scientists and engineers who can effectively work at the intersection of a scientific or engineering discipline, applied mathematics, and computer science. This will require students to be thoroughly grounded in their discipline as well as have an enhanced level of knowledge in the other two areas. And, all of this will be accomplished without substantially increasing the time required to obtain a graduate degree.

Many of the CIC universities have long-established certificate programs designed to provide an interdisciplinary education to computational scientists and engineers, whereby students receiving a PhD in a given discipline, such as chemical engineering or physics, take a sequence of approved courses in computational science, computer science and applied mathematics. Upon graduation, the students receive a certificate in “scientific computation” or some variant thereof. While this has been partially successful at broadening the education and training of computationally-inclined graduate students at those institutions, it falls short in exposing students to the full breadth of computational science and engineering knowledge and opportunities needed for innovation in the 21st century. In many instances, certificate curricula are narrow or outdated. Moreover, students at institutions without these certificate programs have no access to these opportunities.

The Virtual School of Computational Science and Engineering will dramatically increase and enhance the course offerings in computational science available to graduate students at the CIC universities by developing innovative new courses that draw upon the expertise of faculty across these institutions. The Virtual School will also work with CIC member faculty to establish and standardize certificate programs in computational science and engineering as well as sub-disciplines thereof, such as bioinformatics and computational nanoscience, across the CIC universities. In this way, students at all of the CIC institutions can broaden and deepen their computational education. Workshops, seminars, conferences and summer schools will further enhance graduate education in computational science, preparing students to utilize modern high performance computing architectures, including multi- and many-core platforms for petascale computing. The initial focus on CIC institutions will serve as an important testbed for a larger, national effort, allowing for identification of novel curricula and best practices.

Although many major research universities have hired computational science and engineering faculty over the past decade, smaller schools may lack critical mass in this discipline and have relatively few computational faculty, and, accordingly, few course offerings. The Virtual School
Virtual School of Computational Science and Engineering

_of Computational Science and Engineering_ will further serve as a resource to the entire Great Lakes Consortium, by providing access to both core and advanced courses in computational modeling and simulation to students at non-CIC institutions that do not have experts in aspects of computational science and engineering on their faculties.

**Undergraduate Education in Computational Modeling and Simulation**

Although the initial and primary focus of the Virtual School will be on graduate education, it is clear that the goals outlined above will not be fully achieved unless there is a corresponding transformation in the undergraduate science and engineering curriculum. All scientists and engineers must be knowledgeable about computer modeling and simulation, not just those specializing in computational science and engineering, just as all scientists and engineers must be knowledgeable about theory and experimentation/observation.

Undergraduate education must expose students to the full range of activities involved in computer modeling and simulation—from applications of existing models as “black boxes” through understanding the theoretical and mathematical foundations of these models to an examination of how mathematical models are implemented on computers. The Virtual School will provide instructional resources to faculty and students suited for undergraduate education, including virtual laboratories, simulation modules, instructional wikis, digital repositories, etc.

**Infrastructure**

Much of the infrastructure for the proposed Virtual School of Computational Science and Engineering is already in place among the universities belonging to the CIC:

- OmniPop, an ultra-high speed network that connects the CIC campuses, provides the infrastructure to support resource sharing as well as video links for delivery of both synchronous and asynchronous courses. A high definition video link is already operational between the University of Illinois at Urbana-Champaign and the University of Michigan, as well as between the University of Michigan, Michigan State University, and Wayne State University, providing a level of “presence” and interactivity that is not possible with lower resolution technologies.

- CourseShare supports the development and sharing of courses among the CIC universities. CourseShare provides the administrative infrastructure that allows students on one CIC campus to enroll in and receive credit for courses taught by faculty at another CIC university. The program expects to deliver more than 15 courses in Fall 2007, and more than 25 courses in Fall 2008. (See: [http://www.cic.uiuc.edu/programs/CICCourseShare/index.shtml](http://www.cic.uiuc.edu/programs/CICCourseShare/index.shtml).) The Virtual School of Computational Science and Engineering will add significantly to this number.

- Portal technologies built upon the Sakai.org, Liferay, and Hubzero framework, developed by CIC partners University of Michigan and Indiana University (with MIT, Carnegie-Mellon...
Virtual School of Computational Science and Engineering

University, Stanford University, and others, Sakai.org) and Purdue University (Hubzero), respectively.

- Shared Digital Repository, which will provide access to digital library resources, including high definition video courses for asynchronous viewing, from across the CIC universities to faculty, staff and students.

- Partnership with iTunes University to facilitate podcasting and vodcasting of lectures and other instructional materials.

Organization and Management

The organization and management of the Virtual School of Computational Science and Engineering is based in part on the CIC’s American Indian Studies Consortium, see:

http://www.cic.uiuc.edu/programs/AmericanIndianStudiesConsortium/index.shtml

The faculty of the Virtual School will include faculty members engaged in computational science and engineering at each of the CIC institutions. The Virtual School will be headed by a Director and will operate with the assistance of an Associate Director and Operating Council. The Director will be a tenured member of the faculty of one of the CIC universities, appointed by the Provosts from the participating CIC institutions to a three-year term. The Director will:

- Provide vision for and oversee the programs and activities of the Virtual School of Computational Science and Engineering;
- Serve as chair of the Operating Council;
- Establish an agenda in consultation with the Operating Council and associate director and run meetings of the Operating Council;

The Associate Director will be a permanent, full-time staff person located at NCSA and will help manage and execute Virtual School programs and activities. Dedicated staff personnel at the CIC universities and the home institution of the Director will assist the Director, associate director and Operating Council.

The Operating Council will oversee the operation of the Virtual School of Computational Science and Engineering, including appointing ad hoc committees as needed. The Council will provide input on all seminars, workshops, summer schools and other activities to be sponsored by the Virtual School. Members of the Operating Council will help connect the work of the Virtual School to the activities in and interests of the computational science and engineering community in their institutions and shall provide the Virtual School with new ideas and evaluative content.

The Operating Council will consist of one computational faculty member from each of the 12 CIC universities, who will serve staggered, three-year terms, plus the director of NCSA as an ex officio member. All CIC faculty in the Virtual School are eligible for appointment to the Operating Council. The provosts at the individual CIC institutions will appoint the members of
the Operating Council. Appointment of a new director will be conducted by the CIC with recommendations by the Operating Council.

In addition to the Operating Council, a Student Advisory Council consisting of one graduate student from each of the participating universities will advise the Director on educational issues relating to needed or desired courses, curricula, and programs.

Activities of the Virtual School and Financial Support

The activities of the Virtual School of Computational Science and Engineering will be focused on providing significant added value in the education and training of a new generation of computational scientists and engineers at the CIC universities. The foremost activity of the Virtual School will be to drive the development, implementation, and coordination of new instructional approaches for computational science and engineering that delivers advanced topics in innovative ways, leverages expertise across the universities, and increases the overall breadth and depth of computational science and engineering curricula available to students in the CIC universities. Courses offered by the Virtual School are not intended to replace the core courses on individual campuses that already have strong student enrollments, but rather to add courses that universities may not otherwise be able to offer because of insufficient local enrollment or insufficient local expertise. Examples of courses not traditionally offered at many CIC schools that the Virtual School would develop and promote include courses on petascale computing and informatics, addressing specific topics such as: computer architectures for scientific computing; modern languages and programming models for multicore architectures and graphical processing units; programming for performance on massively parallel multicore architectures; debugging, performance and validation tools; I/O and archival storage functionality; analysis and visualization capabilities; co-processor utilization for scientific applications; and application development environments and frameworks. In addition, courses in computational science and engineering would be enhanced to address problems whose solution would be enabled by petascale computing. Many of these courses will also be available to non-CIC schools within the GLCPC, thereby offering students at smaller schools opportunities they would not otherwise have. The Virtual School will establish distance-learning courses for universities and colleges who do not have the expertise needed to teach them locally.

Activities will be run largely by CIC computational faculty with support by the Virtual School. Applications for curriculum, course and instructional technology development awards will be solicited annually. Proposals for workshops, seminars, conferences and summer schools will be open to all interested CIC computational faculty and students and will be solicited twice yearly. The Virtual School will seek partnerships with US industry, with particular emphasis on Midwest corporations, including industrial sponsorship of fellowships, summer internships, student recruiting, workshops, and employee training.

Initial support for the Virtual School will be provided by UIUC/NCSA and the University of Michigan with additional assistance provided by the CIC staff. This funding will support the
Virtual School of Computational Science and Engineering

initial development and pilot activities of the Virtual School. In FY2009 financial support for the Virtual School will be sought from the twelve participating CIC institutions. These funds will be used to support (1) administrative staff at the CIC, NCSA, and Director’s institution to work with the Director, associate director, and Operating Council, (2) technical staff to work with CIC computational faculty to develop and implement new instructional technologies and courses across the CIC campuses, (3) curriculum, course, and instructional technology development grants to individual and teams of CIC computational faculty (e.g. faculty release time), (4) the Director’s time (30% of the academic year salary plus one summer month salary), (5) workshops, conferences, summer schools, seminars, and visits by CIC computational faculty to other CIC schools, (6) Operating Council meetings, and (7) marketing and promotional materials. In one proposed financial model, each institution would be required to provide $50K in cash and $50K-$100K in in-kind contributions annually to support the above costs. It is anticipated that federal funds solicited by CIC faculty for REU, IGERT, GAANN, large centers, and other educational programs will be leveraged by the Virtual School. In FY2009-10, funding agencies will be approached and an industrial consortium will be formed for long term support of a national effort for which the GLCPC, CIC schools and selected partners will serve as a testbed.

Timeline

The proposed timeline for initial development of the Virtual School is outlined in the table.

<table>
<thead>
<tr>
<th>Date</th>
<th>Activity</th>
<th>Status</th>
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<tbody>
<tr>
<td>July 2007</td>
<td>Discuss whitepaper at GLC workshop.</td>
<td>Completed</td>
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<tr>
<td>Summer 2008</td>
<td>Appointment of Virtual School Operating Council</td>
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<tr>
<td>Summer 2008 and annually thereafter</td>
<td>Meetings of the Virtual School Operating Council.</td>
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<tr>
<td>Summer 2008</td>
<td>Establish Virtual School website.</td>
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<tr>
<td>August 2008 and annually thereafter</td>
<td>Summer School(s) on Petascale Computing.</td>
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<tr>
<td>October 2008</td>
<td>Appointment of VS Student Advisory Council</td>
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<tr>
<td>Spring 2009 and annually thereafter</td>
<td>Delivery of courses on topics relevant to petascale computing for science &amp; engineering (the number of courses is expected to roughly double each year)</td>
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3 Funding for the CIC American Indian Studies Program is provided by the CIC institutions in the amount of $150K per year per institution. The scope of the Virtual School of Computational Science and Engineering is expected to be much broader that the AIS program.
Virtual School of Computational Science and Engineering

Contacts

Professor Sharon C. Glotzer  
Department of Chemical Engineering  
University of Michigan  
Telephone: 734-615-6296  
e-Mail: sglotzer@umich.edu

Professor Thom H. Dunning, Jr.  
Department of Chemistry  
University of Illinois at Urbana-Champaign  
Telephone: 217-244-0078  
e-Mail: tdunning@ncsa.uiuc.edu