Compute Canada Overview

Ramses van Zon

Compute/Calcul Canada

June 28, 2016
What is Compute Canada?

www.computecanada.ca

- The national advanced research computing (ARC) facility of Canada,
- The not-for-profit corporation formed to manage that project, and
- A federation of 35 institutions who are members of that corporation. The 35 institutions collectively own the infrastructure and employ the skilled personnel (sysadmins and analysts) that comprise the facilities.

- Provide resources and support for advanced research computing for *all* Canadian academic researchers and collaborators.

*The federated CC Team has been assembled from long-standing institutional consortia that now participate in CC as partner Regional Organizations:*

ACENET, Calcul Quebec, Compute Ontario (SHARCNET, SciNet, CAC) and WestGrid.
Compute Canada Projects

- **ATLAS**: “Tier2” computing and storage for the ATLAS experiment at the CERN Large Hadron Collider.
- **CANFAR**: Computational platform to analyze Canadian astronomy data.
- **CBRAIN**: International project to make brain images and computational tools available to researchers around the world.
- **IceCube**: Compute and storage contribution to the IceCube Neutrino Observatory.

- **LIGO**: Support and Resources for Canadian participants in the Laser Interferometer Gravitational Observatory.
- **SNOLAB**: Data analysis for several major experiments at this underground laboratory.
- **TRIUMF**: Canada’s national lab for nuclear and particle physics.

And >343 projects allocated to individual PIs.
## Compute Canada compute resources

<table>
<thead>
<tr>
<th>Name</th>
<th>Cores</th>
<th>Nodes</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP2</td>
<td>30,984</td>
<td>1291</td>
<td>2011</td>
</tr>
<tr>
<td>GPC</td>
<td>30,912</td>
<td>3864</td>
<td>2009</td>
</tr>
<tr>
<td>Guillimin</td>
<td>20,176</td>
<td>2714</td>
<td>2011</td>
</tr>
<tr>
<td>Orcinus</td>
<td>9,616</td>
<td>930</td>
<td>2011</td>
</tr>
<tr>
<td>Orca</td>
<td>8,320</td>
<td>360</td>
<td>2011</td>
</tr>
</tbody>
</table>

- Plus many smaller systems.
- Growing user base with, for the last 5 years, very little increase in resources.
- Many systems soon to be retired.
Systems Planned for the Near Future

- **GP1**: Cloud system (≥ 3000 cores)
- **GP2**: General purpose system (≥ 18000 cores)
- **GP3**: Similar to GP2
- **LP**: Large parallel machine (≥ 66,000 cores)

(core counts only indicative)
GP1  Cloud system ($\geq 3000$ cores)

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Support and training

- 200 FTE of support staff
- Training on CC level:
  - IHPCSS
  - Tutorials at HPCS, and
  - Contributions to Software Carpentry
- Most training by local consortia
  (local summer schools, courses, workshops)

www.accelerateddiscovery.ca/training/workshops-seminars
www.calculquebec.ca/en/support-and-documentation/training
support.scinet.utoronto.ca/education
www.sharcnet.ca/help/index.php/Main_Page
www.hpcvl.org/support-and-training
www.westgrid.ca/support/training
How to Get an Access

www.computecanada.ca/research-portal/account-management/apply-for-an-account

- Any Canadian academic researcher can request a Compute Canada account, and then request an account with the local consortia.
- Researchers can sponsor their group members, as well as (international) collaborators.
- There is no cost involved.
- Always access to support staff
- Having an account get you ‘default’ status, i.e., you can run at modest scale and at low priority
- PI can submit to the annual Resource Allocation Competition to request compute resources; when granted, this translates in priority in the queue and increased limits on number of cores, etc.
Partnership for Advanced Computing in Europe

International HPC Summer School 2016

Ljubljana, 28 June 2016

Florian Berberich
PRACE Board of Directors
PRACE - OVERVIEW
PRACE is an international not-for-profit association under Belgian law, with its seat in Brussels.

PRACE counts 25 members and 2 observers.

The PRACE Hosting Members are France, Germany, Italy and Spain.

PRACE is governed by the PRACE Council in which each member has a seat. The daily management of the association is delegated to the Board of Directors.

PRACE is funded by its members as well as through a series of implementation projects supported by the European Commission.

28/06/2016
4 Hosting Members offering core hours on 6 world-class machines

**MareNostrum:** IBM BSC, Barcelona, Spain

**JUQUEEN:** IBM BlueGene/Q GAUSS/FZJ Jülich, Germany

**CURIE:** Bull Bullx GENCI/CEA Bruyères-le-Châtel, France

**SuperMUC:** IBM GAUSS/LRZ Garching, Germany

**Hazel Hen:** Cray GAUSS/HLRS Stuttgart, Germany

**FERMI:** IBM BlueGene/Q CINECA, Bologna, Italy
435 scientific projects enabled

11.4 thousand million core hours awarded since 2010 with peer review, main criterion is scientific excellence. Open R&D access for industrial users with >50 companies supported

>7 350 people trained by 6 PRACE Advanced Training Centers and others events

24 Pflop/s of peak performance on 6 world-class systems

530 M€ of funding for 2010-2015, access free at the point of usage

25 members, including 4 Hosting Members (France, Germany, Italy, Spain)
Access through PRACE Peer Review

- **Free-of-charge** BUT required to publish results at the end of the award period
- **Preparatory Access** (2 or 6 months)
- **SHAPE Programme** (2 or 6 months)
- **Project Access** (12, 24 or 36 months)

www.prace-ri.eu/call-announcements/
PRACE TRAINING
PRACE Training Offerings

**PRACE-PP**
- 2 Seasonal Schools
- 2 Workshops
- 1 EU-US Summer School
- PATCs (conception)
- Training Portal (establishment)

**PRACE-1IP**
- 4 Seasonal Schools
- 2 Workshops
- 2 International Summer School
- 6 PATCs (conception)
- Training Portal (establishment)

**PRACE-2IP**
- 4 Seasonal Schools
- 2 Workshops
- 2 International Summer School
- 6 PATCs (establishment)
- Training Portal (content)
- Training Surveys

**PRACE-3IP**
- 3 Seasonal Schools
- 1 International Summer School
- 6 PATCs (sustainability, industry)
- Training Portal (industry)
- Training Surveys

**PRACE-4IP**
- 6 Seasonal Schools
- On-demand Events
- 2 International Summer School
- 6 PATCs (assessment)
- Training Portal InDiCo
- MOOCs
- CodeVault
Seasonal Schools

• Have been running since 2008
• Offering top-quality face-to-face training events
• Organised around / all over Europe
• Topics range from generic intermediate to advanced
• From programming techniques to more specialised topical schools

Upcomming Seasonal Schools
• 27 - 30 September 2016
  PRACE Autumn School 2016, Austria - Modern HPC Development for Scientists and Engineers
• 10 – 12 April 2017
  PRACE Spring School 2017, Sweden - HPC in the Life Sciences
PATC Programme 2016-2017

- 79 courses, 215 training days
- New courses on forward-looking topics
  - New hardware and programming paradigms
  - Data science
- Collaboration with CoEs on several courses
Training and Events Portal

- [www.training.prace-ri.eu](http://www.training.prace-ri.eu)
- Single hub for the PRACE training events, training material and tutorials
- Number of page views increased by 25% and number of users by 45% since 2014
CodeVault and More

• Repository of Open Source code samples
  – Examples and model solutions of common HPC programming tasks
    • Possible to utilise in training and as building blocks of real-world applications
  – Anonymous read access

• Best Practice Guides

• White Papers
  – [http://www.prace-ri.eu/white-papers/](http://www.prace-ri.eu/white-papers/)
Future Training Activities

• On-demand events addressing the needs of the CoEs
  – Needs for basic, intermediate, and advanced training

• Launch of Massive Open Online Courses (MOOCs)
  – Introduction to HPC, coordinated by EPCC
  – Management of massive data, coordinated by Univ. Ljubljana

• PRACE Training Centres (PTCs)
  – Cover basic and advanced needs across Europe
PRACE SUMMER OF HPC
**PRACE Summer of HPC (SoHPC)**

**Goal:** To inspire the next generation of software engineering, system administrators, and general users of HPC.
PRACE Summer of HPC (SoHPC)

**SoHPC 2015**
- 9 Partners/Sites
- 80 applications
- 20 Students chosen
- Training week in Barcelona
- 2 Month internship
- 2 Award winners

**SoHPC 2016**
- 10 Partners/sites
- 110 applications
- 21 students chosen
- *Training week in Juelich*
- 2 month internship
- 2 Award winners
PRACE – JOB OPPORTUNITIES
Job Opportunities

• PRACE is an association of 25 members with over 50 HPC centres involved

• Job offers are announced on the PRACE website: www.prace-ri.eu
  – Approximately one job announcements every week
THANK YOU!

QUESTIONS?
RIKEN AICS Overview

(Coordinator 2016: Toshiyuki Imamura)
RIKEN AICS
Site of AICS and K computer

423km (263miles) west of Tokyo

Kobe

Tokyo

Kobe Airport
Advanced Institute for Computational Science (AICS)

- **Foundation**: July 2010

- **Missions**:
  - Operation of K computer for research including industry applications
  - Leading edge research through strong collaborations between computer and computational scientists
  - Development of Japan’s future strategy for computational science, including development of the post K computer

- **#Personnel**: 239 (1 April 2015)
K computer

- **Specifications**
  - 11.28PFlops with 88,128 nodes
  - 1.27PB (16GB/node) memory
  - 6 dim mesh-torus network (5GB/s x 2)
  - 30PB disk

- **Top 500 rankings**
  - No. 1 in Jun. & Nov. 2011
  - No. 4 in Jun. 2013-Nov. 2015
  - No. 5 in Jun. 2016

- **Graph 500 rankings**
  - No. 2 in Nov. 2014

- **HPCG rankings**
  - No. 2 in Nov. 2014, Jun. & Nov. 2015

Real application performance on K

<table>
<thead>
<tr>
<th>Name</th>
<th>Area</th>
<th># of nodes</th>
<th>Performance</th>
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<tbody>
<tr>
<td>NICAM</td>
<td>Global climate</td>
<td>81,920</td>
<td>1.05PF (10%)</td>
</tr>
<tr>
<td>Seism3D</td>
<td>Earthquake</td>
<td>82,944</td>
<td>2.02PF (19%)</td>
</tr>
<tr>
<td>PHASE</td>
<td>Material</td>
<td>82,944</td>
<td>2.12PF (20%)</td>
</tr>
<tr>
<td>RSDFT</td>
<td>Material</td>
<td>82,944</td>
<td>5.84PF (55%)</td>
</tr>
<tr>
<td>FrontFlow/Blue</td>
<td>Flow analysis</td>
<td>82,944</td>
<td>0.64PF (6%)</td>
</tr>
<tr>
<td>LatticeQCD</td>
<td>Particle physics</td>
<td>82,944</td>
<td>1.59PF (15%)</td>
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versatile performance for a wide spectrum of computing needs
High Performance Computing Infrastructure (as of Mar 2015)

- Seamless access to K and other supercomputers in 11 major academic computer centers in Japan
- Joint selection of proposals for K and other supercomputers

Total 13.5 Pflops
Some recent results from the K computer

**Fundamental science**
- Dark matter with $2 \times 10^{12}$ particles
  - Gordon Bell 2012
- Supernova explosion through neutrino heating

**Materials & Energy**
- Fast Charging mechanism of Lithium Ion battery
  - 2012/11/17
- Charge-fluctuation origin of iron-based superconductors

**Life sciences**
- Artificial heart and blood flow
  - 2014/03/30
- High throughput docking simulation for drug design

**Disaster prevention**
- Cloud resolving NICAM run with less than 1 km mesh
  - 2013/10/18
- Coupled earth quake-plate dynamics - tsunami simulation

**Engineering**
- Large-scale aerodynamics simulation for accelerated vehicle design
  - 2014/03/27
- Fluid flow simulation accelerates design of transport vehicles
Flagship2020 Project
Flagship2020 Project

- **Missions**
  - Develop the next Japanese national flagship supercomputer, Post K
  - Simultaneously develop a wide range of HPC applications, to run on Post K, in order to solve social and science issues

- **Budget**
  - 110 Billion JPY (about 0.91 Billion USD in case of 120 JPY/$)
  - including research, development and acquisition, and application development

- **Hardware and System Software**

  RIKEN AICS is in charge of development
  
  Fujitsu is vendor partner

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<td>Q1</td>
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<td>Q4</td>
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<td>Q1</td>
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<td>Q4</td>
<td>Q1</td>
<td>Q2</td>
<td>Q3</td>
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- **Basic Design**
- **Design and Implementation**
- **Manufacturing, Installation, and Tuning**
- **Operation**
- **Preparation**
- **Research and Study**
- **Implementation**
- **Production**
International Collaborations & Human Resource Development

Research opportunities at RIKEN AICS
Working across computer and computational sciences
Working across computer and computational sciences
International Collaboration

- **JLESC (Joint Laboratory on Extreme Scale Computing)**
  - an international, virtual organization whose goal is to enhance the ability of member organizations and investigators to make the bridge between Petascale and Extreme computing.
  - Partners: INRIA, the University of Illinois, Argonne National Laboratory, Barcelona Supercomputing Center, Jülich Supercomputing Centre and RIKEN AICS.
  - 31 projects are running
  - Workshop:
    Barcelona (Spain) in Jun. 2015, Bonn (Germany) in Dec. 2015, Lyon (France) in Jun. 2016, and we will host the WS at Kobe in Dec.

- Main topics:
  - Applications and mini-apps, with a special focus on (but not limited to) molecular dynamics
  - Parallel Programming, runtime and tools
  - Resilience
  - Big Data, I/O and visualization
  - Numerical methods and algorithms
International Collaboration (cond.)

Other international collaborative works, including the conclusion of MOUs

- Centre National de la Recherche Scientifique Maison de la Simulation (Apr. 2014-)
- Argonne Leadership Computing Facility (Nov. 2013-)
- Juelich Supercomputing Center (Oct. 2013-)
- University of Maryland (Oct. 2013-)
- National Computational Infrastructure (Nov. 2011-)
- The Scuola Internazionale Superiore Di Studi Avanzati (May 2011-)
Researcher Development 1

- **International Summer School by PRACE, XSEDE, Compute Canada and RIKEN AICS**
  NY(USA) in 2013, Budapest(Hungary) in 2014, Toronto (Canada) in 2015, Ljubljana(Slovenia) in 2016
  For graduate students and post-docs
  80 participants for 2016 event (8 students from Japan)

- **AICS Spring (2014 - ) and Summer School (2011 - )**
  5 days at AICS to learn basics of programming for parallel computing
  For graduate students and post-docs, and technical college students
  About 20-30 participants every year
Researcher Development 2

- **Internship Program (2014 -)**
  2-3 weeks at AICS Research Division
  Approximately 10 graduate students will participate
  Planning to become international from 2017

- **AICS Youth Workshop Program (2016 -)**
  3 days at the AICS site
  About 20 international young researchers will participate
  Cooperate with JLESC (Joint Laboratory on Extreme Scale Computing)

- **E-Learning Website (2014 -)**
  On-line, Videos of lectures, presentations, hands-on and slides on web
  Main target is graduate students
Supporting Research Communities with XSEDE

John Towns
PI and Project Director, XSEDE
Executive Director, Science & Technology, NCSA
jtowns@ncsa.illinois.edu
Motivation for XSEDE:

• Scientific advancement across multiple disciplines requires a *variety of resources and services*

• XSEDE is about increased productivity of the community and providing expanded capabilities
  – leads to more science
  – is sometimes the difference between a feasible project and an impractical one
  – lowers barriers to adoption

• XSEDE provides a *comprehensive eScience infrastructure* composed of expertly managed and evolving advanced *heterogeneous digital resources and services* integrated into a general-purpose infrastructure
XSEDE – accelerating scientific discovery

XSEDE’s Vision:

a world of digitally enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing advanced computing resources and sharing data to tackle society’s grand challenges.

XSEDE’s Mission:

to enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research by coordinating and adding value to the leading cyberinfrastructure resources funded by the NSF and other agencies.
Vision/Mission: Enable Realizing Best Science
XSEDE Factoids: high order bits

• 5 year, US$121M project
  – plus US$9M, 5 year Technology Investigation Service
    • separate award from NSF
    – in process of obtaining a new award for an additional 5 years

• No funding for major hardware
  – coordination, support and creating a national/international cyberinfrastructure
  – coordinate allocations, support, training and documentation for >$100M of concurrent project awards from NSF

• ~140 FTE /~250 individuals funded across 20 partner institutions
  – this requires solid partnering!
Significant Contributions to Community by XSEDE: Supporting the Community

• Annually supporting 8,000 researchers and students
  – this is potentially a limit given current resources
• More than 17,000 publications supported to date
  – analysis shows significantly higher citation rate than other publications in the same journals
• Over 12,000 active users of XSEDE User Portal
• Nearly 800 proposals for major compute allocations reviewed annually
  – a comparable number of requests for startup and educational allocations
• More than 60,000 user requests addressed to date
  – answering questions and resolving technical issues
• Through Q3PY5, completed 309 projects that assisted computational research teams
  – users reported an average productivity gain of 18.75 months
  – average three months investment of XSEDE staff time
Total Research Funding Supported by XSEDE to Date

$2.21 billion in research supported by XSEDE July 2011-May 2016

Research funding only. XSEDE leverages and integrates additional infrastructure, some funded by NSF (e.g. Track 2 systems) and some not (e.g. Internet2).
XSEDE offers efficient and effective integrated access to a variety of resources

• Leading-edge distributed memory systems
• Very large shared memory systems
• High throughput systems, including Open Science Grid (OSG)
• Visualization engines
• Accelerators like GPUs and Xeon PHIs

Many scientific problems have components that call for use of more than one architecture.
XSEDE User Portal: THE User Site
portal.xsede.org

• XSEDE User Portal (XUP) is designed to be the only site a user needs to use XSEDE

• XUP presents information relevant to users
  – user info is easier to find
  – XUP also provides dynamic data about XSEDE systems
  – capabilities to manage usage, files, data

• As a user you can
  – request an allocation, and manage allocations
  – sign up for training
  – request help
  – manage file and data, and much more!
  – Portal provides single sign-on to all XSEDE resources
Current XSEDE Compute Resources

- **Stampede @ TACC**
  - 9.5 PFLOPS (PF) Dell Cluster w/ GPUs and Xeon PHIs
- **Comet @ SDSC**
  - 2.0 PF cluster
- **Bridges @ PSC**
  - 1.3 PF w/ large memory (274 TB)
- **XStream @ Stanford**
  - 1.0 PF GPU Cray CS-Storm cluster
- **SuperMIC @ LSU**
  - 925 TF Dell Cluster w/ GPUs and Xeon PHIs
- **Jetstream @ Indiana**
  - 516 TF HPC Cloud
- **Gordon @ SDSC**
  - 341 TF Appro cluster
- **Wrangler @ TACC**
  - 62 TF data analytics system
- **Open Science Grid**
  - 60,000 CPU cores

[https://www.xsede.org/web/xup/resource-monitor](https://www.xsede.org/web/xup/resource-monitor)
Current XSEDE Visualization and Data Resources

• Storage
  – Ranch @ TACC
    • 61 PB tape
  – HPSS @ NICS
    • 17 PB tape
  – Wrangler @ TACC
    • 10 PB disk
  – Data Supercell @ PSC
    • 4 PB disk
  – Data Oasis @ SDSC
    • 4 PB tape

• Visualization
  – Maverick @ TACC
    • 59 TF HP/NVIDIA cluster
    • 20 PB disk

https://www.xsede.org/web/xup/resource-monitor#advanced_vis_systems

https://www.xsede.org/web/xup/resource-monitor#storage_systems
Questions?
Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.