Center for High-Performance Computing @ The University of Utah

News

The University of Utah Fall 2008

Article

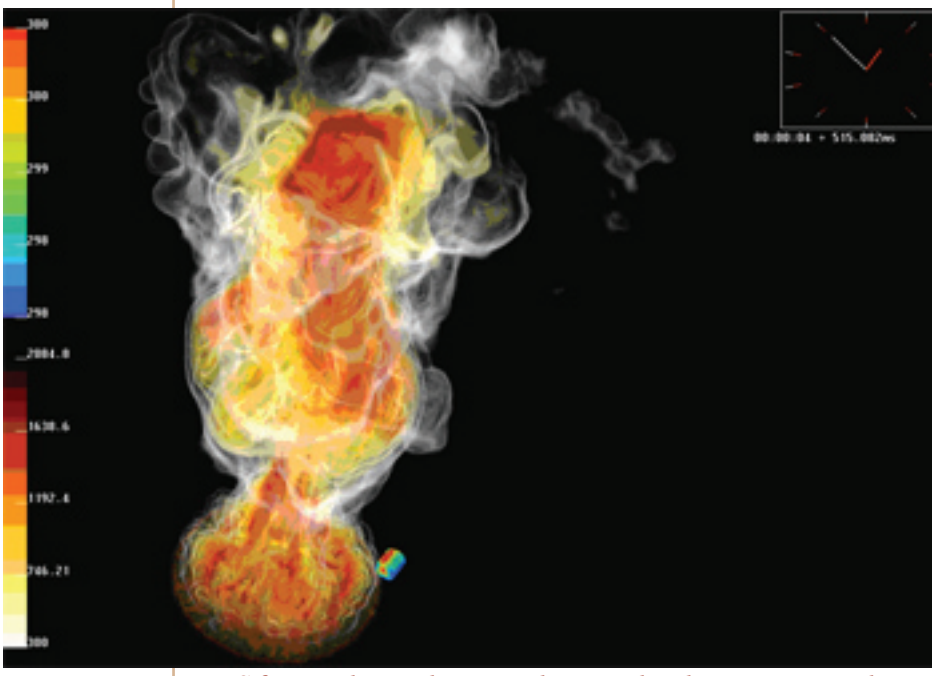
CHPC Supports Research on Clean Energy

By Janet Ellingson, CHPC

$E = MC^2$. If only energy creation were as simple as this beautiful equation. Our crude attempts at turning fossil fuels into energy have produced toxic fumes, greenhouse gases and ugly smoke. The goal of the University of Utah's Institute for Clean and Secure Energy (ICSE) is to expand our understanding of energy development through experimentation, analysis, and simulations and thereby help us produce the energy we need in an environmentally safe way. CHPC's new cluster, Updraft, will be a new significant research access for the Institute (see following box). Directed by Phil Smith, Ph.D., professor of chemical engineering, the Institute houses several programs that include chemists, engineers and computer scientists who are using a multidisciplinary approach to pursue "cradle-to-grave" research and development of energy for electricity generation and for liquid transportation of fuels from our abundant natural resources. In addition, the Institute includes attorneys and economists from The University of Utah's College of Law and The Wallace Stegner Center for Land, Resources, and the Environment who study environmental law and policy. Their work will aid in the implementation of ICSE research.

The Institute's Clean Coal Program is pursuing research and development of electrical power through the clean and efficient use of coal, an abundant national resource with an estimated 250-year reserve at current consumption levels. Coal is responsible for approximately 50% of the energy generated in the United States and 90% of Utah's energy production. Learning how to burn coal cleanly is an important step toward achieving our national independence from foreign fuel sources in a way the does not contribute further to global warming. The Clean Coal Program recognizes the solution will be found in many approaches, "including increased efficiency, co-firing with biomass, retrofitting of existing power plants and CO_2 capture and sequestration." Rather than emitting CO_2 and other pollutants into the atmosphere, power plants can capture the CO_2 and force it into underground caverns such as deep saline aquifers and sites from which oil and coal have been extracted. The Clean Coal Program, in partnership with the University's Energy and Geoscience Institute, is studying the fate of this sequestered CO_2 by creating simulations based on experiments that determine the reactive effects of CO_2, sulfur dioxide, nitrogen oxides and ammonia on materials they may encounter when forced underground. These reactions can be modeled to predict if sequestering in a particular area over time may result in fractures that allow the gases to leak back into the atmosphere. The studies will also guide the development of the technology necessary to successfully sequester the gases.

The Oil Sands and Shale Program, also housed at ICSE, brings together an interdisciplinary group of faculty whose research focuses on unconventional oils, including heavy oil, which is much thicker than the crude oil most commonly refined for our use, and oil found in oil shale and oil sands. Utah has more oil sands resources than any other state, giving us a particular interest in utilizing this resource. However, extracting these oils in a way that is cost efficient and environmentally sound is a huge challenge. Given the national commitment to energy independence accessing



LES fire simulation showing volume rendered temperature and the resulting temperature of a nearby container.

these sources may one day be necessary. The Program is committed to acquiring the knowledge necessary to develop these unconventional oils in a manner that minimizes the carbon footprint of extraction, refinement and use. By involving graduate students in the Program's interdisciplinary research, we will have a new generation of experts who will be well trained in both the science and environmental policy. Last year the Program published the report "A Technical, Economic, and Legal Assessment of North American Heavy Oil, Oil Sands, and Oil Share Resources" for the US Department of Energy.

The Institute's simulations and modeling are based on experiments conducted at an off-site industrial combustion and gasification research facility. The 30,000 square foot site includes two research buildings that house seven combustion and gasification reactors. An integrated distributed control system (DCS) enables engineers to monitor the high-temperatures processes and log research data. In addition to characterizing the combustion process, engineers are able to experiment with the possible technological innovations that will quickly transform research findings into practical applications for the energy industry. The reactors already have an immediate practicality. Companies can bring their biomass waste, such as sugarcane residue and black liquor from the pulp and paper process, and have the Institute determine the most useful way to convert the waste into a usable fuel.

More information about the Institute for Clean and Secure Energy can be found at their website http://www.icse.utah.edu.

ICSE's industrial combustion and gasification research facility

Coming Soon - UPDRAFT - a 2048 core cluster for capability computing!

by Julia Harrison, Associate Director, CHPC

CHPC has recently taken delivery of a new cluster for capability computing. Traditionally CHPC has tuned cluster usage for highest throughput. The new cluster, named UPDRAFT, will be used primarily for large jobs which require huge amounts of compute power, such as the ISCE research described in the above article. The queues on the new system will be optimized to accommodate these large jobs. The new cluster will have 2048 cores for computation running over an InfiniBand interconnect. Each of the 256 Sun Fire X2250 server nodes will have 2 quad core processors (Intel Xeon) running at 2.8 Ghz. In addition there will be 2 interactive nodes for job submission, short compiles and editing. Each interactive node has 2 Intel 3.16 Ghz – Quad core processors (8 per node). There will also be a large scratch space attached and available to all of the nodes of 24 Terabytes (raw) which translates into 18 Terabytes of usable space. At the time of this writing we have achieved 17.5 Tflops on the HPL benchmarks (a flop is a floating-point operations per second)!

Article

The University's Cyberinferstructure Evolves to Meet Research Needs

By Janet Ellingson, Ph.D., CHPC

Many academic disciplines have expanded their use of computational methods for data collection, analysis, modeling, and simulation in basic and applied research. These fields now require significant computational capabilities along with storage for vast amounts of accessible data. CHPC continues to be a primary on-campus computational resource for researchers at the University of Utah. However, the increasing demand now requires a rethinking of the entire research IT infrastructure – also known as cyberinfrastructure (CI) – at the University. Dr. Steve Corbató, the new director of Cyberinfrastructure Strategic Initiatives in the Office of Information Technology, is doing just that. His work is done under the guidance of the Campus Cyberinfrastructure Council, chaired by Prof. Martin Berzins, head of the School of Computing. The Council's mission is to develop strategies for an evolving, customizable set of integrated, high-performance, and cost-effective research IT services to the University community. In coordination with the strategic planning efforts of Prof. Tom Parks, the vice president for research, and Steve Hess, the vice president for information technology, Dr. Corbató is doing the initial planning for a cyberinfrastructure that will enable university researchers to be more effective, more collaborative and more competitive.

The challenge will be to keep pace with the growing needs and requirements on campus by creating an infrastructure that is both cost effective and adaptive to the rapidly changing technology base. This will require plans that incorporate the existing campus CI services at CHPC and capabilities in the faculty-led research institutes, in addition to taking advantage of funding opportunities reflective of the increasing focus on CI among national R&D funding agencies. The Campus CI Council is considering several high performance computing opportunities available to institutions through the National Science Foundation. Some level of institutional and state support currently exists for cyberinfrastructure. The University has purchased a new off-campus data center that will address the future computing needs of the University and to house major CI related activities. [See accompanying article below.] With high-capacity electricity feeds and plans for a state-of-the-art water cooling process, the new data center will be structured to meet the needs of University research faculty as they move toward a Petascale (Peta = 10^{15}) regime of computation.

One of Dr. Corbató's current projects is leading the development of an optical fiber network that will connect the University's principal on-campus network nodes with the new data center and several of the University's key local partners, including the Utah Higher Education offices and potentially the Salt Palace. The current design calls for many of the optical fiber segments to run in conduits along the Utah Transit Authority TRAX lines.

Dr. Corbató is now working with the University's science, engineering and medicine faculty, many of whom already have developed successful computationally oriented collaborations, to better understand their cyberinfrastructure needs. At a data curation workshop planned for later this year, faculty, researchers and library staff will hear from national experts and then will help identify more precisely the data management needs of the University's research community and discuss the role of the libraries in this process. Increasingly, funding agencies are expecting that research data be made available to other researchers and the public at large on an open access basis in many cases after some period of time.

While serving in leadership positions at Internet2, the organization dedicated to developing leading-edge Internet technologies for higher education, Dr. Corbató worked on many national and international networking projects. He oversaw the Abilene Network for four years, developed the Manhattan Landing exchange point in New York City, and created the FiberCo dark fiber acquisition and holding vehicle that purchased national-scale optical fiber segments from telecommunications companies selling off unused fiber assets. Before joining Internet2, Dr. Corbató helped develop Washington State K-20 Network, a video and data network for its public and higher education systems.

Dr. Corbató also understands first hand the needs of the researchers whose work the new CI will serve. Before he chose to spend his time facilitating the movement of photons along optical fibers, he studied the movement of high-energy particles that blasted through the Earth's atmosphere. His academic background is in experimental astrophysics. He earned his B.A. from Rice University and his Ph.D. from the University of Pennsylvania, both in physics. As a post-doctoral researcher, he joined the University of Utah's Cosmic Ray research group that then studied high-energy particles with the Fly's Eye and High Resolution Eye telescope arrays situated near Dugway, Utah. He is also an avid alpine skier, which may be one reason he values fast, unimpeded movement of both data and skis along the most direct route.

Steven Corbató on a hike in the western Utah desert.

FYI

University Purchases Building for New Data Center

By Joe Breen, Assistant Director, Networking, CHPC

This summer the University of Utah purchased a large building downtown to use as a central campus data center. The data center will offer potential opportunities for all campus groups. Two committees, a business committee and a design committee, are overseeing the building's transformation. The business committee is working on the financial picture of monies and how to work with co-location partners such as other schools in the state, Board of Regents, and other commercial partners. The design committee, with representation from enterprise, cyberinfrastructure, computational research, campus design and others, will obtain requirement info from different groups and coordinate with consultants. Over the next few months, the design committee will decide on a consultant group to take the university through a Strategic Planning and Design process. At the end of this process, the University will have a set of schematics by which to proceed on build out of the data center. The business committee has approved funding for the consultants and has requested a two-year timeline for completion of the project.

The building is a 75,000 sq. foot building with a seismically-hardened shell that is completely empty inside. The building is in an industrial area and has 2.5 MegaWatt of power available to it today and can easily grow in power. The building has no flooring, internal electrical, cooling or any developed space at this time and looks like a giant empty warehouse. It has a large raised dock that allows two 18 wheel semi-truck trailers to park and unload. The building also has another smaller ground-level dock entrance. The design and construction of the building will build out the necessary infrastructure to become a hardened data center in which one can install many racks.

The University will develop 25,000 sq. feet initially. Another 30,000 sq. feet will house "traditional data center" material known as medical records. The medical records will be on the other side of a large structural concrete wall and some limited office space and therefore offer very limited liability to a datacenter environment.

The University is developing a metro-optical network ring that will go to the data center. This optical ring will support multiple 10GigE and some SAN protocols. This ring will pick up several sites in the Salt Lake metropolitan area, as well as connect to the carrier Points of Presence (PoPs).

Earl Lewis is the project manager for the Metro Optical network project, the Data Center project and the Medical Records project. He will be coordinating with the consultants' project management group as they come on board.

Staff Research

Access Grid Infrastructure for Telematic Performances

By Jimmy and Beth Miklavcic, Multimedia Communications, CHPC

Jimmy and Beth Miklavcic presented *The Poetics of Challenge – Developing Artistic Works in an Emerging Digital Tool Set* for The Digital Resources for the Humanities and Arts Conference September 14-17, 2008 held at the University of Cambridge, England. The conference took place on Cambridge University's Sidgwick Site, the home of the humanities facilities on campus.

Mary Jacobus, the DRHA08 Local Committee Chair states that Cambridge University is an appropriate place to bring DRHA and sow the seeds for new exploration into 'e-Humanities' through discussions around new collaborative electronic environments, collective knowledge, crossing disciplinary boundaries and innovations in the humanities and the arts. The e-Humanities are flourishing as never before, bringing new scholarly communities and knowledge into being.

On September 16, in the West Road Concert Hall, Jimmy and Beth presented their paper about the challenges of telematic performances using examples from the recent performance of InterPlay: Carnivale, held at the University of Utah Intermountain Network and Scientific Computation Center March 28-30, 2008. The purpose of the presentation was to examine the challenges faced in project development processes and to find solutions for improvements in the creation of network collaborations. Questions regarding the process of using Access Grid Technology were discussed.

Beth and Jimmy Miklavcic at Cambridge, England

Feedback from audience members included statements such as, "I feel as though I just watched NASA scientists at work." One attendee asked "When will it be possible to meet with as many sites as one's system can sustain?" Jimmy and Beth responded, "Now."

Staff Research

Computer Modeling of Complex Geometric Forms

In July the 11th Annual Bridges Conference for Mathematics, Music, Art, Architecture and Culture was held in Leeuwarden, Netherlands, the town where M.C. Escher was born. Escher's drawings are well known for their impossible and fantastical architecture. CHPC staffer Robert McDermott, Ph. D., presented the paper, "A Computer Aided Geometric Model of a Ten-Plane Polyhedral Transformation," the culmination of his work with University of Utah student Will Hawkins. Together they created a computer aided geometric model for a polyhedral transformation written in C++, OpenGL and GLUT. This geometric model allows a user to interactively change the shape of a closed convex polyhedron derived from 10 face planes in a fundamental region. Given different inputs, a variety of polyhedron were created. For some inputs, the output was a Platonic or Archimedean polyhedron or more complex polyhedrons.

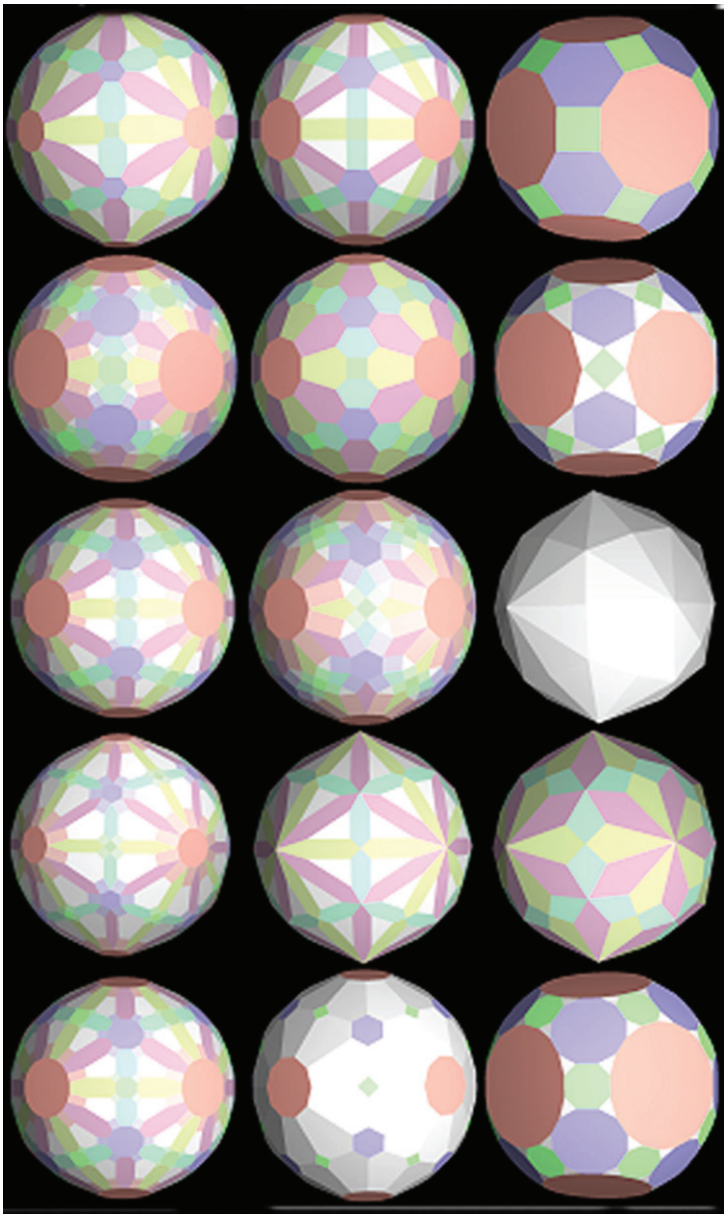
For nearly 30 years, Dr. McDermott's research has focused on computer-generated complex geometric forms, starting with a 3-plane computer model created while he was a staff scientist at the NYIT Computer Graphics Laboratory, to the present 10-plane model. He is now interested in the animation of these models and using them in audience interactive presentations, as he successfully demonstrated at this year's Bridges Conference.

Dr. McDermott's current research is on tensegrity models, which are physical models composed of compression members made of 1/2 inch PVC pipe and tension members made of fishing line. The overall effect of the construction is to give the compression members the appearance of floating within space. The models can be used in public school math classes to teach geometric principles.

Upcoming Presentations at INSCC

Chemistry Packages - Nov. 13 - 1:00 PM
Dr. Anita Orendt will give an overview of the computational chemistry software packages, including Gaussian, Amber, NWChem, Molpro, Dalton, Babel, GaussView, GAMES, that are available on CHPC computer systems.

Gaussian03 and Gaussview - Nov. 20 - 1:00 PM
Dr. Orendt will give more details on the use of Gaussian03 and Gaussview on the CHPC arches clusters. She will discuss batch scripts and input file formats, parallel scaling and timings with the different scratch options (TMP, MM, SERIAL), as well as the scratch needs of Gaussian03. Finally, she will demonstrate the use of GaussView to build molecules, input structures, set up input files and analyze output files.



Fifteen polyhedra from a continuous ten-plane computer-aided geometric model.

FYI

CHPC maintains on its web site a listing of publications and talks that acknowledge the use of CHPC's resources. You can find the current listing at the following address:

http://www.chpc.utah.edu/docs/research/CHPCBibliography.pdf

If you utilize CHPC resources in your research, please include an acknowledgement in your publications and presentations. Also, please give us a copy for our records.

CHPC at SC08

CHPC staffers Irv Allen, Steve Harper and Wayne Bradford at SC07.

CHPC with again be taking part in the ACM/IEEE Super-Computing Conference held this year in Austin, Texas. We will be highlighting research projects supported by CHPC at the University of Utah.

We will also be highlighting our involvement in the Utah Cyberinfrastructure Consortium (UtahCI), which consists of groups from the Utah State University, Southern Utah University, Weber State University, Utah Valley University and the University of Utah. The mission of UtahCI is to create and advance collaborative technological infrastructure that supports and enhances the research and educational mission of institutions in Utah.

FYI

CHPC Statitician Wins Ping Pong Championship

Dr. Byron Davis, CHPC's staff consultant for statistics, successfully defended his gold medal in the mixed doubles competition in this year's Huntsman World Senior Games held in St. George, Utah. Dr. Davis and his wife Carol Davis have competed in doubles team tournaments for more than twenty years. They have both held individual state and national titles, in addition to their current title in the mixed doubles category.

Dr. Davis is also an expert in serving up statistal data. CHPC's statistics server, Turretarch, currently runs the following software: SAS 9.1.3, R 2.5.1, S-Plus 7.0.3, HLM3, and WEKA. This server and software is available free of charge to University researchers. Dr. Davis is available to assist users in the mode of accessing the server and using the software to analyze their research data. He can be reached via email at byron.davis@utah.edu or by phone, 585-5604.

Byron and Carol Davis in championship form

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ACKNOWLEDGEMENTS

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"A grant of computer time from the Center for High Performance Computing is gratefully acknowledged."

If you use the NIH portion of Arches (delicatearch, marchingmen or tunnelarch), please add: "partially supported by NIH-NCRR grant # 1S10RR17214."

Please submit copies of dissertations, reports, preprints, and reprints in which the CHPC is acknowledged to: Center for High Performance Computing, 155 South 1452 East, Rm #405, University of Utah, Salt Lake City, Utah 84112-0190