Center for High-Performance Computing @ the University of Utah

News

University of Utah Spring, 2006

Article

Common Grid Architecture for Scientific Applications: Application to MGAC (Modified Genetic Algorithms for Atomic Clusters and Crystals)

by Ron Price, Victor Bazterra, Wayne Bradford, Julio C. Facelli

Center for High Performance Computing

There are many sites across the country that have grid infrastructure[1] without any grid applications running them, but many applications could use efficient grid based resources. For instance MGAC (Modified Genetic Algorithms for Atomic Clusters and Crystals)[2-4] is an application that for very large size problems shows significant load balancing issues that can be mitigated using a grid architecture. We are modifying MGAC to become a custom grid application (MGAC-CGA). Creating MGAC-CGA will allow the application to have access to more resources, improve load balancing and automate tedious and time consuming tasks such job submission and "baby sitting" in multiple computer systems. The tasks that will be automated will take care of queue related problems such as finding a suitable queue, submitting to the queue and checking job status in the queue. Eventually, in later stages of development we will add some fault tolerance which will resubmit a job if system related issues occur (i.e. network down, scheduler unavailable). The grid functionality will be provided by calls to Globus Toolkit 4.0 (http://www.globus.org/) application program interface (API). CHPC is also using this architecture as a template for researchers at the University to implement similar CGAs for other applications, such as distributed flexible docking (in collaboration with Prof. Thomas Cheatham) and combustion simulations (in collaboration with Prof. Phil Smith).

The implementation is being done in three phases. During phase one, which has been completed, we have installed GT4 on two machines at our center and created the following proof of concepts: submit a job manually from one machine to the other using the Web Service Grid Resource Allocation Manager (WS-GRAM), write a program that submits a job from one machine to the other using WS-GRAM and lastly write a program that submits a Job from one machine to the other using WS-GRAM and act on notifications provided from the external states of the managed job services in WS-GRAM: un-submitted, stage in, pending, active, suspended, stage out, clean up, done and failed. In phase one the events that occur are limited since the scheduler will be a Unix fork by default, although it will be the perfect opportunity to work out the complexities of the Grid Security Infrastructure (GSI), WS-GRAM API and firewall related issues.

We have taken the first step towards creating MGAC-CGA by installing, configuring and testing GT4 on one of the machines at our center. Currently GSI, WS-GRAM and all of its dependent services/protocols are functional. Next we will setup the second machine and continue with phase one. Our primary target is TeraGrid since MGAC needs more resources than our policies allow for and TeraGrid just began to test GT4.

In phase two, that is under way, we will have to reconfigure GSI in order to establish trust between a secure local machine at our center (depicted as "Local Host" in figure 1) and all TeraGrid sites. At this point we will implement the following architecture:

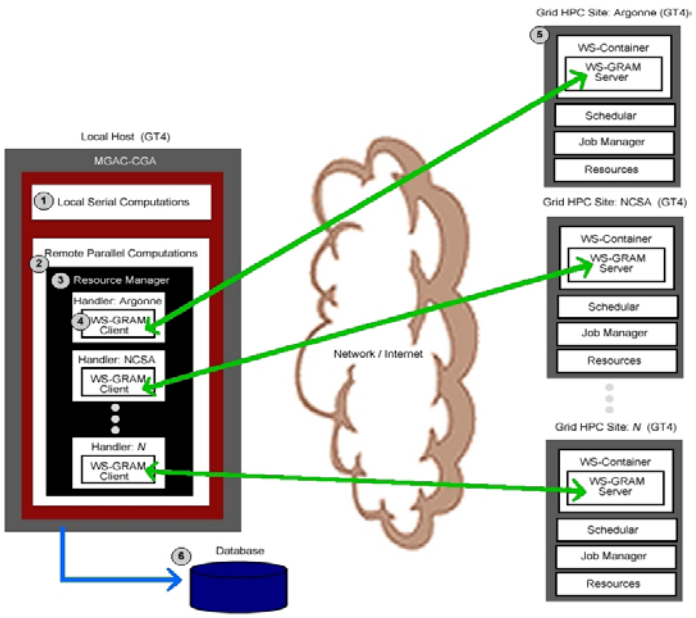


Figure 1

** MGAC-CGA will be composed of two types of computations: serial and parallel. The serial computations that need be completed locally and the parallel computations that need to be completed remotely. Here, local computations are being executed to create the next generation of atomic clusters.*

** The remote parallel computational portion of MGAC-CGA requires parallel resources to evaluate optimizations of*

** The Resource Manager portion of MGAC-CGA will be multi threaded. The Resource Manager will be responsible for managing up to N Handlers by spawning, deleting, waiting on and restarting handler instances.*

** Handlers are individual processes running in the resource manager controlling the execution of WS-GRAM Clients; each handler instance is responsible for one WS-GRAM Client. The handlers receive commands from the Resource Manager that tell the handler what to run and what type of resource is needed. The handler then interprets the commands and feeds them to a WS-GRAM client that will take care of staging files, job submission and listening for notifications.*

** At the Grid HPC Site the WS-GRAM server will receive the WS-GRAM clients request and act upon it by submitting a job to the scheduler and sending notifications back to the WS-GRAM client. The notifications will be the same notifications used in phase one, only now that we have a scheduler to help form the notification the WS-GRAM Client will be provided with more precise information. Since MGAC-CGA can have N handlers it will be able to submit jobs to N Grid HPC sites that have GT4 enabled.*

** Once the Handler has returned its results to the Resource Manager the core MGAC logic becomes aware of the results and saves them off to a database.*

Phase three will be to add some fault tolerance to MGAC-CGA and a web interface. Also we will investigate implementing Monitoring and Discovery client logic as Grid HPC sites such as TeraGrid begin to test them.
As the Global Grid Forum solidifies its decision on a high level Grid API through the Simple API for Grid Applications Research Group (SAGA-RG) we will migrate to that API. Currently we are evaluating the Grid Application Toolkit (GAT) and so is SAGA-RG. The advantage to using GAT is that as standards change the GAT API will not change. Also, standards will inevitably change and technology will evolve therefore we expect to re-factor portions of our code base.

Successful implementation of MGAC-CGA has several significant benefits to our center and the scientific community as a whole. This would benefit our center by laying the foundation for other applications to be grid enabled, but most importantly MGAC-CGA would provide the computational power necessary to obtain results that MGAC itself couldn't obtain. This would benefit the scientific community by acting as a case study on how to turn a computationally demanding application in to a custom grid application and provide the application with resources it needs. Another benefit to the community would be proof that our frame work for grid enabling an application is valid.

REFERENCES

1 F. Berman, G. Fox, and T. Hey, (John Wiley & Sons, London, 2003), p. 1080.
2 V. E. Bazterra, M. Cuma, M. B. Ferraro, et al., J. of Parallel and Distrib. Comput. 65, 48 (2005).
3 G. M. Day, W. D. S. Motherwell, H. Ammon, et al., Acta Crystall. B B61, 511 (2005).
4 O. Oña, V. E. Bazterra, M. C. Caputo, et al., Phys Rev. A 72, 053205 (2005).

Article

State of the Art Clinical Skills Testing Facilities in the New Health Sciences Education Building

by Jimmy Miklavcic
Multimedia, Telematics & Digital Communications, Center for High Performance Computing, University of Utah

Clinical Skills System's monitor and control room.

The University of Utah Health Sciences Center is home of one of the most state of the art Clinical Skills education facilities in the intermountain region. Located on the third floor in the newly constructed Spencer F. and Cleone P. Eccles Health Sciences Education Building (HSEB), the Clinical Skills Suite is the most technological intensive facility in the building. It is designed to support clinical education, utilizing standardized patients.

An interior core is provided for the preparation of the standardized patients, with access to each of the eighteen examination rooms. Students access the examination rooms via a surrounding hallway. Each examination room is equipped with an examination table and associated equipment. The student/standardized patient experience is managed using the B-Line Medical's Clinical Skills System. This system captures in real-time, a video/audio record of the experience for review by the student and/or instructor, provides facility management and tracks student performance.

In May of 2003, Wayne Peay, director of the Spencer S. Eccles Health Sciences Library, approached the Center for High Performance Computing to assist in either developing or locating technology that could be utilized in such a facility. Developing a system from the ground up seemed a daunting task and one that, we thought, would be a task of last resort.

A search was first initiated to locate other health science facilities that might have developed an automated Clinical Skills System and at that time, none were found. We tried to look for any current technology that could be adapted and we felt that the Access Grid™ system, developed by Argonne National Laboratory, had many aspects that could be adapted upon and modified to fit. One major component was missing. The ability to record and playback, on demand, any of thetwenty-two possible examinations was grossly underdeveloped and unreliable. Without this cru-cial functionality, we realized that Access Grid technology would be too cumbersome to build upon in the short time that we had before us.

We continued our search for a system that could be modified to fit the needs of the HSEB. During a perusal of security systems we came across Vicon Security Systems. This was very promising. The Vicon system had the crucial function of recording each examination room as well as the ability to play back, on demand, any recorded examination. Although the format of the recording was a proprietary implementation of MPEG-4 that forced to use their playback software, we felt that we were on the right track. In fact, a system, configured to fit the Clincal Skillls Suite, was ordered.

Clinical Skills System's student exam station outside each of the exam rooms.

The B-Line Express Clinical Skills System's integrated hardware.

In November of 2004, B-Line Express, a new start-up company that was developing a clinical skills system for George Washington University and Ohio State University, contacted Wayne Peay. Investigating B-Line's web site we realized that they had created a complete solution to clinical skills education and testing. We contacted the two institutions to get inside information on the system and how it was being used. Upon hearing the successes of both the Ohio State University and the George Washington University implementations of B-Line's product, we decide to forego the Vicon Security System and replace it with an implementation of the B-Line Express Clinical Skills System.

The hardware of the B-Line Express Clinical Skills System is a heterogeneous integration of off-the-shelf components that are controlled and monitored by a well-

conceived software system. The solution revolutionizes the way institutions create, administer, record and score Clinical Skills encounters with standardized patients and simulators. Through a remarkably easy to use, web-based application, the system includes user management and exam content creation, exam management, scoring and reporting, and professional quality audio and video.

Some of the hardware components include twenty-two MPEG-4 video encoders, video storage and on demand video server, video router, application server, and web server. The system is programmed to activate for a scheduled examination, automatically initiating the exam content on networked PC systems inside and outside each exam room. The standardized patient uses the system in the exam room and the student being tested uses the system outside. Once the exam has been completed, the exam is scored and immediately available to the student for review. The system resets and initiates the next scheduled exam. Both the student and instructor can review the exam scores and the recorded examination experience from anywhere in the building with proper network authorization.

Since its opening, the Clinical Skills Suite is scheduled constantly by nearly every department and college in the University of Utah Health Sciences Center. It is managed by the Clinical Suite Subcommittee, which includes representatives from the School of Medicine, College of Nursing, College of Pharmacy and the Eccles Health Sciences Library.

B-Line Express has since changed its name to B-Line Medical and has now installed several Clinical Skills Systems in health facilities across the country. It also provides a software solution for those who choose to purchase and install their own hardware. For more information about B-Line Medical visit *www.blinemedical.com.*

Upcoming Presentations

CHPC has developed a series of courses to help users make the most use of CHPC resources. Please mark your calendars. These presentations are all held in the INSCC Audtitorium and begin at 1:30pm on the scheduled date, unless otherwise stated:

April 20th: Network Communication Tools:
From Skype to Access Grid

April 27th: Chemistry Packages at CHPC
(10:30 - 12:00)

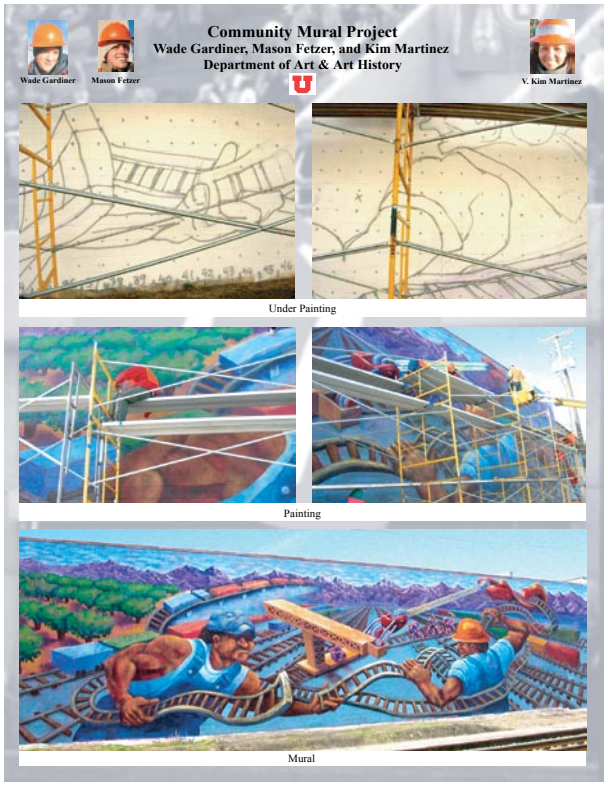
May 4th: Using Gaussian03 and Gaussview

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.

Report

Research Posters on the HIII 2006

by Robert McDermott
Staff Scientist for Visualization, Center for High Performance Computing, University of Utah



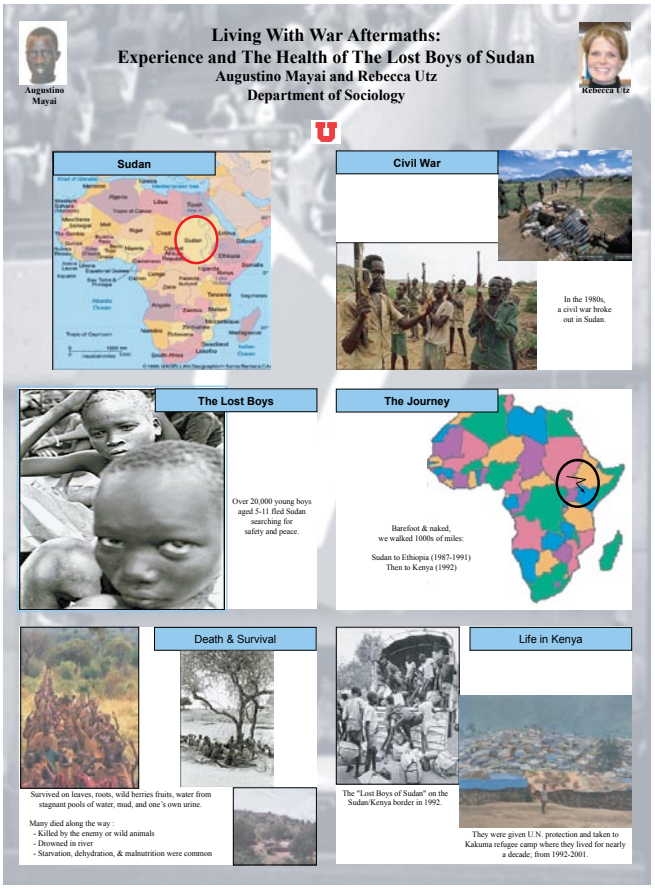
This year's Research Posters on the Hill event took place on Thursday, January 26th in the Auditorium of the State Office Building on Capitol Hill from 8:00am to 1:00pm. As has been the case for the past six years the event is shared with students from Utah State University. All of the participating students have graduated high school within the state of Utah.

Every year we make efforts to improve the event and this year was no different. Firstly, we assigned all senators and all representatives to students this ensured that our students would make contact with every senator and every representative. Secondly, letters from each student were placed in envelopes and hand delivered to their assigned legislator's mail boxes, inviting legislators to attend the event. Thirdly, handouts were printed to include a picture of their poster on one side of a page and their abstract for their work on the other side of a page. These pages were placed in envelopes and also hand delivered to legislator's mail boxes.

This year we featured the work of fine art students, Wade Gardiner and Mason Fetzer, who were two of eight students painting a large scale mural (100 foot long by 25 foot high), located along the UTA TRAX Line. A set of posters were produced to show this work and other murals painted by University students. In addition to these students and their work we drew attention to three other poster projects. In one project a Fine Art Ceramics student, Kristen

McDermaid, had collected clay from a number of sites across to state. She used these clays to produce slips for glazing her ceramics. Each of her clays produced a distinctive slip which in turn produced a distinctive coloration for her ceramics. Kristen exhibited pieces of her ceramics in addition to her poster. A Fine Art Printmaking student, LeGrand Olsen, exhibited his woodcuts depicting scenes of Salt Lake City in addition to his poster. The printmaking process was the focus of his poster. A third poster from Eric Sahm and Mike Davis from the Department of Geology had a set of posters depicting work of WEST (Water, the Environment, Science and Teaching): implementing inquiry-based learning in K-12 classrooms. These two students had supporting posters exhibited additional work of WEST with Birds, Erosion and Insects projects.

In addition to these four featured posters we had 30 posters from across campus representing a wide variety of disciplines. Of particular note was a poster by Augistino Mayai from the Department of Sociology. He had made the very long walk with the Lost Boys of the Sudan. When civil war broke out in Sudan they walked to Ethiopia and when civil war broke out there they walked back to Sudan and then on the Kenya. In Kenya the U.N. set up stable camps and schools. After a time these boys were resettled in the U.S. and in particular a small group including Augistino settled in Salt Lake City.

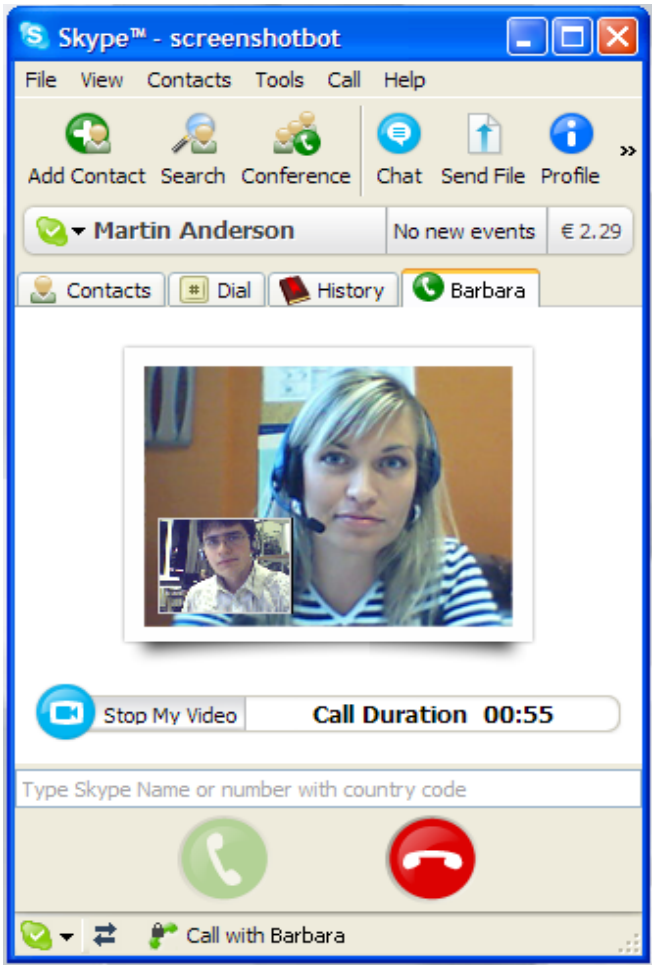


The work of two other students to be considered was a poster by William McKean a Department of Biology student working in a Human Genetics Laboratory with Chicken Embryos and a poster by Jeremy Alvord another Department of Biology student working in a Pediatrics Laboratory with Lamb Embryos. These two posters are strong examples of fundamental research being conducted in the Medical Sciences

Report — Video Conference and Access Grid Facilities

by Jimmy Miklavcic
Multimedia, Telematics & Digital Communications
Center for High Performance

Video and audio conference technology has now expanded into a wide spectrum of hardware and software products for the laptop up to the large meeting facility with a cost ranging from free to more than fifty thousand dollars. Here at CHPC we can offer services with systems that span this wide range.



FYI

For the latest news, system status, and downtimes, see the CHPC home page: *http://www.chpc.utah.edu/*

Skype

The simplest and most cost effective system available is Skype. Most noted for its voice over IP functionality, it now offers video capabilities. You can download the product from www.skype.com and the installation only takes a few minutes. The free version allows you to contact any other Skype user free of charge or make conference calls with up to four other people. You can talk or chat for as long as you like. For an extra cost, you can call any landline. The video service is just as easy to use but is limited to one-on-one video conversations.

H.323 ViaVideo II

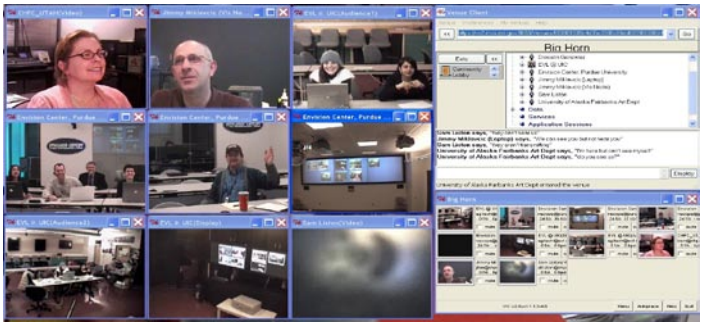
H.323 is the IP based equivalent to the H.320 videoconference technology that utilizes standard and ISDN phone lines. We have two ViaVideo II H.323 cameras available for checkout. We can supply a laptop or you can use your own. The ViaVideo II will work for up to five local participants in a point-to-point meeting. It can be expanded to two or more sites if one of the remote sites offers a connection to an H.323 Multipoint Conference Unit (MCU).

To initiate a meeting you just dial up the other site's IP address. With this system, when you are in a conference with more than two sites, you will only see the site that is speaking or, if you are speaking, the last site that spoke. You do not get the full experience of the other sites connected to the meeting.

Access Grid

The Access Grid™ (AG) is ideal for individual to large network wide meetings and seminars. CHPC has several ways to assist you in participating in Access Grid activities. In the INSCC Auditorium (RM 110) we have a full AG system for large-scale meetings, presentations and remote seminars. We will be soon upgrading the an AG system in the Visualization Lab (RM 294) that will be ready in late summer. We also have desktop and laptop systems for those individuals who want to meet or attend remote seminars.

The Access Grid software is available for various versions of Linux, Windows XP and MacOS X. CHPC staff is available to assist anyone who would like to use or setup their own Access Grid system. For more information about the Access Grid you can visit *http://www.accessgrid.org* or contact Jimmy Miklavcic at jimmy.miklavcic@utah.edu.



CHPC Security Policies

Please read and comply with the University of Utah Information Resources Policies, particularly sec. 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.

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:

www.chpc.utah.edu/docs/research/CHPCBib.html

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 Staff Directory

Administrative Staff	Title	Phone	Email	Location
Julio Facelli	Director	556-2426	Julio.Facelli@utah.edu	410 INSCC
Julia Harrison	Associate Director	652-0019	julia.harrison@utah.edu	430 INSCC
Guy Adams	Assistant Director, Systems	554-0125	gadams@chpc.utah.edu	424 INSCC
Joe Breen	Assistant Director, Networking	550-9172	jbreen@chpc.utah.edu	426 INSCC
DeeAnn Raynor	Administrative Officer	581-5253	dee@chpc.utah.edu	412 INSCC
Janet Ellingson	Administrative Assistant	585-3791	janet@chpc.utah.edu	405-2 INSCC

Scientific Staff	Expertise	Phone	Email	Location
James Agutter	Information Visualization	581-8779	agutterja@arch.utah.edu	235 AAC
Thomas Cheatham III	Biomolecular Modeling	587-9652	cheatham@chpc.utah.edu	306 INSCC
Martin Cuma	Scientific Applications	587-7770	mcuma@chpc.utah.edu	418 INSCC
Byron L. Davis	Statistics	585-5604	byron@chpc.utah.edu	416 INSCC
Julio Facelli	Molecular Sciences	556-2426	Julio.Facelli@utah.edu	410 INSCC
Stefano Foresti	Information Visualization	581-3173	stefano@chpc.utah.edu	322 INSCC
Robert McDermott	Visualization	581-4370	mcdermott@chpc.utah.edu	420 INSCC
Anita Orendt	Molecular Sciences	231-2762	orendt@chpc.utah.edu	422 INSCC
Alun Thomas	Bioinformatics	587-9309	alun@gene.pi.med.utah.edu	Research Park

Systems/Network Staff	Title	Phone	Email	Location
Irvin Allen	System Administrator	231-3194	iallen@chpc.utah.edu	405-40 INSCC
Wayne Bradford	System Administrator	243-8655	wayne.bradford@chpc.utah.edu	405-41 INSCC
Erik Brown	System Administrator	824-4996	erik@chpc.utah.edu	405-29 INSCC
Brian Haymore	Lead, Comp. Cluster Admin.	558-1150	brian@chpc.utah.edu	428 INSCC
Samuel T. Liston	Digital Communication & Visualization	232-6932	stliston@chpc.utah.edu	405-30 INSCC
Jimmy Miklavcic	Multimedia, Telematic & Digital Communication	585-9335	jimmy.miklavcic@utah.edu	296 INSCC
Ron Price	Software Engineer & Grid Architect	560-2305	rprice@eng.utah.edu	405-4 INSCC
David Richardson	Computer Technician	550-3788	drr@chpc.utah.edu	405-23 INSCC
Steve Smith	System Administration	581-7552	steve@chpc.utah.edu	405-25 INSCC
Matthew Thorley	Network Assistant	560-3438	ruach@chpc.utah.edu	405-20 INSCC
Neal Todd	System Administrator	259-3495	neal@chpc.utah.edu	405-31 INSCC
Alan Wisniewski	Network Engineer	580-5835	quantix@chpc.utah.edu	405-21 INSCC

User Services Staff	Title	Phone	Email	Location
Iris Boanta	Technical Assistant	N/A	iris@chpc.utah.edu	405-10 INSCC
Jason Duhaine	Systems Assistant	N/A	jason@chpc.utah.edu	405-28 INSCC
Shawn Lyons	Network Assistant	N/A	slyons@chpc.utah.edu	405-22 INSCC
Beth Miklavcic	Multimedia Design, Digital Video	585-1066	bam@chpc.utah.edu	111 INSCC
Liza Newren	Technical Assistant	N/A	liza@chpc.utah.edu	405-9 INSCC
Paul Vandersteen	Technical Assistant	N/A	paul@chpc.utah.edu	405-19 INSCC

The University of Utah seeks to provide equal access to its programs, services, and activities to people with disabilities. Reasonable prior notice is needed to arrange accommodations.

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

Welcome to CHPC News!

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

Janet Ellingson
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:
Phone:

Department or Affiliation:
Email:

Address:
(UofU campus or U.S. Mail)

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.*"

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