Center for High-Performance Computing

NEWS

THE UNIVERSITY OF UTAH

SPRING 2014

Research

Autism Research within CHPC's Protected Environment

By Sabree Crowton and Nicole Fisher, UT-ADDM

CHPC has a robust protected environment that allows researchers using protected health information (PHI) to gather, process and store data. In addition to providing access to high performance computing power, other tangible benefits for researchers using PHI is that CHPC handles systems management issues, such as rapid response to electrical power issues, provision of reliable cooling and heating, VPN support for a work-anywhere computing experience, and ensures a hardened, secure environment compared to office computers or departmental servers. This resource allows much better compliance and reduces the vulnerabilities of exposure of PHI data.

One example of current research within this environment is the Utah Autism and Developmental Disabilities Monitoring Project (UT-ADDM) headed by Deborah Bilder, M.D. and William McMahon, M.D. in the Department of Psychiatry at the University of Utah's School of Medicine. UT-ADDM is part of the Utah Registry of Autism and Developmental Disabilities (URADD), a partnership between the Utah Department of Health, the Utah State Office of Eduction and the University of Utah.

Autism Spectrum Disorders (ASDs) have recently been a topic of interest in the United States media. The news media speculate on the causes behind the startling rise of these disorders over the past decade. Utah is often in the spotlight as an example of significant increase in the number of children with an ASD. The 2013 Utah Department of Health Status Update reports: "Utah rates are among the highest in the nation and nearly double the national average." Research indicates that the measured prevalence of ASDs in Utah children eight years of age more than doubled from 2002 to 2010.

The Utah Autism and Developmental Disabilities Monitoring Project (UT-ADDM) was established in 2003 as one of the Centers for Disease Control and Prevention (CDC)'s ADDM Network sites. In collaboration with the Utah Department of Health and investigators from the University of Utah, UT-ADDM partners with state and local agencies and organizations that serve children with developmental disabilities and their families to track the number of 4-year-old children and 8-year-old children with ASD, intellectual disability, or both. This program also gathers information on the characteristics of children with ASD and on factors that are associated with risk for this condition. UT-ADDM data can be used to promote early identification, plan for training and service needs, guide research, and inform policy so that children and families in our community get the help needed.

According to The American Psychiatric Association's Diagnostic and Statistical Manual-IV (DSM-4), a child must meet the following criteria in order to be identified as having an autistic spectrum disorder: 1) qualitative impairment in social interaction; 2) qualitative impairment in communication; 3) restricted repetitive and stereotyped patterns of behavior, interests, and activities; 4) delays or abnormal functioning, with onset prior to age 3 years, in social interaction, language as used in social communication, and/or symbolic or imaginative play; and 5) the disturbance is not better accounted by Rett's Disorder or Childhood Disintegrative Disorder. The newer DSM-5, which came out in May 2013, will be incorporated in Study Year 2014

The project's most recent study year concluded on March 27, 2014 with the release of data from Study Year 2010. These estimates are based on information collected from the health and special education records of children who were 8 years old and living in Salt Lake, Davis and/or Tooele counties in 2010. Overall, UT-ADDM identified 442 children with ASD, including children with and without a diagnosis documented in their records. The estimates for 2010 indi-

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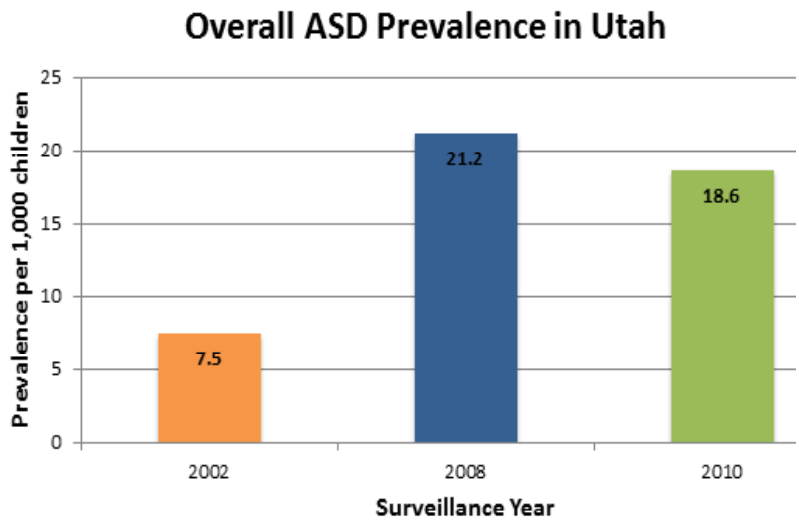
cate that 1 in 54 children (or 18.6 per 1,000 8-year-olds) were identified with ASD. This estimate is higher than the average number of children identified with ASD (1 in 68) in those areas of the United States where the CDC tracks ASD. Boys were almost 5 times more likely to be identified with ASD than girls. One in 34 boys was identified with ASD compared to 1 in 135 girls. Thirty-three percent of children identified with ASD were evaluated for developmental concerns by the time they were three years old. Eighty percent of children identified with ASD had a diagnosis documented in their records. On average, those children were diagnosed at age 4 years and 5 months, even though children can be diagnosed as early as age two.

With the assistance of the University of Utah's Center for High Performance Computing, the UT-ADDM team is able to process, organize, and analyze the data collected for their report within CHPC's PHI protected environment. In addition, CHPC provides essential storage and technological support for the computational needs of the researchers. Indeed, the safety and reliability of CHPC has been indispensable to the UT-ADDM project. In addition to maintaining and updating the current database, CHPC is building a database to house information from previous study years in a secure manner that is easily accessible and non-corruptible.

By studying the prevalence of ASDs and other developmental disabilities in Utah over time, UT-ADDM will be gathering important information that will inform public policy decisions, improve community awareness, assist in the identification of risk factors and identify underserved populations.



Further research is required to determine the causes behind the dramatic upsurge in ASD cases. Some increase is likely due to improvements in screening, diagnosis and treatment, awareness, and record keeping/documentation. However, there may be other developmental, genetic or environmental factors playing a role in the increased prevalence of ASDs. Researchers from multiple disciplines have begun investigating possible causes of the disorder. Ongoing research has been looking into the roles of air pollution and chemicals. In addition, neuroscientists are trying to find specific genes or neural pathways that may be contributing to ASD.

This winter CHPC staff moved the center's computational resources from the Komas and SSB Data Centers to the University's Downtown Data Center. Updraft was retired and ember was divided, with Phil Smith's nodes creating the new cluster ash. Kingspeak continues to expand as research groups purchase nodes. CHPC has also added storage capacity. Photo by Sam Liston.

News

CHPC Joins Consortium to Share HPC Expertise

by Janet Ellingson

The National Science Foundation has awarded a grant of $5.3 million to a consortium of university high performance computing centers that includes CHPC. With Clemson University as the lead, the group includes the centers at University of Utah, University of Hawaii, Harvard, University of Southern California, and University of Wisconsin. The purpose of the grant is to establish a peer group of "research and education facilitators" (REFs) whose experience and expertise will be a resource for researchers throughout the nation who need greater computing power than their desktops provide, yet don't have the expertise in advanced cyberinfrastructure (ACI) or the experience in massively scaled cluster computing. The need for these ACI-REFs has become more apparent as researchers in disciplines that have not traditionally used high performance computing now realize the benefits of computational power.

CHPC's REFs -- Wim Cordoen, Anita Orendt and Martin Cuma

CHPC's scientific staff, Dr. Anita Orendt, Dr. Martin Cuma and Dr. Wim Cardoen, are the University of Utah's REFs who will join with the other staff members from the other sites in the consortium as they begin to create a national infrastructure support model that will help faculty and staff achieve their research goals. The REFs from the consortium institutions will gather together at the University of Utah during the first week in June 2014. During this initial meeting, the ACI-REFs will become well acquainted with each other and develop a plan, according to the grant proposal, to create "a community of practitioners that shares resources, experience, and expertise to facilitate new knowledge discovery." Once the community is established, if researchers on our campus need assistance in a particular science domain where our local ACI-REFs don't have expertise, they will be directed by our staff to this nation-wide pool where the needed expertise may already exist. Likewise, our REFs will assist researchers from other institutions, thus providing access to a bigger pool of knowledge.

University of Utah researchers, however, need not wait for the creation of a national network of experts, as Anita, Martin and Wim are eager to help faculty and students whose research would benefit from CHPC's computational resources. CHPC staff can also assist researchers, when appropriate, in the use of national infrastructure such as Extreme Science and Engineering Discovery Environment (XSEDE) and the Open Science Grid (OSG).

CHPC staff is looking forward to the additional resources that will be available to researchers through this program.

Sam Liston's photo of CHPC's pod 1 hot aisle at the Downtown Data Center. This pod holds the VM servers and storage.

XSEDE Workshops

CHPC will host three XSEDE workshops this summer:

Harness the Power of GPUs: Intro to GPGPU Programming
(June 16 - 20, 2014)

Harness the Power of GPUs, an Intro to GPGPU Programming, is a mixture of lecture and labs that introduces all levels of parallelism as well as common approaches for parallelization in order to achieve the following goals: 1) better utilization of the GPUs by enabling more scientists to use them; 2) better understanding of the efficiency in the GPU utilization by the application developers; and 3) a higher job throughput by enabling more resources and shortening job runtimes. In addition, participants will understand and avoid the common pitfalls of parallel computing, learn CUDA and OpenACC, understand the basic principles of data parallel computing, tap into enormous computing power, even on a laptop, and speed up research.

All-in-one Hybrid Computing Workshop
(June 24 - June 27, 2014)

This 4-day event will include MPI, OpenMP, OpenACC and accelerators and run June 24-27. We will conclude with a special hybrid exercise contest that will challenge the students to apply their skills over the following 3 weeks and be awarded the First Annual XSEDE Summer Boot Camp Championship Trophy - worth up to $8.

Data Intensive Summer School
(June 30 - July 2, 2014)

The *Data Intensive Summer School* focuses on the skills needed to manage, process and gain insight from large amounts of data. It is targeted at researchers from the physical, biological, economic and social sciences that are beginning to drown in data. We will cover the nuts and bolts of data intensive computing, common tools and software, predictive analytics algorithms, data management and non-relational database models. Given the short duration of the summer school, the emphasis will be on providing a solid foundation that the attendees can use as a starting point for advanced topics of particular relevance to their work.

Registration will be found at this site: **https://www.xsede.org/web/xup/course-calendar.** CHPC will be posting more specific information on its website as the dates approach.

SC14 New Orleans, LA | hpc matters.

This year's SuperComputing Conference will be in New Orleans, November 16 - 21, 2014. The conference attracts over 11,000 attendees from all over the world. Sam Liston is now planning the University's exhibit for the convention floor. At CHPC's booth he highlights University of Utah research that uses CHPC's computational resources. As you can see from the photo below of last year's booth, Sam creates a bold and colorful display using posters and video monitors. If you would like your group's research highlighted, contact Sam Liston.

"CHPC plays a central role in multiple aspects of the research carried out in my lab. We own two compute nodes on the ember computer cluster and 35 TB of storage space. In addition, we use the common compute nodes on the kingspeak and ember clusters on a daily basis. Our research program uses genomics based approaches to uncover novel mechanisms that regulate brain function, behavior and susceptibility to psychiatric disorders. We require CHPC resources on a daily basis to analyze genome and transciptome data, to model gene networks and gene interactions in the brain, and to identify novel disease-linked gene pathways. My lab places constant demands on CHPC staff to help with data storage, analyses and the installation of new software. We are very grateful for the outstanding support this team provides. "

Assistant Professor Christopher Gregg, Neurobiology & Anatomy and Human Genetics

News

What's New at CHPC?

By Anita Orendt

- The migration of all hardware from SSB and Komas to the Downtown Data Center has been completed. This allows us to change our downtime scheduling policy as we no longer need quarterly downtimes for maintenance of the cooling systems at Komas. See the new downtime policy at **https://wiki.chpc.utah.edu/display/policy/1.7+Downtime+Policy**

- Kingspeak general CHPC nodes now include four 20-core nodes along with the original 32 16-core nodes. This results in new ways to request general nodes. These have been added to the "Resource Specification Section" of the Kingspeak User Guide found at **https://wiki.chpc.utah.edu/display/DOCS/Kingspeak+User+Guide**

- There are new options for guest access to CHPC clusters. Jobs run in this manner are pre-emptible by any jobs submitted by the owner of the nodes your job is using:

  - For owner nodes on kingspeak and ember use '#PBS -A owner-guest' (starting Apr 15, 2014)

  - For ash.chpc.utah.edu use '#PBS -A smithp-guest' (use ash-guest.chpc.utah.edu to access general ash interactive nodes).

  - For telluride.chpc.utah.edu use '#PBS -A cheatham-guest'

- CHPC has recently deployed FastX, a tool to interact with remote linux systems graphically in much more efficient, effective way than by using simple X forwarding. The new tool allows users to display individual applications or whole desktop environments, and also allows for detaching/reattaching (from the same or a different location) to the graphical sessions. For more information about this along with details of how to download a client and CHPC's usage policies for this tool please see: **https://wiki.chpc.utah.edu/display/DOCS/FastX**

- We are upgrading the license server for commercial software licenses administered by CHPC to a set of three redundant servers. This setup should improve availability of the licenses and also enable us to change license definitions without stopping the license services. Users will also be able to see the status of the licenses by pointing their web browser to **http://alecto.inscc.utah.edu:8090**

- Watch for announcements of the availability of a freecycle cluster named lonepeak. It should be available in June.

Selection of Recent Research Using CHPC Resources

Austin, D. (2013). Verification and Validation of a geomechanical model aimed at simulating wellbore completion via shape-charge jet perforation of metal and penetration into sandstone. Ph.D. Dissertation, University of Utah.

Baron, R. (2013). "Fast Sampling of A-to-B Protein Global Conformational Transitions: From Galileo Galilei to Monte Carlo Anisotropic Network Modeling." Biophysical Journal 105: 1545 - 1546.

Bergonzo, C. Galindo-Murillo, R; Cheatham, TE (2013). "Molecular modeling of nucleic acid structure: Electrostatics and solvation." Current Protocols Nucleic Acid Chemistry 55: 7.9.1 - 7.9.27.

Bradford, W., Hurdle, J.F., LaSalle, B., Facelli, J.C. (2014). "Development of a HIPAA-compliant environment for translational research data and analytics." J Am Med Informatics 21: 185 - 189.

Edalatpour, S., Francoeur, M. (2014). The Thermal Discrete Dipole Approximation (T-DDA) with Surface interaction: Formulation and Preliminary Results. NanoRad 2014. Shanghai, China.

Fleming, A. M., Orendt, A.M., He, Y., Zhu, J., Dukor, R. (2013). "Reconciliation of Chemical, Enzymatic, spectroscopic and Computational Data to Assign the Absolute Configuration of the DNA Base Lesion Spiroiminodihydantoin." J of American Chemical Society 135: 18191 - 18204

Levkova, L., DeTar, C. (2014). "Quark-gluon plasma in an external magnetic field." Phys. Rev. Lett. 112: 012002.

Milo, A., Bess, E. N., Sigman, M.S. (2014). "Interrogating selectivity in catalysis using molecular vibrations." Nature 507: 210 - 215.

Rutz, J. S., Steenburgh, W.J.; Ralph, F.M.(2013). "Climatological characteristics of atmospheric rivers and their inland penetration over the western US." Mon. Wea. Rev. 142: 905 - 921.

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." J. of Geophysical Research: Solid Earth 118: 1 - 11

Zgarbova, M, Luque, FJ, Sponer, J, Cheatham TE: Otyepka, M, Jurecka, P.(2013). "Toward improved description of DNA backbone: Revisiting epsilon and zeta torsion force field parameters." J Chem Theor Comput 9: 2339 - 2354.

Owner Nodes and VM Agreements

by Anita Orendt

Over the last several months CHPC staff has been working with the CHPC User Council and the University IT Research Portfolio Governance group to develop Faculty Resource User Agreements for both owner nodes and for the provisioning of Virtual Machines (VMs). One of the motivations for establishing these agreements is the growth in the number of owner nodes and VMs that CHPC now runs. CHPC currently has 25 different groups that own nodes on kingspeak and/or ember; in terms of node counts these groups own 122 of the 158 kingspeak nodes, and 75 of the 142 ember nodes. CHPC also runs two clusters that are owned by individual groups, ash which has 251 nodes and telluride with 89 nodes. For VMs, CHPC currently has 219 running – with 38 of them in the protected environment.

For the owner nodes, the agreement details both the provisioning and the support of the node. This provides owners with a written document outlining the operation, support, and life cycle of the owner node, the costs of the nodes, their acceptable use and a list of responsibilities that both the owner and CHPC have in the operation of the nodes. This agreement was emailed in late March to all PIs who own nodes. It is also posted here: **https://wiki.chpc.utah.edu/display/policy/2.3+Adding+Nodes+to+CHPC+Clusters**

For VMs, the agreement contains two documents. The first is a general agreement covering the creation and acceptable usage of any VM provisioned by CHPC in a similar manner as the owner nodes. The second document outlines the specific terms for a given VM, covering the PI request with the manner of usage, as well as the specification of the VM size and OS, any software that will be installed, and a listing of what CHPC will provide and what is the PI's responsibility. CHPC will be working with VM owners to finalize individual agreements and a general agreement will eventually be posted in our online policy manual.

"The impact of the CHPC computer farms is enormous for the Cosmic Ray Group of the Department of Physics and Astronomy. We collect large amounts of data from the Telescope Array Experiment, and analyze it on CHPC computers. We use even more CPU time on CHPC computer systems to generate large numbers of events for our Monte Carlo simulations of the experiment. The CHPC is a crucial resource for us and I don't know what we would do without it."

Prof. Gordon Thomson, Physics and Astronomy

NFS Grants at CHPC

by Joe Breen

With funding from the National Science Foundation, CHPC staff is working on two projects that promise to improve access to computational resources for the University of Utah's diverse research groups.

The first, "CC-NIE Integration," will create a sliceable network to meet the numerous complex requests from researchers who need special network treatment, including higher bandwidth, increased security, and access to space outside the firewall (referred to as the "Science DMZ"). For example, slices for the "DMZ," network experiments, and dedicated student experiments will all reside simultaneously on the same hardware yet maintain their unique characteristics. Steve Corbató, Deputy CIO and CHPC's interim director, is the PI along with Adam Bolton (Astronomy), Tom Cheatham (Medicinal Chemistry), and Rob Ricci (Computer Science). Joe Breen, CHPC's lead on advanced network initiatives, coordinates the work.

The second project, "MRI: Development of APT, a Testbed Instrument with Adaptable Profiles for Network and Computational Science," has a similar goal of providing our diverse research community access to shared computational resources. A testbed control system will allow the efficient use of the hardware by easily repurposing hardware to meet the changing profiles and time demands of the participating groups. The project is headed by Rob Ricci, the project's PI, and School of Computing's FLUX group, with CHPC staff providing the networking and hardware expertise. The VP of Research provided matching funds for the hardware, which now resides at the Downtown Data Center.

In Memorium
Steve Smith - 1955 - 2014

Steve Smith was hired at the Center for High Performance Computing (CHPC) in 2003 as a desktop Windows system administrator. He consistently took the users' needs to heart. He spent countless extra hours weeknights and weekends recovering data and cleaning machines from malware infections so that the users would not lose their research data. He was a great co-worker and we miss him.

CHPC Staff Directory

Administrative Staff	Title	Phone*	Email	Location
Steve Corbató	Interim Director			
Julia D. Harrison	Associate Director			
Guy Adams	Assistant Director, Systems & Network			
Anita Orendt	Assistant Director, Research Consulting & Faculty Engagem			
Janet Ellingson	Administrative Manager & Newsletter Editor			

Scientific Staff	Expertise	Phone*	Email	Location
Wim Cardoen	Scientific Applications			
Martin Cuma	Scientific Applications			
Sean Igo	Natural Language Processing			
Albert Lund	Graduate Assistant			

Project Leads		Phone*	Email	Location
Wayne Bradford	Security			
Joe Breen	Advanced Network Initiatives			
Steve Harper	Virtualization			
Brian Haymore	HPC & Storage			
Sam Liston	Special Events/SC			

Technical Support Staff	Group	Phone*	Email	Location
Irvin Allen	Systems Admin			
Nathaniel Ellingson	Tech Assistant			
Jake Evans	Network Engineer			
David Heidorn	Systems Admin			
David Richardson	Systems Admin			
Walter Scott	User Services			
Alan Wisniewski	Network Support			

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

What is CHPC?

The University of Utah's Center for High Performance Computing (CHPC) purview is to support University faculty and research groups whose main focus requires computing and advanced networking as core instrument(s) central to their research. The Center provides large-scale computer systems, storage, networking, and the expertise to optimize the use of these high-end technologies. CHPC facilitates advancement in academic disciplines whose computational requirements exceed the resources available in individual colleges or departments. CHPC also provides a protected environment for health science researchers. Since 1996 these resources have resulted in more than 900 scientific publications.

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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.*"

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