Center for High-Performance Computing @ the University of Utah

News

University of Utah Fall, 2005

Article

Computational R&D for Industrial Applications

by Prof. Feng Liu

Department of Materials Science & Engineering, Center for Computational Design & Testing of Novel Nanomaterials, University of Utah

Recent advances in high-speed supercomputer and computational algorithms have brought us into a new era of computational materials science. These advances make it possible to investigate many existing materials systems that were previously considered intractable and also predict and design novel materials that did not exist in nature but possess desirable and superior properties. Computer modeling and simulation has not only emerged as an additional method for scientific research in parallel to experimentation and theory, but has also become a new and effective method for industrial design, testing, and development. Most exciting, computational research and development (R&D) has been rapidly emerging in many sectors of industry, with increased hiring of graduate students with computational backgrounds.

The need for computational R&D becomes even more prominent in view of the emergence of nanotechnology. The continued miniaturization of electronic and optoelectronic devices is increasing the need for nanoscale structural assemblies to perform the function of computer, laser, data storage, sensor, and satellite communication. However, the nanostructured materials and devices are generally not existing themselves in nature and thus have to be designed and made in laboratories. Also, their properties are not *a priori* known. Therefore, the fabrication and characterization of novel nanostructured materials and devices are both exciting and challenging. To this end, computational R&D has obvious advantages over the conventional experimental R&D in terms of the cost effectiveness, repetitiveness, and versatility.

For the materials industry, the cost effectiveness, the repetitiveness, and the versatility of computational prediction and design of novel materials prior to laboratory synthesis and production have shown great commercial potentials. "Computational experimentation" may now develop products that would otherwise be too costly to develop in the laboratory. Therefore, to meet the demands of the broad interests of materials industries, reliable and efficient state-of-the-art computational packages that are capable of characterizing a wide spectrum of material properties of technological interest must be developed. They must produce results that compare accurately with known properties in the representative existing materials systems and hence be applied to predict and design yet-to-be-explored novel materials. Also, such computational packages themselves possess a great market value

First-principles computational methods based on density functional theory (DFT) have been well established for predicting materials properties. They are capable of predicting the equilibrium structural and mechanical properties as well as dynamic diffusion energy barriers with an accuracy within a few percent of the experimental values and have been successfully applied to a variety of materials systems of semiconductors, metals, and ceramics. They have also made it possible to predict the non-equilibrium materials properties, such as electrical transport, from first principles by performing DFT analysis within the framework of nonequilibrium Green's function (NEGF) formalism. Such quantum mechanics-based computations are also becoming more and more efficient due to the recent advance in high-speed parallel computers and computational algorithms. The Center for High Performance Computing (CHPC) at the University of Utah hosts one of the largest parallel computational platforms for such computations.

In 2002, we established "The Center for Computational Design and Testing of Novel Nanomaterials" (CCDT, http://ccdt.coe.utah.edu/) as part of the Utah Centers of Excellence Program sponsored by the Governor's Office of Economic Development. The mission of CCDT is to develop and commercialize computational packages for materials design and testing and license designs of novel nanostructured materials and device components. Two first-principles computational engines have been developed: a "Materials Designer" (**MaDes**) for predicting the structural, mechani-

cal, and dynamic properties and a "Device Simulator" (**DeSim**) for predicting the electrical transport properties. In addition, a Web-based interface has been developed for visual, interactive, and on-line computational applications. In 2003, a spin-off company, Visual Interactive Scientific Computing, Inc. (VISCO), was founded to commercialize and market our center's technologies.

Recently, **Fairchild Semiconductor Corp.**, the world's leading silicon wafer supplier and the largest semiconductor firm in the Salt Lake valley, has granted a service contract to our center for computational characterization of oxygen diffusion in heavily arsenic (As) doped silicon (Si) to help optimize their Si wafer processing technology. It demonstrates a unique industrial application for computational materials characterization, as we briefly discuss below.

Heavily doped Czochralski-grown silicon wafer is a substrate used most frequently in power discrete devices. Arsenic has been used as one of the most important doping species for source and drain in deep submicron complementary metal oxide semiconductor (CMOS) technology. For the node smaller than 90 nm, the concentration of As in the ultra shallow source and drain is approaching a range of 10^{20}~10^{21} cm^{-3}. Knowledge about the interaction between interstitial oxygen (Oi) and As dopant and diffusion of Oi in such a heavily As-doped Si substrate will help us to better understand this system, so as to optimize the Si wafer processing for current leakage reduction.

When we computationally characterized the Oi-As interaction and diffusion barrier in the heavily As-doped Si, we found that the direct As-O bond formation is prohibitive with a large energy cost, and the optimal lowest-energy configuration is for As and O to be at the second nearest-neighbor positions forming a -Si-O-Si-As- complex, as shown in Fig. 1. Oi can therefore be trapped by As to form such a complex when Oi diffuses in As vicinity. Also, we found that Oi can easily diffuse around As with a low barrier from one complex structure to another (see Fig. 1). But it must overcome a larger barrier to escape from As. Thus, the overall Oi mobility is decreased in comparison with that in intrinsic Si. Our findings have provided key information for Farichild Semiconductor Corp. in explaining the retardation of Oi diffusion and precipitation observed in their heavily As doped Si wafer samples, and provided important guidance for improving their Si wafer process. Currently, we are extending such computational characterization to other types of dopants, including phosphorus (P), boron (B), and antimony (Sb).

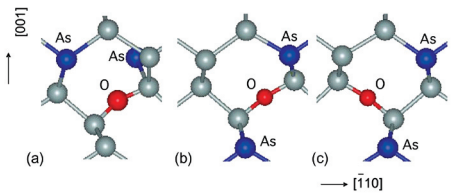


***Fig. 1**: Computational characterization of binding and diffusion of interstitial O (red) in heavily As (blue) doped Si (grey), illustrating the formation of a -Si-O-Si-As- complex*

Computational R&D can be applied not only for industrial materials characterization (which is what we are doing for Fairchild Semiconductor Corp.) but also for industrial design of new materials and devices. For example, an invention disclosure on "in situ continuous human organ pressure monitor" has been filed at University of Utah Technology Commercialization Office and a patent of "carbon nanotube electromechanical pressure sensor" has been filed through Hon Hai Precision Industry Co., both based on our center's computational R&D.

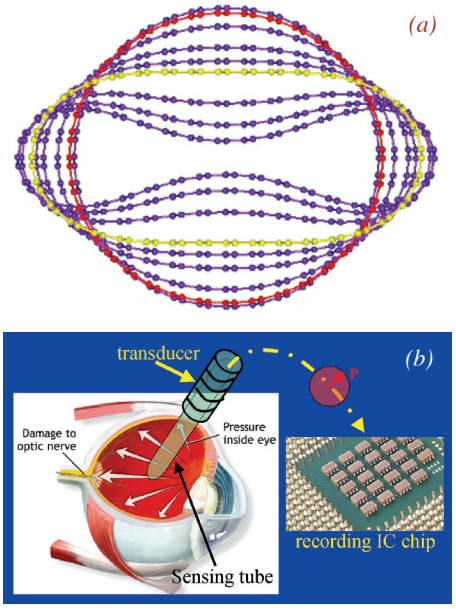


***Fig. 2**: (a) Simulated cross-sections of a carbon nanotube under pressure, displaying a series of shape transitions from circle to oval (red) and then to peanut (yellow); (b) Schematic illustration of an in situ continuous IOP monitor, based on the discovery of pressure induced tube shape transition and P-V relations*

Using Materials Designer, we have discovered novel pressure induced shape transitions and a universal constant defining such transitions for carbon nanotubes, as shown in Fig. 2a. Such a transition is further found to be universal, not limited to carbon nanotubes but apply to tubes made of any materials and of any size. Because of the derivation of a quantitative pressure-volume (P-V) relation of such transitions and its applicability to very small size, the discovery has stimulated some unique designs of minute pressure devices that can be put inside human body for medical applications. This has led to the invention of "in situ continuous human organ pressure monitor", as illustrated in Fig. 2b for an intraocular pressure (IOP) monitor for diagnosis of Glaucoma.

Using the Device Simulator, we discover also the pressure induced shape transition of carbon nanotubes in turn induces an electrical transition: the original metal tube becomes a semiconductor beyond a critical transition pressure. Such correlated mechanical and electrical response of carbon nanotube to external pressure provides an effective method for designing nanoscale electromechanical pressure sensors. The critical pressure is found to decrease with in- creasing tube radius, which allows sensing of different pressures by using different radii of tubes. Figure 3

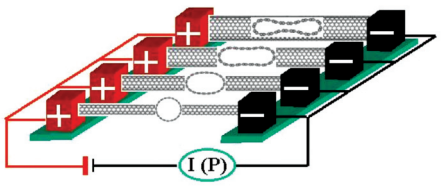


***Fig. 3**: Schematics of a tunable electromechanical pressure sensor consisting of an array of different sizes of tubes, sensing a broad range of pressures*

shows the principle-of-design of such a pressure sensor. Under a given pressure, each tube transforms into different shapes and hence exhibits different conductance. By measuring the current under a given voltage, it will be capable to detect a wide range of pressures. A patent of this pressure sensor has been filed.

To make the computational R&D a viable industrial sector, one must make the computational engines user-friendly. To this end, we have been developing a web laboratory for visual interactive on-line computational applications. An on-line 'DEMO" is available at our center's web site: http://ccdt.coe.utah.edu/. The virtual laboratory is built by integrating web interface programs with materials computational engines to provide an on-line interactive environment for computational R&D. The architecture of the web laboratory is shown in Fig. 4. It consists of a client-side interface program, a web server, a server-side interface program, an archive of computational engines, and a database server.

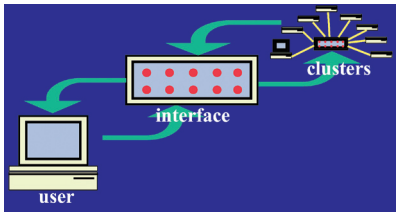


Fig. 4: Schematic illustration of the architecture of the web laboratory for computational R&D

The client side interface works as a gateway for users to log in, manage accounts, upload input files, submit jobs, run simulations, monitor the simulation process, view results in 2D and 3D graphics, and download reports. The server-side interface will perform account management, pass client-side messages to simulation programs or the database server, activate simulation programs, process simulation results, prepare reports, and pass messages from simulation programs or database server back to client-side interface. The web laboratory can be customized for individual industrial applications.

In summary, computational R&D saves time and money! We foresee that computational R&D will have broad applications in future industries, especially those industrial sectors derived from emerging nano and biotechnologies.

FYI

CHPC, in conjunction with the Scientific Computing and Imaging Institute (SCI) and the Center for the Simulation of Accidental Fires and Explosions (C-SAFE), will have a presence at this year's SC2005 conference. Hosted by the ACM/IEEE, SC2005 provides an opportunity for industry and institutions to come together, make new contacts, and learn about the leading edge in high performance computing.

Our booth this year will showcase posters from groups around our campus, highlighting work that has been aided by our HPC systems. We will also have several demos in our booth, including Jimmy Miklavcic's work *Interplay*.

Article

CHPC and Another Language: Partners in a Box of Loose Minds

by Jimmy Miklavcic

Multimedia, Telematic, and Digital Communication, Center for High Performance Computing, University of Utah

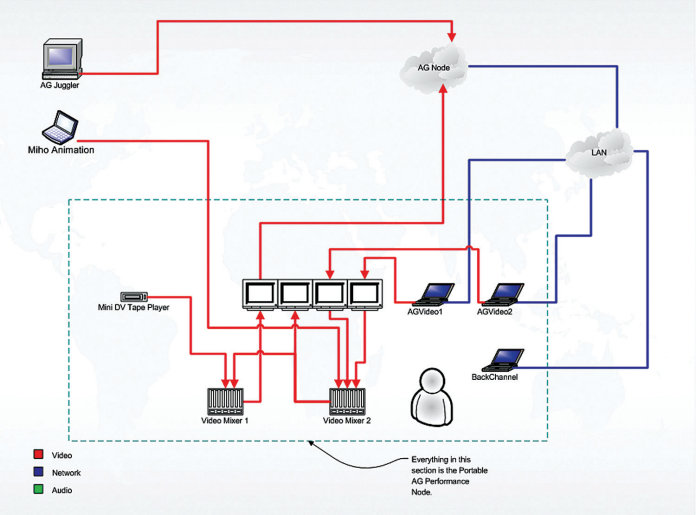
On August 3 - 4, 2005, the Center for High Performance Computing at the University of Utah, in partnership with Another Language Performing Arts Company of Salt Lake City, Utah, presented a national, real-time telematic collaborative performance titled *InterPlay: Loose Minds in a Box*. This unprecedented event took place at the Los Angeles Convention Center in Los Angeles, California, as part of the Access Grid's introduction into the Emerging Technologies program at the recent ACM SIGGRAPH 2005 Computer Graphics Conference.

InterPlay is a multi-faceted telematic collaborative event that consists of two or more performances that occur simultaneously at multiple sites throughout the world. The performances are concurrently captured, mixed, encoded and streamed onto the network. The director of the InterPlay manipulates each video stream to appear in any of several video windows. This creates a work that takes individual events and weaves them into a multi-layered distributed tapestry: the unique thought processes of each artist influence the artistic performance, then the director moves the performances to a new level by incorporating them into his/her own thought and creative process.

InterPlay: Loose Minds in a Box premiered in Salt Lake City at the University of Utah Intermountain Network and Scientific Computation Center's auditorium on April 15 – 17, 2005. It is the third performance of the InterPlay form following *InterPlay: Intransitive Senses* and *InterPlay: Hallucinations*.

Reunited to perform *InterPlay: Loose Minds in a Box* from their respective states and institutions were Scott Deal

(ARSC University of Alaska, Fairbanks), Charles Nichols (University of Montana, Missoula), Tina Shah, Helen Kostis, (Electronic Visualization Lab at University of Illinois, Chicago), T.J. Rogers, Joe Hayes, Carol Cunningham (Envision Center for Data Perceptualization at Purdue University, Indiana), Nadja Masura and Peter Rogers (Department of Theatre at University of Maryland), and Erik Brown (CHPC at University of Utah). Performing locally in the Los Angeles Convention Center were Beth Miklavcic and Jimmy Miklavcic (Another Language/CHPC at the University of Utah), Miho Aoki (ARSC at University of Alaska, Fairbanks) and Dioselin Gonzalez (Envision Center for Data Perceptualization at Purdue University, Indiana).



The performance incorporated fourteen individual video streams into a live, real-time, surrealist cinematic experience. Beth Miklavcic — assistant director, performer and Access Grid node operator — enhanced the InterPlay experience by creatively choreographing the video streams across thirty-six feet of projection screen surface. Scott Deal (percussion) and Charles Nichols (electronic violin) combined their musical virtuosity over distances of more than two thousand miles to fill the L.A. space with rich, exotic sounds. Nadja Masura and Peter Rogers transformed a classroom into their personal performance space while Tina Shah and Helen Kostis explored the solitary aspects of confinement. Joe Hayes performed within a local VR environment designed by Miho Aoki; their manifestations were sent over Internet 2 to fortify the artistic concept.

In the final scene, Joe Hayes at Purdue used the motion of his body within a motion capture system to send MIDI control information to Montana, which then manipulated a text/sound composition created by Charles Nichols. Miho contributed her incredible 3D computer animations while Dioselin manipulated characters in the VR world from a remote system. All this sonic and visual material was integrated into a cohesive, collaborative mix within the L.A. performance space.

All of the technology that Another Language used in InterPlay projects has been provided by the Center for High Performance Computing at the University of Utah. I designed a mobile AG performance system (MAGP) that was comprised of three laptops and two SIMA digital video mixers and a rack mounted LCD monitor with four four-inch color monitors. Two laptops were used to collect the incoming video streams from the various participating sites. The video output of each of these systems was connected to inputs of the pre-mixer and the master mixer. The video stream of Beth's performance connected to the pre-mixer. Miho's 3D animations connected to the master mixer. With this configuration I could select, process, and composite any three of the video sources into the main video mix..

InterPlay: Loose Minds in a Box was an exceptional demonstration of how Access Grid technology can be used to fulfill artistic ideas. Another Language has the unique opportunity to be among many of today's foremost authorities in telematic, collaborative, multimedia and computer aided arts such as Roy Ascott, Margaret Dolinsky and Don Forresta.

Another Language stepped up to the challenge of showcasing this rare quality of art coming out the state of Utah. With hard work, we met with great success. Another Language could not have done this with out the great work of those at SIGGRAPH 2005 and the technical support of those at each remote site. We especially would like to thank Donna Cox, Jeff Carpenter (NCSA), Jeff Schwab (Purdue University), Jennifer Teig von Hoffman (Boston University) and the additional support staff. Additional recognition goes out to Many Amyrolo (Ryerson University, Toronto Canada) for his work on the MIDI multicast service.

Another Language would also like to thank the University of Utah Center for High Performance Computing for supporting these projects and sponsoring our presence at SIGGRAPH 2005.

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/#chpcbib

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.

Upcoming Presentations

CHPC has developed a series of courses to help users make the most of their use of CHPC resources. We continuously add to and improve this series and present it every Fall-Winter. Please mark your calendars. These presentations are all held in the INSCC Audtitorium and begin at 1:30pm on the scheduled date:

9/29/05: OVERVIEW OF CHPC

This presentation gives users new to CHPC, or interested in High Performance Computing an overview of the resources available at CHPC, and the policies and procedures to access these resources.

The topics that will be covered include:

- The platforms available
- Filesystems
- Access
- An overview of the batch system and policies
- Service Unit Allocations

10/13/05: INTRO. TO PARALLEL COMPUTING

In this talk, we first discuss various parallel architectures and note which ones are represented at the CHPC, in particular, shared and distributed memory parallel computers. A very short introduction into two programming solutions for these machines, MPI and OpenMP, will then be given followed by instructions on how to compile, run, debug and profile parallel applications on the CHPC parallel computers. Although this talk is more directed towards those starting to explore parallel programming, more experienced users can gain from the second half of the talk, that will provide details on software development tools available at the CHPC.

10/20/05: INTRO. TO PROGRAMMING WITH MPI

This course discusses introductory and selected intermediate topics in MPI programming. We base this presentation on two simple examples and explain the MPI parallel development of them. The first example encompasses MPI initialization and simple point to point communication (which takes place between two processes). The second example includes introduction to collective communication calls (where all active processes are involved) and options for effective data communication strategies, such as derived data types and packing the data. Some ideas on more advanced MPI programming options are discussed in the end of the talk

10/27/05: MATHEMATICAL LIBRARIES AT CHPC

In this talk we introduce the users to the mathematical libraries that are installed on the CHPC systems, which are designed to ease the programming and speed-up scientific applications. First, we will talk about BLAS, which is a standardized library of Basic Linear Algebra Subroutines, and present few examples. Then we briefly focus on other libraries that are in use, including freeware LAPACK, ScaLAPACK, PETSc and FFTW, and commercial NAG and custom libraries from Compaq.

11/10/05: FAST PARALLEL I/O AT THE CHPC

Fast parallel I/O at the CHPC In this talk we explain how to perform fast parallel I/O operations on the CHPC computers. It should be beneficial for all users who are interested in speeding up their parallel applications via faster file operations. First, we describe in detail PVFS (Parallel Virtual File System), installed on Icebox. Then we go over several examples on how to perform parallel I/O on this file system, in particular, MPI-I/O extension to the MPI standard and native PVFS function calls. Subsequently we detail ways how to compile and run MPI-I/O applications on both PVFS (icebox/arches) and on the Compaq Sierra's AdvFS. We conclude the talk with an insight into some more advanced aspects of MPI-I/O.

11/17/05: CHEMISTRY PACKAGES AT CHPC

This talk will focus on the computational chemistry software packages - Gaussian, Amber, NWChem, Molpro, Amica, Babel, GaussView, ECCE - that are available on CHPC computer systems. The talk will be an overview of the packages and their capabilities, and will focus on details of how users can access the installations at CHPC.| This talk is the precursor for a second talk scheduled for next month that will focus on the use of Gaussian 98/03 and GaussView.

12/1/05: USING GAUSSIAN03 AND GAUSSVIEW

This presentation will focus on the use of Gaussian03 and Gaussview on the CHPC systems. The discussion will focus on the functionality of Gaussian as well as the format and construction of input files and PBS scripts. Restrictions on memory usage and disk space will be discussed. Timings of several jobs will be presented to demonstrate the parallel scaling that Gaussian achieves on icebox. Demonstrations on the use of GaussView will also be presented.

1/19/06: DEBUGGING WITH TOTALVIEW

This talk introduces Totalview, a debugger that has become a standard in the Unix code development comunity. After short introduction to its major features, we will present three examples, serial, parallel OpenMP and parallel MPI codes. Using these examples, we will show common and specific features for debugging these codes, as well as point out differences in using Totalview on different CHPC platforms.

1/26/06: PROFILING WITH VAMPIR/GUIDEVIEW

In this talk, we introduce a new profiling package, Vampir/Guideview, capable of profiling serial, parallel OpenMP and MPI applications. We will explain how to set up basic profiling session for serial and parallel codes, and hint on advanced features such as code instrumentation and object-oriented performance analysis. Within the talk, we will provide several hands-on examples of application profiling.

Slides from CHPC's presentations are archived on the CHPC web site. You may access them at any time by going to http://www.chpc.utah.edu/docs/presentations/ and selecting the name of the presentation either from the menu tree or the presentation list in the central content area.

CHPC Security Policies

Please read and comply with the University of Utah Information Resources Policies (http://www.admin.utah.edu/ppmanual/1/1-15.html), particularly section C and D.

CHPC does not allow clear text passwords when accessing our systems. We require the use of Secure Shell (SSH).

You may not share your account with anyone under any circumstances.

Do not leave your terminal unattended while you are logged in to your account.

Do not introduce classified or sensitive work on CHPC systems.

Protect your password and follow the password policies outlined at http://www.chpc.utah.edu/docs/policies.

Do not try to break passwords, tamper with system files, look into anyone else's directories, or otherwise abuse the trust implicit in your account.

Do not inspect, modify, distribute, or copy privileged data or software without proper authorization, or attempt to do so.

If you suspect a security problem, report it promptly to CHPC's Help Desk. Phone: (801) 971-3442 email: problems@chpc.utah.edu. If your concerns are an emergency during non-University working hours, please contact the campus help desk at 581-4000.

PASSWORD POLICY

Most systems administered by CHPC share a password database.

Choose a good password (see recommendations below). CHPC will periodically attempt to crack all passwords on the systems maintained by the center.

CHPC reserves the right to lock cracked accounts at any time, however we may attempt to notify users of weak accounts and give them an opportunity to remedy the situation prior to taking this action if operational conditions allow for it to happen.

Once this action has been taken, users will be required to contact the help desk to get their accounts unlocked. Phone: (801) 971-3442, email: problems@chpc.utah.edu

Passwords are not to be shared. If you have a student or colleague who needs to use our systems, they must apply for a separate account.

* *Do not use passwords from other facilities.*
* *Do not write your password down anywhere.*
* *Do not transmit your password via electronic mail.*

Please note: No one from CHPC will EVER ask you your password! If anyone contacts you and asks for your password, (claiming to be a CHPC employee) refuse and report it immediately to the CHPC help desk.

CHOOSING A PASSWORD

A good password is at least six, preferably seven or eight characters long. There are four classes of characters: Lowercase, Uppercase, Numbers and Symbols. You should incorporate at least two of these four classes into your new password.

Do not use actual words, whether they are in English or another language. Password cracking programs can be fed dictionaries of words, both English and foreign. These dictionaries are easily available on the net.

Avoid the names of fantasy characters.

Do not use the special codes from games (like xyzzy), which are very well known.

Do not use a word followed or preceeded by a number (like python6 or Python6).

Exchanging l's (ells) and 1's (ones) or 3's and e's can be easily broken.

Do not use your license plate number, phone number, or your spouse's/child's/lover's name or birthday.

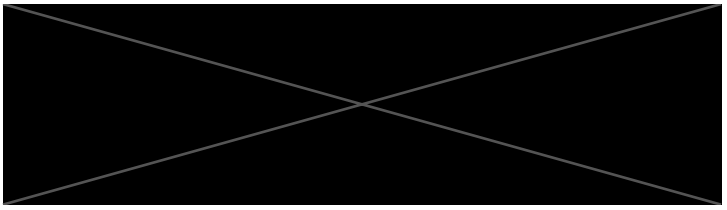
Do not use repeated patterns (C!C!C!C!) or simple keyboard patterns (qwerty).

FYI

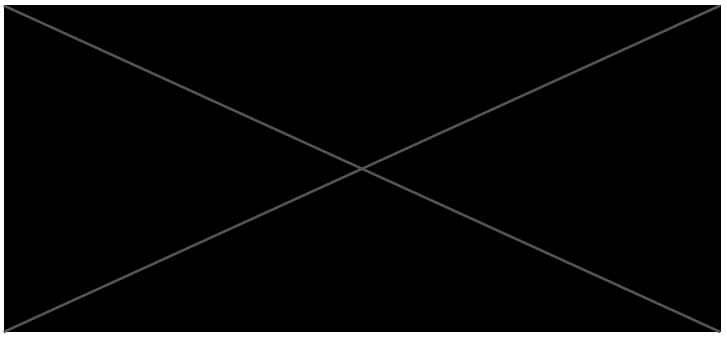
You can find CHPC security policies in their entirety on our web site: http://www.chpc.utah.edu/docs/policies/security.html

CHPC Staff Directory

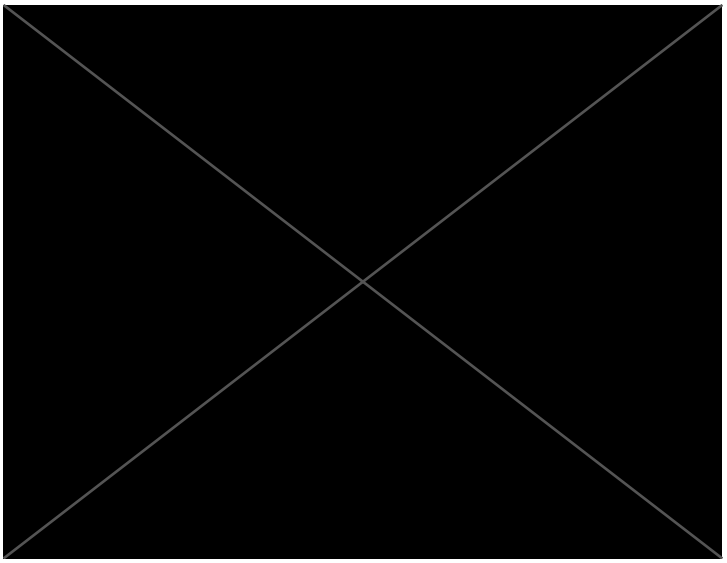
Administrative Staff	Title	Phone	Email	Location
Julio Facelli	Director			
Julia Harrison	Associate Director			
Guy Adams	Assistant Director, Systems			
Joe Breen	Assistant Director, Networking			
DeeAnn Raynor	Administrative Officer			
Victoria Volcik	Administrative Assistant			



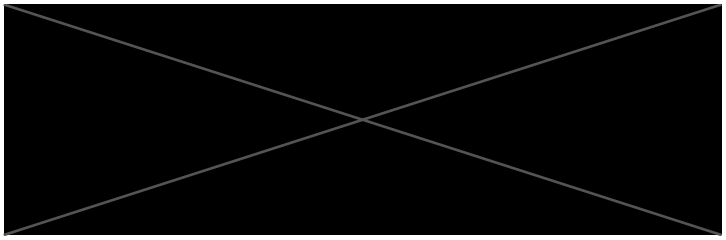
Scientific Staff	Expertise	Phone	Email	Location
James Agutter	Information Visualization			
Victor Bazterra	Molecular Sciences			
Thomas Cheatham III	Biomolecular Modeling			
Martin Cuma	Scientific Applications			
Byron L. Davis	Statistics			
Julio Facelli	Molecular Sciences			
Stefano Foresti	Information Visualization			
Robert McDermott	Visualization			
Anita Orendt	Molecular Sciences			
Alun Thomas	Bioinformatics			



Systems/Network Staff	Title	Phone	Email	Location
Irvin Allen	System Administrator			
Wayne Bradford	System Administrator			
Erik Brown	System Administrator			
Steve Harper	System Administrator			
Brian Haymore	Lead, Comp. Cluster Admin.			
Samuel T. Liston	Digital Communication & Visualization			
Shawn Lyons	Network Engineer			
Jimmy Miklavcic	Multimedia, Telematic & Digital Communication			
Ron Price	Software Engineer & Grid Architect			
David Richardson	Computer Technician			
Steve Smith	System Administration			
Matthew Thorley	Network Assistant			
Neal Todd	System Administrator			
Alan Wisniewski	Network Engineer			



User Services Staff	Title	Phone	Email	Location
Iris Boanta	Technical Assistant			
Jason Duhaine	Systems Assistant			
Derick Huth	Technical Assistant			
Beth Miklavcic	Multimedia Design, Digital Video			
Liza Newren	Technical Assistant			
Erik Ratcliffe	Graphic & Web Design			
Paul Vandersteen	Technical Assistant			



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Please help us to continue to provide you with access to cutting edge equipment.

ACKNOWLEDGEMENTS

If you use CHPC computer time or staff resources, we request that you acknowledge this in technical reports, publications, and dissertations. Here is an example of what we ask you to include in your acknowledgements:

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

If you use Arches, 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