Community Update - June 2012

Upcoming Events

SHARCNET Literacy (New User) Webinars:
Monday, July 23 @ 2pm &
Monday, July 30 @ 11am

Western Summer Workshop on Scientific and High Performance Computing
Parallelization Overheads (part II)
Thursday, July 19 @ 10am
Western Science Centre, Room 148
Speaker: Marc Moreno Maza, Department of Computer Science, Western University

Building and Linking Local, Regional, and National Cyber infrastructure to Advance Science
Friday, July 20 @1pm EDT
University of British Columbia
Speaker: Daniel Katz, Sr. Fellow in the Computation Institute (CI), University of Chicago and Argonne National Laboratory
Compute Canada is arranging for his talk to be shared via videoconference to sites across Canada.
(Please note that SHARCNET AccessGrid rooms do not support Vidyo, we encourage remote attendance via the desktop).

Ontario Summer School on HPC – East
July 23-26
University of Ottawa
We are pleased to announce the Ontario High Performance Computing Summer School - East, hosted by HPCVL and jointly organized by the Ontario HPC consortia: SHARCNET, SciNet and HPCVL. This 4-day series of workshops will cover introductions to shared and distributed parallel programming using OpenMP (for multicore machines), MPI (for clusters), CUDA (for GPU's) and much more.

For help attending a webinar, see the SHARCNET help wiki.

Note: SHARCNET events can also be found online.

SHARCNET Research Support Programmes

Click here for information on the revised Continuous Small Dedicated Resources Programme.

Questions about our research support programmes may be e-mailed.

Equipment Update

Whale's replacement nodes were delivered in June and will be combined with *orca* to replace the computational capabilities lost with the decommissioning of *whale*.

Click here to help select the proper system for your jobs or e-mail help.
SHARCNET training wiki also provides help in selecting the proper cluster for your work.
SHARCNET system updates are posted online.

SHARCNET™

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Compute Canada

Compute Canada is currently undergoing significant restructuring to refine and improve its governance model. As part of this process, a Governance Advisory Committee was struck by the Board with the support of the Canada Foundation for Innovation (CFI), to provide Compute Canada with recommendations about how to restructure the governance model going forward for a strong and successful organization. This committee held its first face-to-face meeting June 27-29. The committee is currently drafting recommendations, which will receive preliminary review by the Board before being released to the community for feedback in July. This information is also contained in the Compute Canada July newsletter.

Site Leader Updates

Thomas Wolf gave the following talks:

- June 13-16: *Travelling waves and conservation laws for complex mKdV-type equations*, 2012 SIAM Conference on Nonlinear Waves and Coherent Structures in the session Novel Symbolic Methods to Investigate (Integrable) Nonlinear Differential Equations that was co-organized with Willy Hereman
- June 18-21: *A solver for linear algebraic systems resulting from filtering discrete structures*, the SIAM Conference on Discrete Mathematics DM12 at session MS41 Interactions between Computer Algebra and Discrete Mathematics - Part I of III Dalhousie University, Halifax, Nova Scotia.
- June 24-28: *Recent extensions of the package CRACK for the solution of non-polynomial differential systems of equations*, Canadian Applied and Industrial Mathematics Annual Meeting, CAIMS 2012 in MS 4279 Minisymposium Applications of computer algebra in applied and industrial mathematics 2 Fields Institute in Toronto.

These talks report on research that made use heavily of SHARCNET computer resources. *More*

Hugh Couchman and John Morton attended HP-CAST 18 in Hamburg, Germany, June 15-16.

We would like to collect user-generated visualization to showcase results on our website, for presentations & training materials, and for reporting to our funding agencies. We would also like to learn more about challenges that researchers face when trying to visualize their multi-dimensional/massive datasets, as we may be able to offer our expertise. If any researchers have examples of great visualization based on their calculations on SHARCNET, please e-mail these.

SHARCNET Events Held

SHARCNET Literacy (New User) Webinars:
June 4, 11, 18, 25

Ontario Summer School on HPC – West
June 4-8 – Western University

Ontario Summer School on HPC – Central
June 25-28 – University of Toronto

VCL training
June 25-27
Western University

Western (UWO) Summer Workshops on Scientific and High Performance Computing:
June 14: *Serial, threaded, MPI and GPU execution models*. Speaker: Tyson Whitehead.
June 21: *Parallel solution of PDEs: Algorithms and software*. Speaker: Ge Baolai.
July 5: *Optimizing algorithms and code for data locality and parallelism*. Speaker: Marc Moreno Maza.
July 12: *Parallelization Overheads (Part I).* Speaker: Marc Moreno Maza.

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SHARCNET In the News

Sheridan Awarded $1 million for New NSERC Industrial Research Chair (SHARCNET researcher Dr. E. Sykes)

Do you twitter? Send your twitter handle to info@sharcnet.ca and we'll add you to the feed. SHARCNET's twitter is "@sharcnet", or follow Compute Canada "@computecanada".

New User Spotlight

This month we highlight Rebecca Harrop who is working with Dr. Scott Hopkins in the Chemistry Department at the University of Waterloo. Rebecca is researching the process of sulphur adsorption on rhodium nanoclusters, with the view that such studies will shed light on the process of sulphur poisoning of bulk rhodium catalysts. The SHARCET systems are used to run quantum chemical calculations that predict isomeric structures and physico-chemical properties for small RhnSm+ clusters ($n \leq 12$, $m \leq 3$). These predictions will aid in the interpretation of experimental data acquired during spectroscopic and chemical dynamic studies. Such studies also provide a deeper understanding of the evolution of bulk phase properties from those of the constituent atoms and molecules, and in some cases may be used to identify unique nanocluster properties, which can be employed in the design of new nanostructured materials. SHARCNET has been an invaluable tool for the computational aspects of this research. Identification of the low energy RhnSm+ cluster structures requires several thousand electronic structure calculations, which must be undertaken at the density functional theory level. *Without the aid of a HPC cluster, these calculations would take many years to complete. SHARCNET is very efficient and user friendly and it has been a great asset to our research team*.

Upcoming Workshops and Conferences

Perimeter Institute Scientific Seminars
Waterloo, ON

SC'12, The International Conference for High Performance Computing, Networking, Storage and Analysis
November 10-16, 2012
Salt Lake City, Utah

---*SHARCNET is one of seven HPC consortia in Canada that operates under the umbrella of Compute/Calcul Canada.*