Center for High-Performance Computing

NEWS

THE UNIVERSITY OF UTAH

SPRING 2013

Research

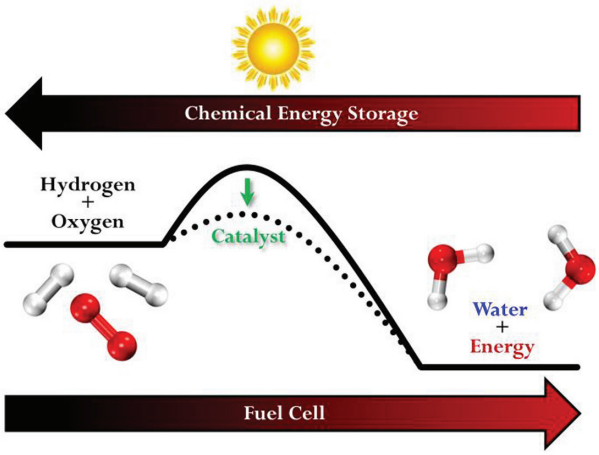
Quantum Chemistry at CHPC

By Prof. Ryan P. Steele, Dept of Chemistry

Chemistry powers the world. From combustion reactions that propel automobiles to photosynthesis reactions that harness the power of sunlight, chemistry drives the conversion from molecules to useful energy. Quantum chemistry research at CHPC includes the study, simulation, and design of these processes in new areas.

Renewable Energy Applications

The world's energy appetite is perpetually growing, and factors ranging from environmental concerns to national security motivate the search for clean, renewable sources of energy. Solar technologies are a potentially viable source, but this option also highlights the need for new chemistry. Rather than direct conversion of sunlight into energy, as in the ubiquitous solar panel, our current focus is on the chemical storage of solar energy. Simply put, energy demands continue when the sun sets and on cloudy days, and current battery technology is not sufficient or economical for widespread solar energy storage.

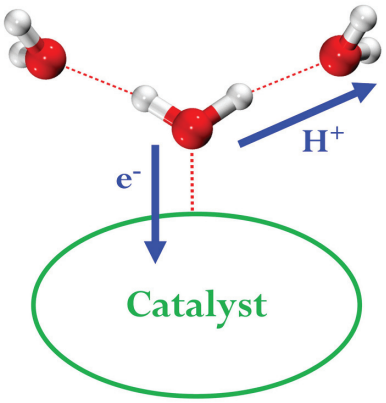


A traditional hydrogen fuel cell forms the basis of our approach. This cell combines hydrogen and oxygen to form water, along with a release of energy. This process is exquisitely environmentally friendly; the sole chemical byproduct is water itself. Along the way, the chemical energy that is stored in hydrogen and oxygen bonds is released to power devices.

A major caveat to the so-called "green" label for this process is that a significant source of hydrogen and oxygen must be available. Rather than turning to fossil fuel-based feedstocks for hydrogen, for example, sunlight can be harnessed to run the reaction in reverse.

This reverse process is called "water splitting" and stores the sun's energy in chemical bonds. Instead of its traditional role as a benign solvent, this process involves the chemical activation of water as a reactive species. The fuel cell (forward) releases energy while forming water, and water-splitting (reverse) reactions take energy from the sun as input and store the energy as hydrogen and oxygen. This process requires an uphill climb on the energy landscape, which is not naturally viable. However, the energy of the sun can be used to enable this reaction.

Traversing a large energy barrier en route to these chemical storage species is inefficient and does not make optimal use of the sun's energy. Catalysts lower these barriers, thereby increasing chemical efficiency. A handful of promising catalysts have appeared in recent years in the chemical and engineering communities. These catalysts generally offer as much promise for renewable energy as they do ambiguity for chemistry. Their catalytic mechanisms are, quite simply, poorly understood. This lack of mechanistic information is a formidable bottleneck for catalyst optimization and improvement.



Water Oxidation

$$2\,H_2O \rightarrow O_2 + 4H^+ + 4e^-$$

Work in our lab has recently focused on the detailed mechanism of water oxidation. During water splitting, a four-electron oxidation (loss of electrons) must occur to eventually yield O_2. By simulating the atomic behavior of this ionization process using quantum chemistry tools, key mechanistic details have been determined. In the figure

(Continued on Page 2)

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above, the solar catalyst enables the loss of an electron from water, which drives proton transfer to neighboring water molecules. This initial step—loss of an electron inducing atomic motion—is the key interaction between electronic and nuclear movement. But it also is only the first of several important steps.

Quantum Chemistry

The simulation of chemical motions, including the intricate, correlated dance of the electrons (i.e., bonds), requires chemists to delve into the rather bizarre world of quantum mechanics. In doing so, these simulations provide a bottom-up modeling approach with the potential for an exact simulation of chemical processes.

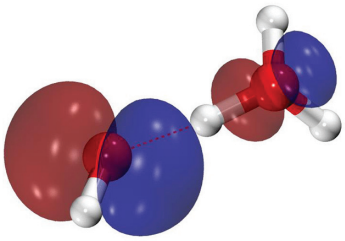
In quantum mechanics, particles behave as waves. This wavefunction describes all of a particle's properties and behavior. Two aspects seemingly preclude this knowledge: 1) the principles of quantum mechanics dictate that a wavefunction is an experimentally unobservable object; and, 2) for all but the simplest of systems, this wavefunction cannot be calculated analytically.

> *The fundamental laws necessary for the treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.*
>
> *- Paul Dirac, 1933 Nobel Prize winner*

Using novel simulation algorithms, however, as well as the high-powered computing resources of CHPC, very accurate simulations of molecules and their electrons can be obtained. Such simulations form the core of the field of quantum chemistry. Along with other members of the Henry Eyring Center for Theoretical Chemistry at the University of Utah, our research group develops faster and more accurate methods for performing such simulations and solving problems at the forefront of chemistry.

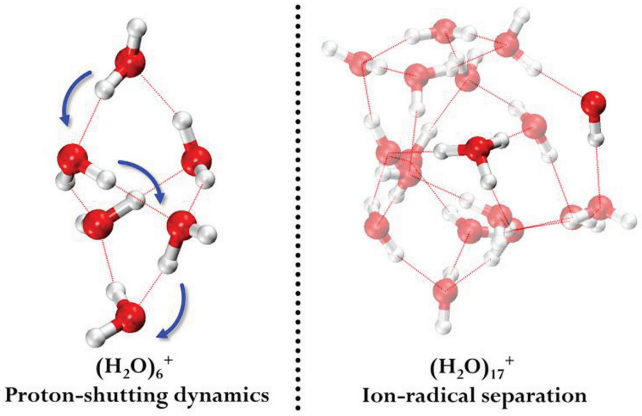
Water-Splitting Mechanisms: Electrons & Nuclei "Talk"

The water-splitting chemistry mentioned above involves the motion of atoms following removal of an electron from water. In the ionized water dimer, $(H_2O)_2^+$, which has been the prototypical species studied to date, removal of an electron occurs from the hydrogen-bonding acceptor. Rapid proton motion drives this system toward an open-shell radical species, nominally considered $HO\cdots H_3O^+$. The remaining unpaired electron is shared between the two partners, however, suggesting that they continue to interact.



Indeed, using newly developed techniques for sampling the quantum mechanical motion of the atoms, we have discovered a rather peculiar structure, in which the hydrogen-bonded proton and the terminal hydrogen atoms undergo large-amplitude motion. This structure is far more fluxional than a static picture implies. In short, every hydrogenic moiety in the complex is delocalized, in spite of the fact that this complex is stable.

The most interesting questions arise when larger water clusters are examined. While the dimer prototype exhibits the initial proton movement indicative of water ripping apart, what happens when other water molecules are present? Does this ion-radical contact pair remain intact?



Quantum chemistry simulations of the structure and dynamics of larger clusters reveal that it does not. Instead, the hydronium cation (H_3O^+) is found to diffuse away from the hydroxyl radical (OH) via a Grotthuss proton-hopping mechanism. This mechanism allows protons to quickly diffuse through solution by hopping between water molecules, rather than via the crowd-parting motions required for diffusion of more standard ions though solution. Solvation of hydronium serves as a driving force for separation of the ion-radical pair, and this behavior is confirmed by our calculations in large clusters. This result promisingly suggests that hydronium does not linger to become involved in the catalytic mechanism and can quickly diffuse from the reactive center to complete the balance of charge in an electrolytic cell.

While this result is a key piece of the water-splitting story, it is only one of four total oxidation steps and, most notably, ignores the catalyst! Current work in our group is deciphering the role that the catalyst now plays compared to this reference mechanism. Recent methodology developments will also provide computational access to these previously intractable problems.

For CHPC Users:

View The Users in Your Project

By Walter Scott, CHPC Web Developer

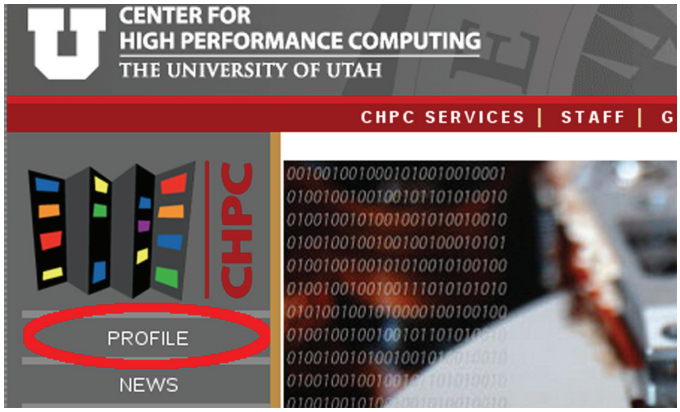
At CHPC we try to keep our account records as up-to-date as possible. Keeping accurate records not only helps us know who is utilizing our services, but it also improves our security position by allowing us to limit access to only our current users. Principal investigators (PIs) are our greatest asset when it comes to keeping account records updated because they can more easily tell us who is in their group and who has moved on.

We have implemented a utility on our web site to help principal investigators view a list of the users we have on file for their group. We ask that our researchers review this list periodically and inform us of any changes that need to be made.

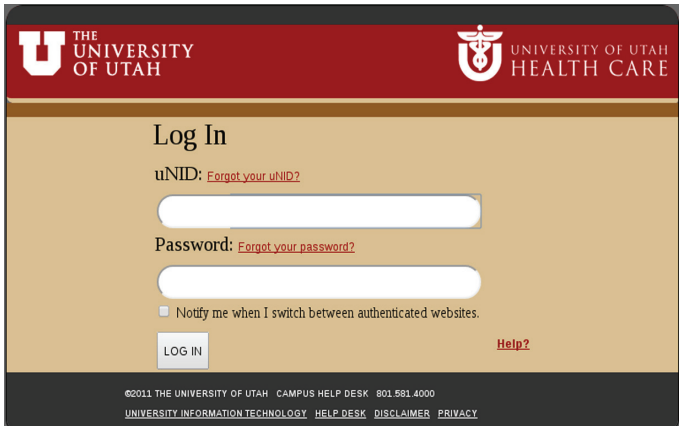
Here are the steps to access this utility:

1. Point your web browser to our web site at http://www.chpc.utah.edu

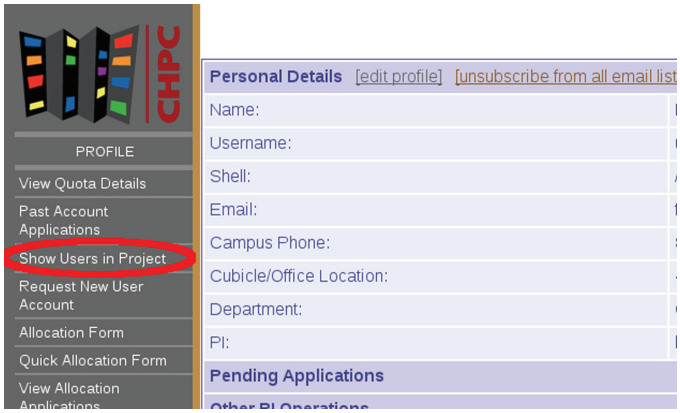
2. Click “PROFILE” on the left hand side of the page .



3. Log in using your uNID and campus password.



4. Click “Show Users in Project” on the left hand side of the page.



5. You will be presented with a list of the users in your project. For each user, you will be able to see his or her full name, uNID, the group name (most researchers will only have one group, but some have more than one), the email address, and whether we have the account currently locked (see image below).

Now that we have this utility in place, CHPC will send PIs periodic requests that they check for users who are no longer in their group. Please let us know if you want any users removed from the system by sending a list (please include names and uNIDs) to issues@chpc.utah.edu.

*Note: user deletions are permanent and the home directories of users are removed, usually 30 days after we have received the PI’s request for removal.

Name	UNID	Group	Email	Account Locked?
Full Name	u0000000	lastname	full.name@utah.edu	No
First Last	u0000001	lastname	first.last@utah.edu	Yes

News

XYZ in 3D

by Jimmy Miklavcic, CHPC Media Manager

The Center for High Performance Computing and Another Language Performing Arts Company presented the world premiere of XYZ (2013) on February 22, 2013. XYZ was a telematic cinema performance integrating live performance and 3D stereographic cinema performed in INSCC's VisLab Blackbox Theater.

XYZ was written by Elizabeth Miklavcic as a digital poem where four transcendental entities from space arrive to Earth, posing questions that engage our existence within the cosmos. The fifth character, Gaia, played by Elizabeth Miklavcic, represented the planet Earth. Gaia prepared the audience for the pending visit of Colored-By-Numbers (Hanelle Miklavcic), Ghost (Alexis Leavitt), Marooned (Jimmy Miklavcic) and Rose (Elizabeth Miklavcic) and returned after the visit to aid the audience become reacquainted with solid ground.

The performance incorporated 3D active stereographic cinema, made possible by the aid of Nvidia's Quadro 5000 graphics card and an Acer h5360bd 3D DLP Projector. Actors were recorded in front of a green screen. The video was then processed and edited with Apple's Final Cut Pro 7 and the rendered image sequences were mapped onto plane surfaces in Maya 2012. Thin circular objects, with one character in each object, were created by using a Boolean intersection between the planar surface and a flattened cylinder 720 pixels in diameter. These circular objects were then placed inside clear bubble objects that were floated, by animation, throughout the various scenes of the piece. NASA images of several different space environments such as the Green Ring Nebula, the Eagle Nebula and the Fantastic Four Galaxies were incorporated to establish a place in space for the entities to float about.

The entire production was developed by co-directors Elizabeth and Jimmy Miklavcic. This included image processing, editing original video, animating the choreographic movement of the entities and rendering left and right eye image sequences. The left and right eye image sequences were then imported and edited again in Final Cut Pro where audio and original music was added. Once completed, a final stereo video pair was exported for playback in a stereographic player and displayed on the large screen in the VisLab Blackbox Theater. Further development includes creating an anaglyph (red/cyan) video for additional screenings in larger venues and video streaming over the Internet.

Back Up Your Data!

On February 25th CHPC experienced a major file system failure that affected the home directories for users in 23 of our research groups. The incident was the result of a rare simultaneous failure of a disk and the disk controller that should have recognized the disk failure and prevented data corruption. Within a week the majority of users had their home directories fully restored and back online. Restoration for the remaining users had to be handled individually. All restores were completed by March 22nd.

CHPC does not back up /scratch file systems and the HPC general file system. For the space that is backed up, there is a complete backup every weekend, with daily incremental backups. Users should not rely on this backup as their only protection. We strongly encourage you to make copies of your own data. Having multiple copies of your most crucial data is the only guarantee that you will have the data should a machine failure occur. Hardware can and does periodically fail. This can be done in a few ways:

- Keep a copy on an external storage device.
- If you have multiple filesystems have the data on more than one.
- Take advantage of the CHPC archival service. Users can buy tapes and have us make a copy of their data. We will do this for a group only once a quarter.
- Explore other backup services offered by campus. See the UIT website for their cloud services: http://it.utah.edu/services/cloud/index.html

Congratulations to Dr. Anita Orendt, CHPC staff scientist, who received the W.W. Epstein Outstanding Educator Award from the Department of Chemistry. She is seen here (back row far left) with chemistry students and co-advisor Dr. Holly Sebahar (back row right) at the American Chemical Society's national meeting. The group was honored with the Commendable ACS Student Chapter Award.

Examples of Recent Research Using CHPC Resouces

Kochanski, A., Jenkins, M.A., Krueger, S., Mandel, J., Beezley, J. (2013). "Real time simulation of 2007 Santa Ana fires." Forest Ecology and Management 294: 136 - 149.

Olson, J. K., Boldyrev, A.I. (2013). "Planar to 3D Transition in the B6Hy Anions." J Phys Chem A 117(7): 1614 - 1620.

Staten, P. W. (2012). Understanding the causes and mechanisms of atmospheric circulation change. Ph.D., Department of Atmospheric Sciences, University of Utah.

Thorne, M. S., Zhang, Y., Ritsema, J. (2013). "Evaluation of 1-D and 3-D seismic models of the Pacific lower mantel with S, SKS, and SKKS travetimes and amplitudes." Journal of Geophysical Research: Solid Earth 118: 1 - 11.

Thorne, M. S., Garnero, E.J., Jahnke, G., Igel, H., McNamara, A.K. (2013). "Mega ultra low velocity zone and mantel flow." Earth and Planetary Science Letters 364: 59 - 67.

Yeager, K. N., Steenburgh, W.J., Alcott, T.I. (2013). "Contributions of lake-effect periods to the cool-season hydroclimate of the Great Salt Lake Basin." J. Appl. Meteor. Climate 52: 341 - 362.

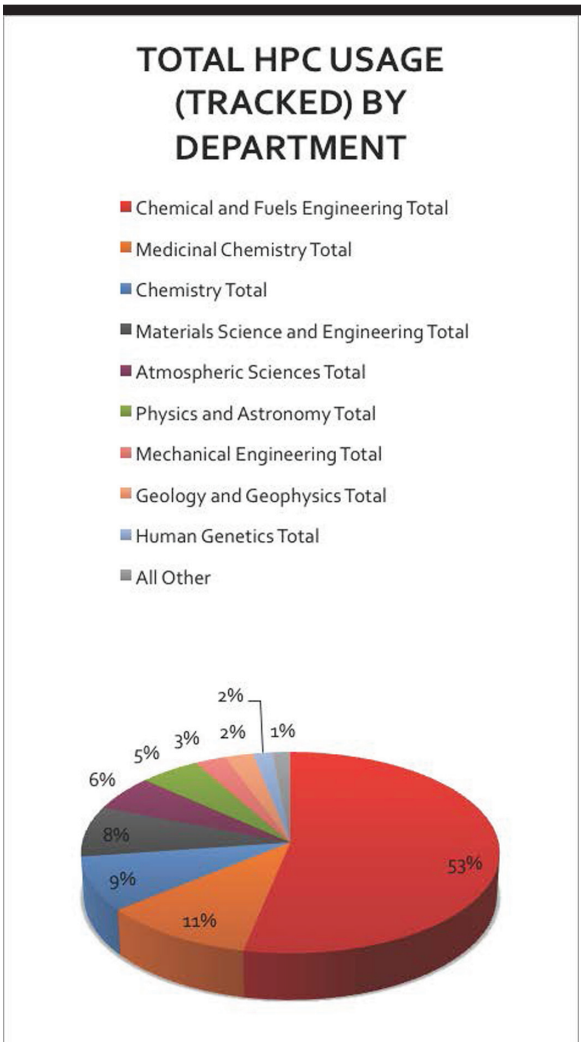
For a full bibliography go to: http://www.chpc.utah.edu/docs/research/CHPCBibliography.pdf

What is CHPC?

The Center for High Performance Computing provides large-scale computing resources to University faculty and research staff to facilitate their research. CHPC is located in the INSCC building (just north of the Park administration building) and is responsible for the operation, maintenance and upgrade of computing resources housed at data centers in INSCC, SSB, Komas and the new Downtown Data Center.

The projects currently supported by CHPC come from a wide array of University disciplines that require large capacity computing resources, both for calculating the solutions of large-scale, two and three dimensional problems and for graphic visualization of the results.

If CHPC resources would be of use in your research, please go to our website www.chpc.utah.edu for more information.



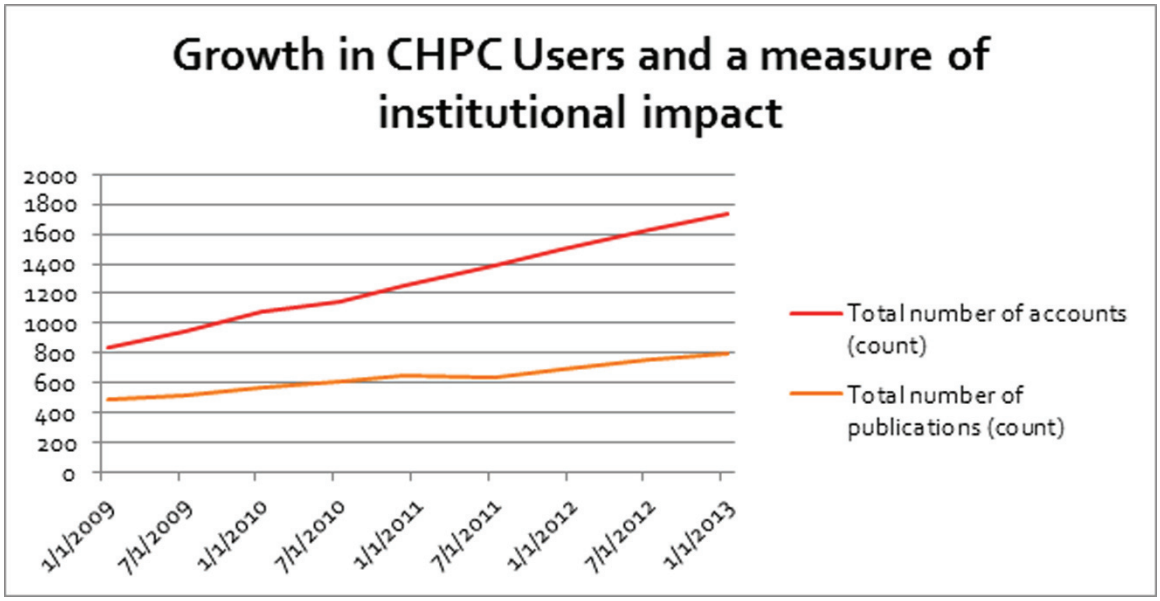
For a summary of CHPC's activities over the past two years, see our bi-annual report at http://www.chpc.utah.edu/docs/CHPCActivities_2011-2012.pdf

CHPC Growth

CHPC has experienced considerable growth over the last two years. This growth is illustrated in two graphs from CHPC recent bi-annual report. There have been significant increases in the number of groups and users. The number of research groups grew from 379 in 2011 to 447 by the end of 2012. The number of user accounts has steadily increased linearly at a rate of 6% per year. We now have nearly 1800 users, although not all are currently using our resources.

Growth is also shown in the increase in usage data. We measure usage in service units. A service unit is one hour walltime per core normalized to a 2 Ghz speed. We split usage into two categories: tracked and non-tracked. The tracked metrics on the computational nodes contains usage at the user, PI, department and college levels. The non-tracked data are more coarsely summarized only by the "ownership" of the computational resource. Examples of non-tracked data are interactive nodes on the clusters, mid-range nodes owned by departments, virtual machines and other miscellaneous computation resources supported by CHPC. The tracked usage data shows a 25% increase over the past two years: in 2011 our users used 56,906,106 service units while in 2012 they used 71,156,043 service units.

As shown in the graph to the left, half of our tracked usage comes from users in Chemical and Fuels Engineering; however, many other departments are well represented. Among those identified on this graph as "All Other" are users from Biology, Mathematics, Finance, and Internal Medicine.



CHPC Staff Directory

Administrative Staff	Title	Phone*	Email	Location
Julio Facelli	Director	585-3791	julio.facelli@utah.edu	410 INSCC
Julia D. Harrison	Associate Director	585-1869	julia.harrison@utah.edu	430 INSCC
Guy Adams	Assistant Director, Systems	554-0125	guy.adams@utah.edu	424 INSCC
Joe Breen	Advanced Network Initiatives	550-9172	joe.breen@utah.edu	426 INSCC
Jimmy Miklavcic	Manager, Media Services	585-9335	jimmy.miklavcic@utah.edu	296 INSCC
Janet Ellingson	Administrative Manager & Newsletter Editor	585-3791	janet.ellingson@utah.edu	405 INSCC

Scientific Staff	Expertise	Phone*	Email	Location
Wim Cardoen	Scientific Applications	971-4184	wim.cardoen@utah.edu	420 INSCC
Martin Cuma	Scientific Applications	587-7770	martin.cuma@utah.edu	418 INSCC
Sean Igo	Natural Language Processing	N/A	sean.igo@utah.edu	405-16 INCSS
Anita Orendt	Molecular Sciences	231-2762	anita.orendt@utah.edu	422 INSCC
Ron Price	Software Eng/Grid Architect	560-2305	ron.price@utah.edu	405-4 INSCC
Jody Smith	Database Manager	647-3042	jody.d.smith@utah.edu	405-12 INSCC

Technical Support Staff	Group	Phone*	Email	Location
Irvin Allen	Systems Admin	231-3194	irvin.allen@utah.edu	405-40 INSCC
Robert Bolton	Systems Admin	528-8233	robert.bolton@utah.edu	405-24 INSCC
Wayne Bradford	Systems Admin	243-8655	wayne.bradford@utah.edu	405-41 INSCC
Erik Brown	Systems Admin	824-4996	erik.brown@utah.edu	405-29 INSCC
Brandon Day	Tech Assistant	N/A	N/A	405-20 INSCC
Nathaniel Ellingson	Tech Assistant	N/A	N/A	405 INSCC
Jake Evans	Network Engineer	718-1526	jake.evans@utah.edu	405-22 INSCC
Steve Harper	Systems Admin	541-3514	s.harper@utah.edu	405-31 INSCC
Brian Haymore	HPC Systems	558-1150	brian.haymore@utah.edu	428 INSCC
Eric Hughes	Systems Admin	879-8449	eric.hughes@utah.edu	405-18 INSCC
Samuel T. Liston	Systems Admin	232-6932	sam.liston@utah.edu	405-39 INSCC
Beth Miklavcic	Multimedia	585-1066	beth.miklavcic@utah.edu	111 INSCC
Michael Palmer	Systems Admin	435-720-3261	michaelj.palmer@utah.edu	405-28 INSCC
David Richardson	Network Engineer	550-3788	david.richardson@utah.edu	405-38 INSCC
Walter Scott	User Services	309-0763	walter.scott@utah.edu	405-13 INSCC
Steve Smith	Systems Admin	581-7552	steve.smith@utah.edu	405-25 INSCC
Neal Todd	Systems Admin	201-1761	neal.todd@utah.edu	405-30 INSCC
Alan Wisniewski	Network Support	580-5835	alan.wisniewski@utah.edu	405-21 INSCC

*All phone numbers are preceded by area code 801 unless otherwise noted.

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THE UNIVERSITY OF UTAH

Center for High Performance Computing
155 South 1452 East, RM #405
SALT LAKE CITY, UT 84112-0190

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If you would like to be added to our mailing list, please fill out this form and return it to:

Janet Ellingson
THE UNIVERSITY OF UTAH
Center For High Performance Computing
155 S 1452 E ROOM 405
SALT LAKE CITY, UT 84112-0190
FAX: (801)585-5366

(room 405 of the INSCC Building)

Name:
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Department or Affiliation:
Email:

Address:
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Thank you for using our Systems!

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.*"

Please submit copies or citations of dissertations, reports, pre-prints, 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