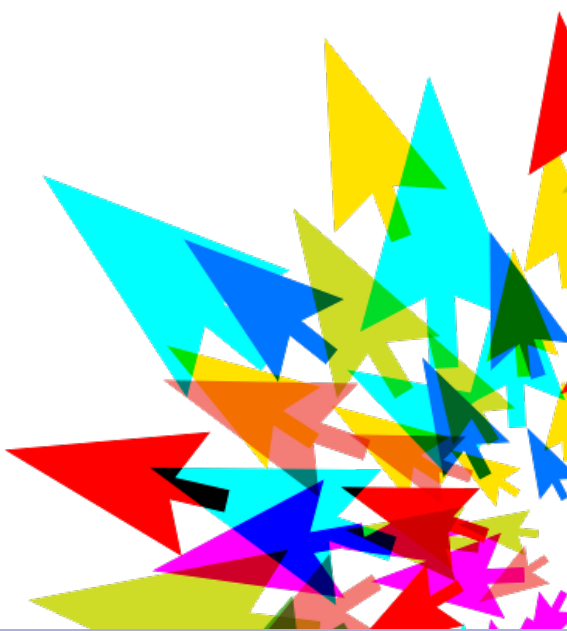
Compute Canada Overview

Ramses van Zon

Compute/Calcul Canada

June 28, 2016



What is Compute Canada?

www.computecanada.ca

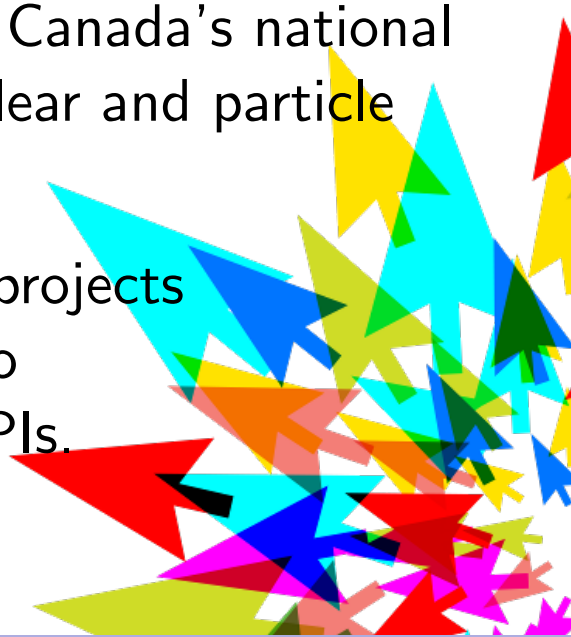
- The national advanced research computing (ARC) facility of Canada,
- The not-for-profit corporation formed to manage that project, and
- A federation of 35 institutions who are members of that corporation. The 35 institutions collectively own the infrastructure and employ the skilled personnel (sysadmins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

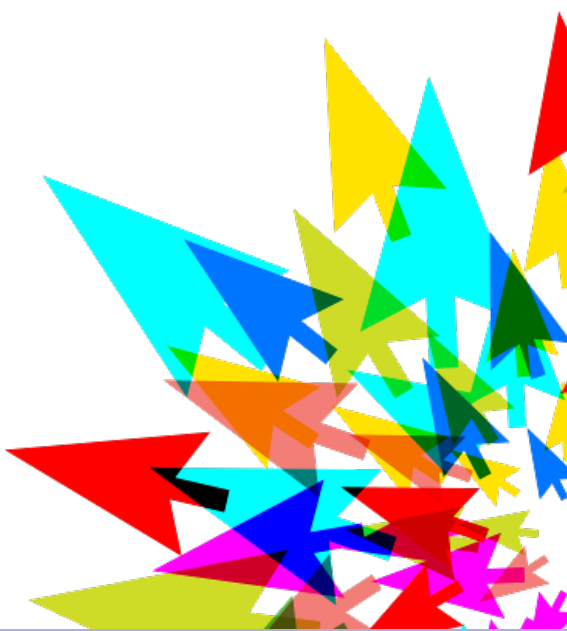
- **ATLAS**: "Tier2" computing and storage for the ATLAS experiment at the CERN Large Hadron Collider.
- **CANFAR**: Computational platform to analyze Canadian astronomy data.
- **CBRAIN**: international project to make brain images and computational tools available to researchers around the world.
- **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.



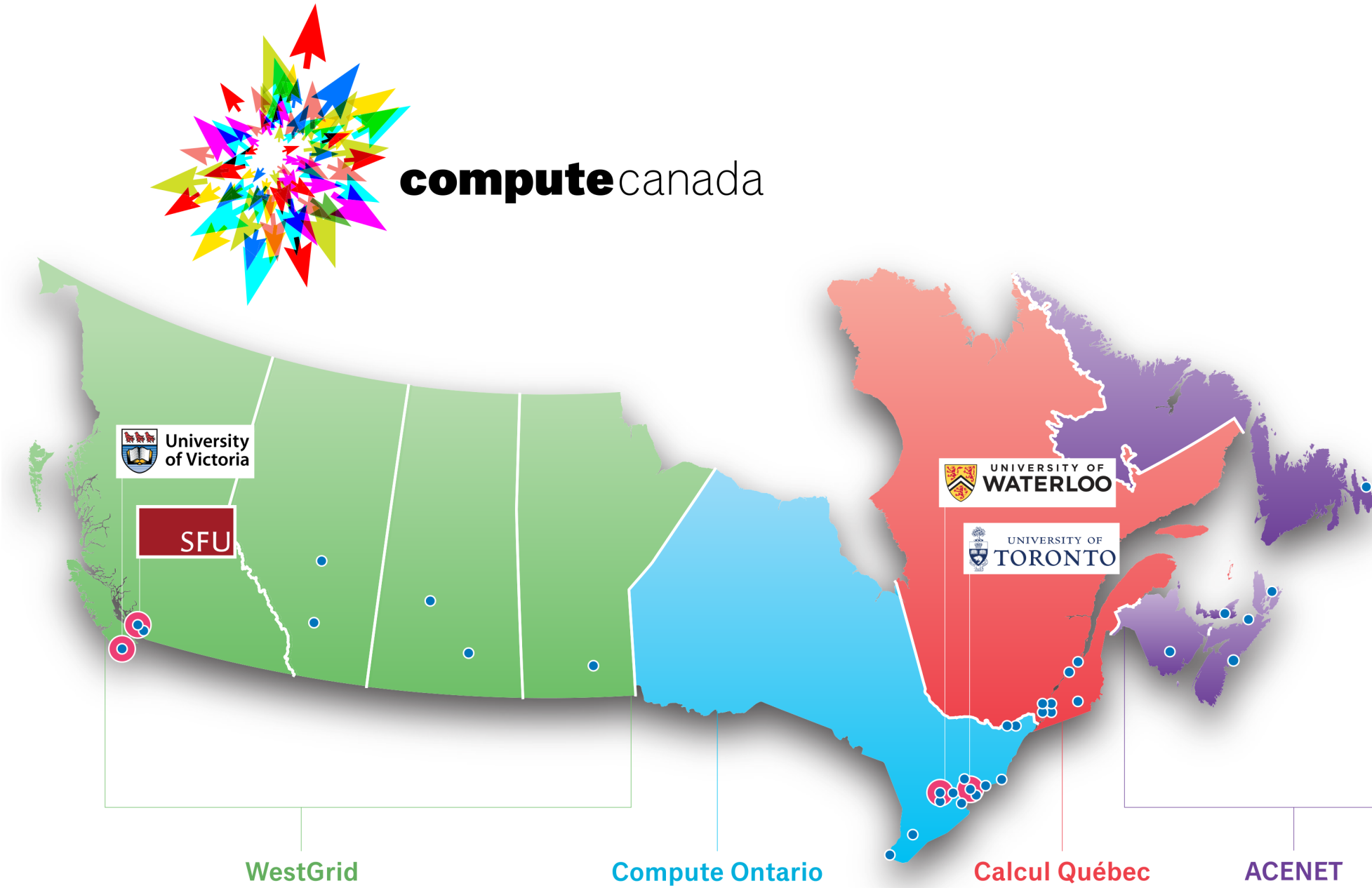
Compute Canada compute resources

Name	Cores	Nodes	Year
MP2	30,984	1291	2011
GPC	30,912	3864	2009
Guillimin	20,176	2714	2011
Orcinus	9,616	930	2011
Orca	8,320	360	2011

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

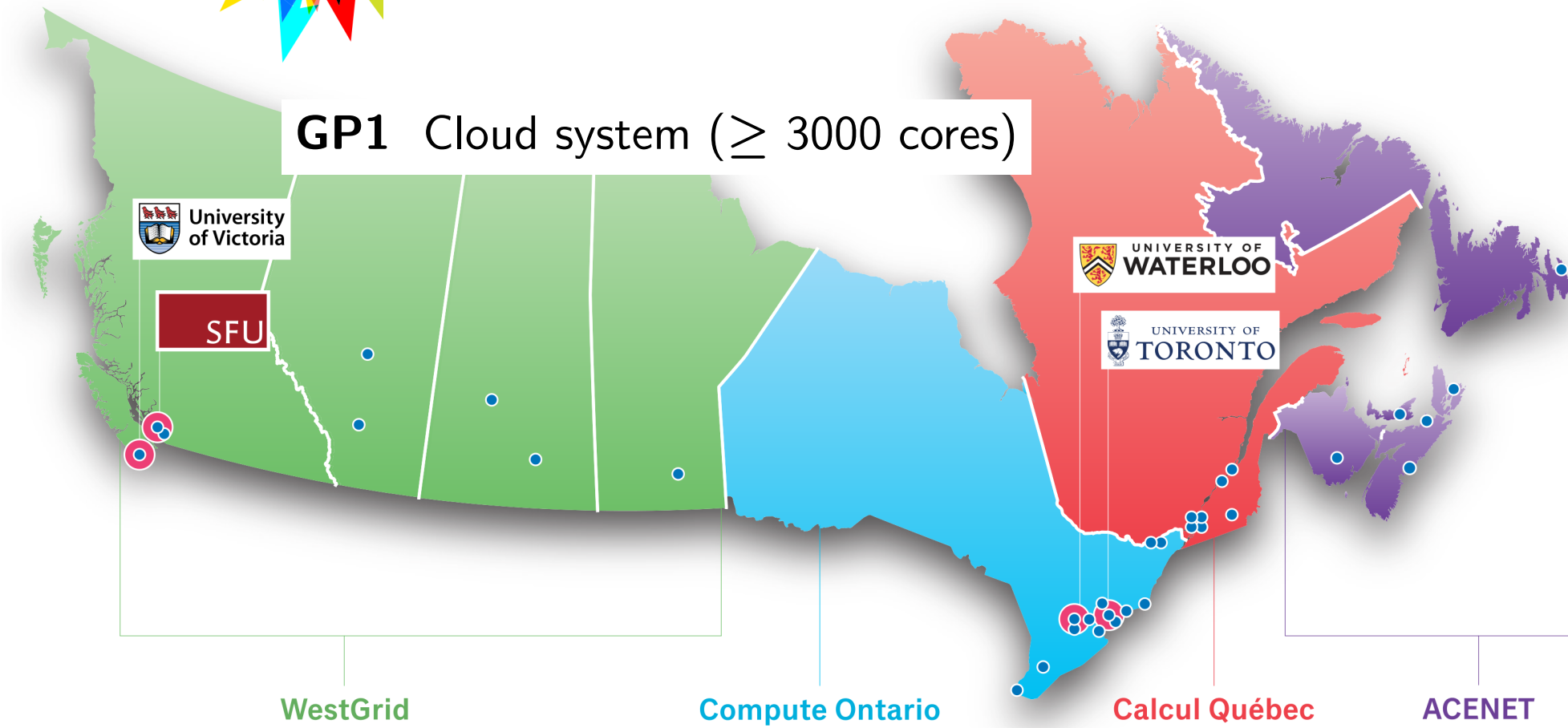


Systems Planned for the Near Future



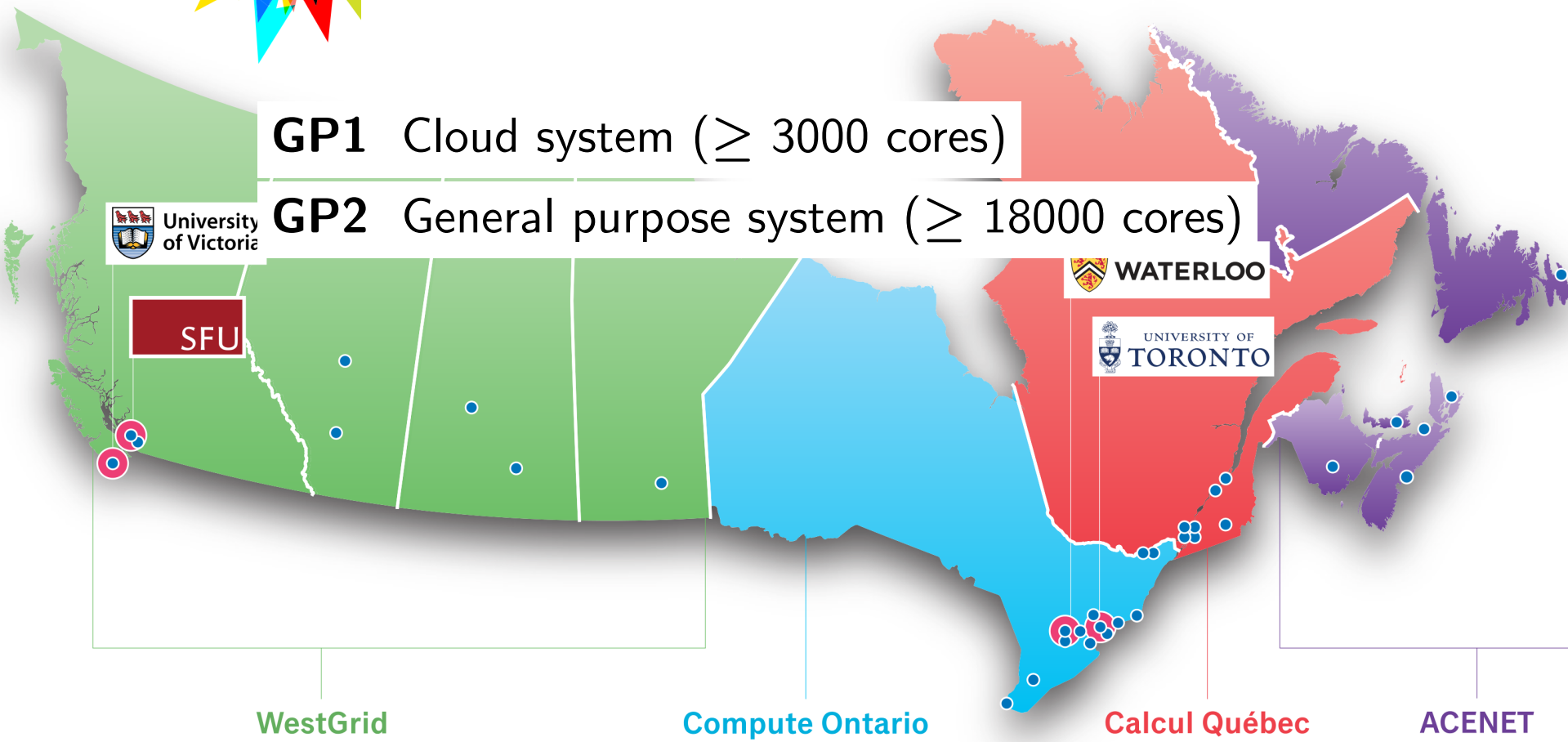
Systems Planned for the Near Future

computecanada



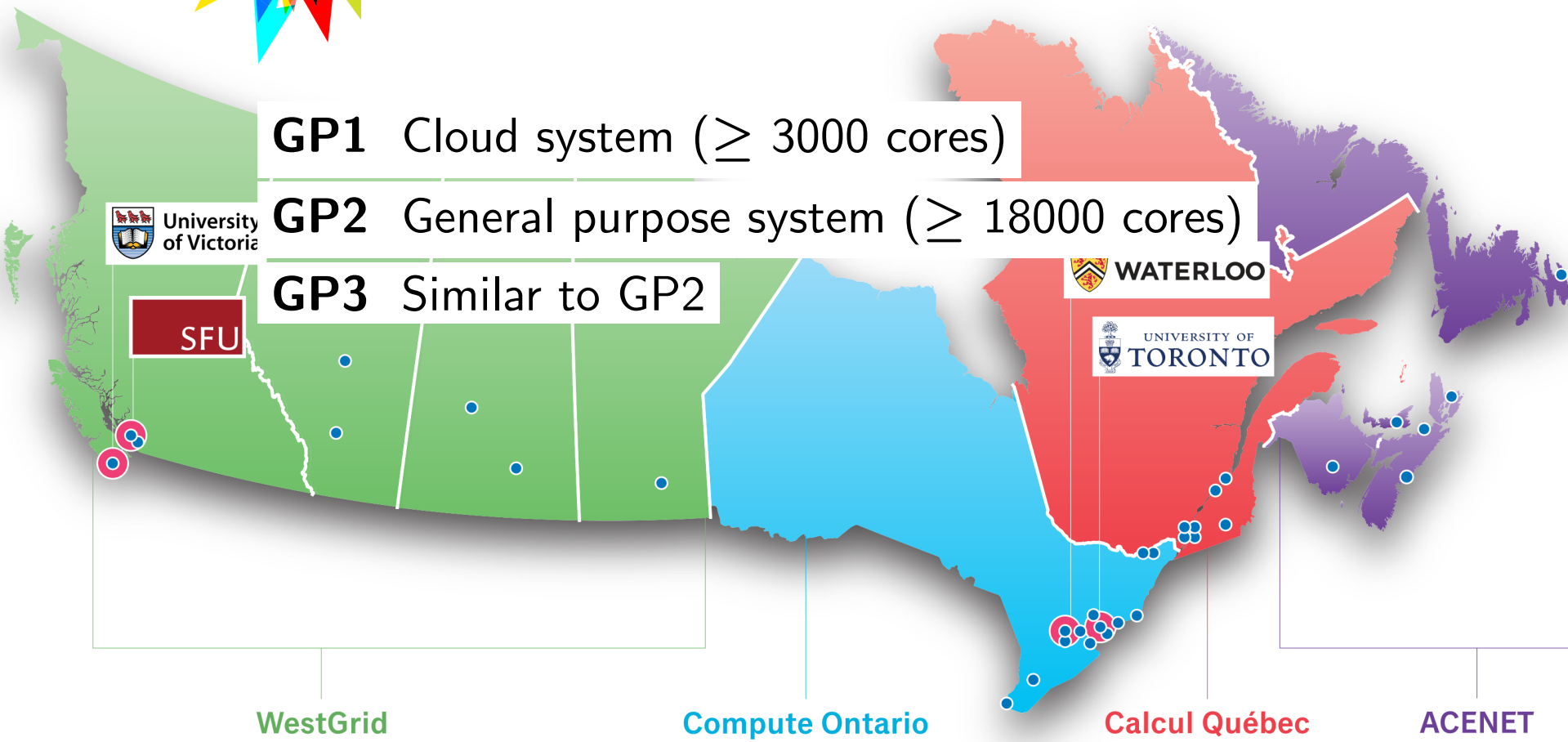
Systems Planned for the Near Future

computecanada



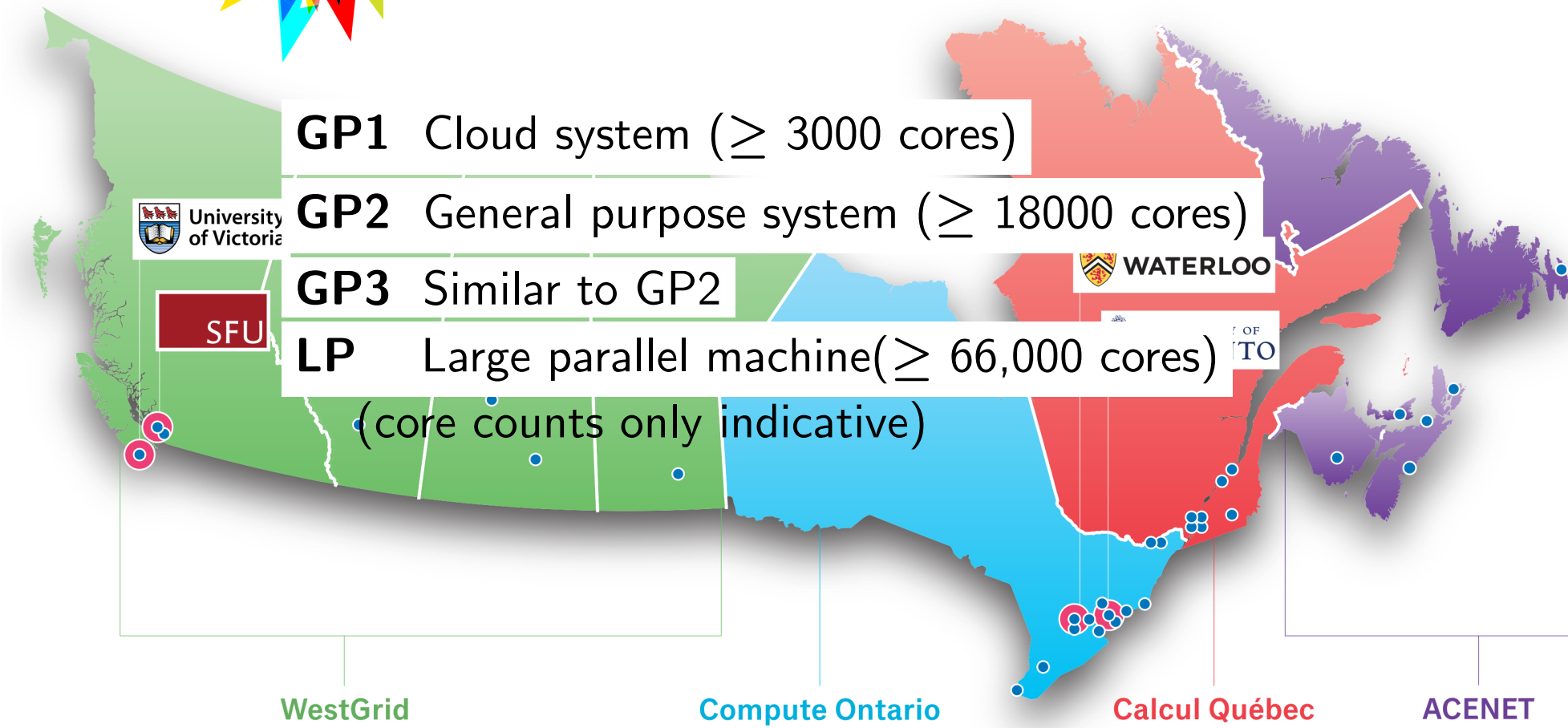
Systems Planned for the Near Future

computecanada



Systems Planned for the Near Future

computecanada



GP1 Cloud system ($\geq$ 3000 cores)

GP2 General purpose system ($\geq$ 18000 cores)

GP3 Similar to GP2

LP Large parallel machine($\geq$ 66,000 cores)

(core counts only indicative)

WestGrid | Compute Ontario | Calcul Québec | ACENET

Support and training

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

www.acceleratediscovery.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 reserarcher 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 incresed 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

Partnership for Advanced Computing in Europe

PRACE is an international not-for-profit association under Belgian law, with its seat in Brussels

PRACE counts 25 members and 2 observers

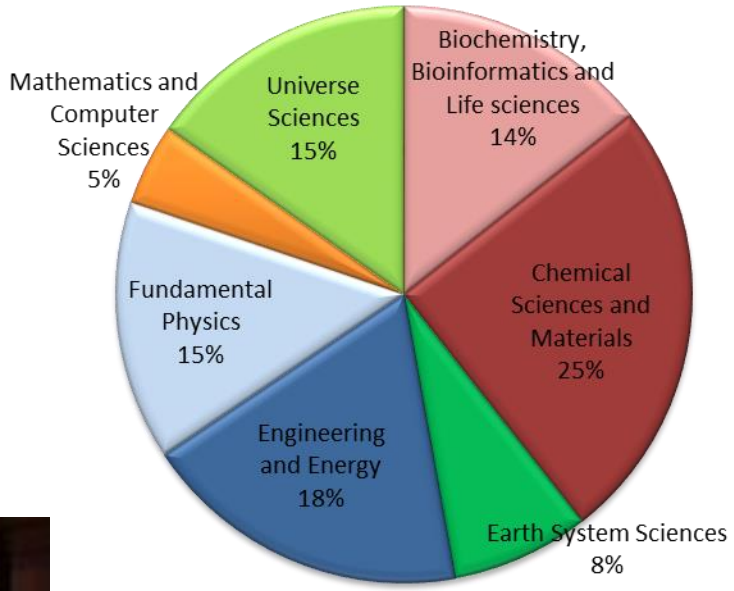
The **PRACE** Hosting Members are France, Germany, Italy and Spain

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

4 Hosting Members offering core hours on 6 world-class machines

MareNostrum: IBM
BSC, Barcelona, Spain



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

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

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***)

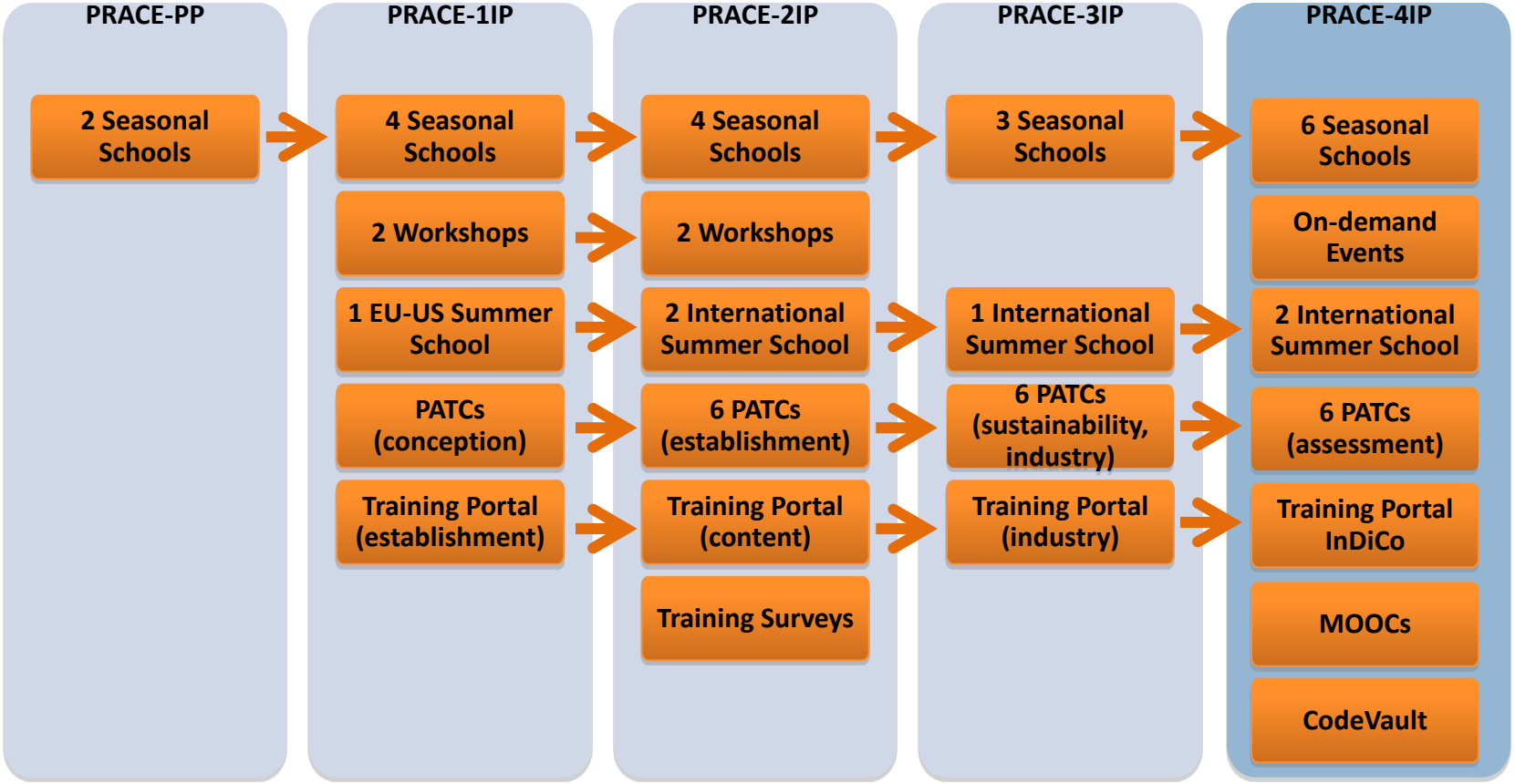
Project Access (***12, 24 or 36 months***)

Criterion: Scientific Excellence

www.prace-ri.eu/call-announcements/

PRACE TRAINING

PRACE Training Offerings



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

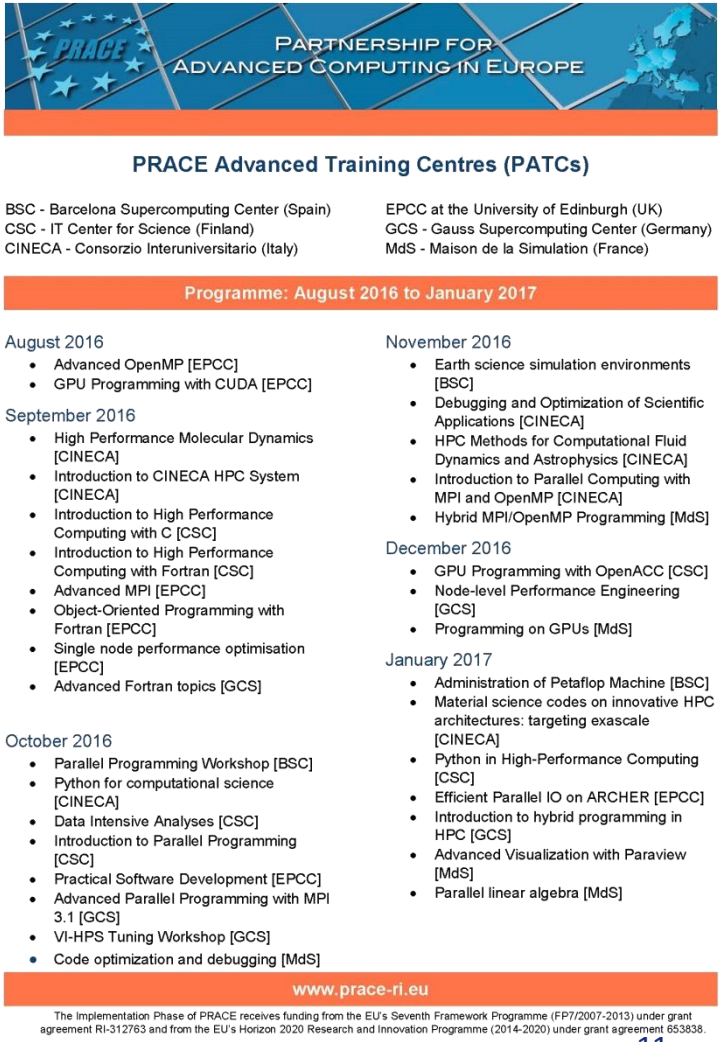
  PRACE Autumn School 2016, Austria - Modern HPC Development for Scientists and Engineers

- 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



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE Advanced Training Centres (PATCs)

BSC - Barcelona Supercomputing Center (Spain)
CSC - IT Center for Science (Finland)
CINECA - Consorzio Interuniversitario (Italy)
EPCC at the University of Edinburgh (UK)
GCS - Gauss Supercomputing Center (Germany)
MdS - Maison de la Simulation (France)

Programme: August 2016 to January 2017

August 2016
- Advanced OpenMP [EPCC]
- GPU Programming with CUDA [EPCC]

September 2016
- High Performance Molecular Dynamics [CINECA]
- Introduction to CINECA HPC System [CINECA]
- Introduction to High Performance Computing with C [CSC]
- Introduction to High Performance Computing with Fortran [CSC]
- Advanced MPI [EPCC]
- Object-Oriented Programming with Fortran [EPCC]
- Single node performance optimisation [EPCC]
- Advanced Fortran topics [GCS]

October 2016
- Parallel Programming Workshop [BSC]
- Python for computational science [CINECA]
- Data Intensive Analyses [CSC]
- Introduction to Parallel Programming [CSC]
- Practical Software Development [EPCC]
- Advanced Parallel Programming with MPI 3.1 [GCS]
- VI-HPS Tuning Workshop [GCS]
- Code optimization and debugging [MdS]

November 2016
- Earth science simulation environments [BSC]
- Debugging and Optimization of Scientific Applications [CINECA]
- HPC Methods for Computational Fluid Dynamics and Astrophysics [CINECA]
- Introduction to Parallel Computing with MPI and OpenMP [CINECA]
- Hybrid MPI/OpenMP Programming [MdS]

December 2016
- GPU Programming with OpenACC [CSC]
- Node-level Performance Engineering [GCS]
- Programming on GPUs [MdS]

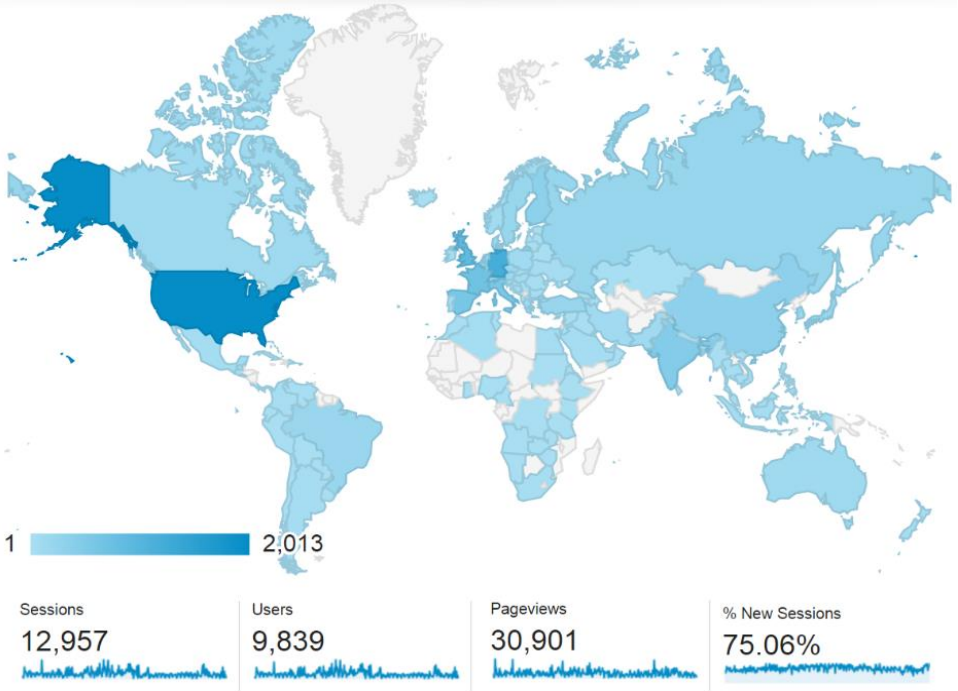
January 2017
- Administration of Petaflop Machine [BSC]
- Material science codes on innovative HPC architectures: targeting exascale [CINECA]
- Python in High-Performance Computing [CSC]
- Efficient Parallel IO on ARCHER [EPCC]
- Introduction to hybrid programming in HPC [GCS]
- Advanced Visualization with Paraview [MdS]
- Parallel linear algebra [MdS]

www.prace-ri.eu

The Implementation Phase of PRACE receives funding from the EU's Seventh Framework Programme (FP7/2007-2013) under grant agreement RI-312763 and from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 653838.

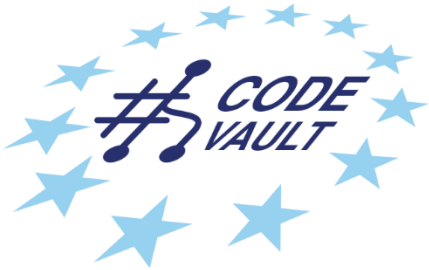
Training and Events Portal

- 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
  - https://gitlab.com/PRACE-4IP/CodeVault
  - 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
  - http://www.prace-ri.eu/best-practice-guides/
- White Papers
  - http://www.prace-ri.eu/white-papers/



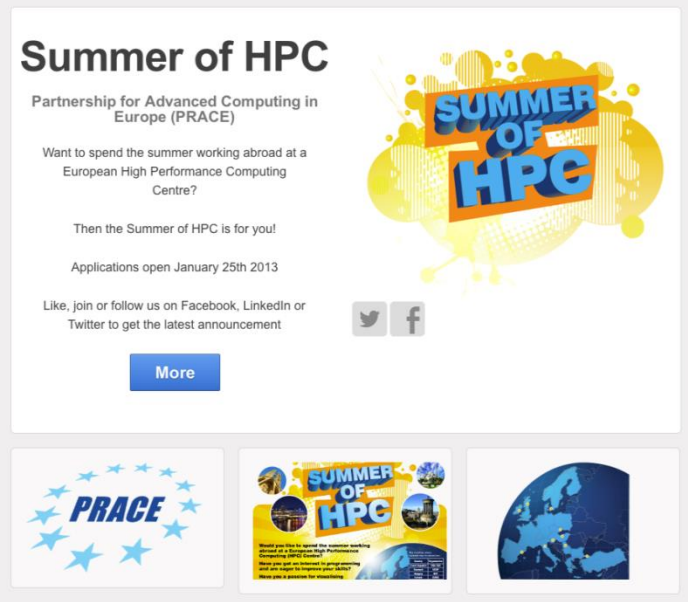
Future Training Activities

- 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*

HPC

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

PRACE
PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE
JÜLICH FORSCHUNGSZENTRUM
lrz
MPCDF
Inria INVENTEURS DU MONDE NUMÉRIQUE
POLITÉCNICA "Engineering the future"
SURF SARA
UMEA UNIVERSITET
UNIVERSITAS OSLOENSIS MDCCCXI
NTNU
GCS Gauss Centre for Supercomputing
cea
cnrs
epcc
KTH VETENSKAP OCH KONST
CYFRONET
UNIVERSIDADE DE COIMBRA
HLRS High-Performance Computing Center | Stuttgart
UPPSALA UNIVERSITET
GENCI
CINES
UPC
CSIC
RISC Software GmbH
WCSS
grnet
Science & Technology Facilities Council
CSC
JKU JOHANNES KEPLER UNIVERSITÄT LINZ
University of Ljubljana
Inter-University Computation Center
CSCS
BSC
CINECA
IT4Innovations national supercomputing center
PRACE
TÉCNICO LISBOA
LINKÖPING UNIVERSITY
PSNC
CESGA
Fakulteta za informacijske študije Faculty of information studies
UNINETT
ICHEC Irish Centre for High-End Computing
İTÜ
THE CYPRUS INSTITUTE
NCSA NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS
KØBENHAVNS UNIVERSITET
UNIVERSIDADE DE EVORA
Ihsan Doğramacı Bilkent University

THANK YOU!

QUESTIONS?

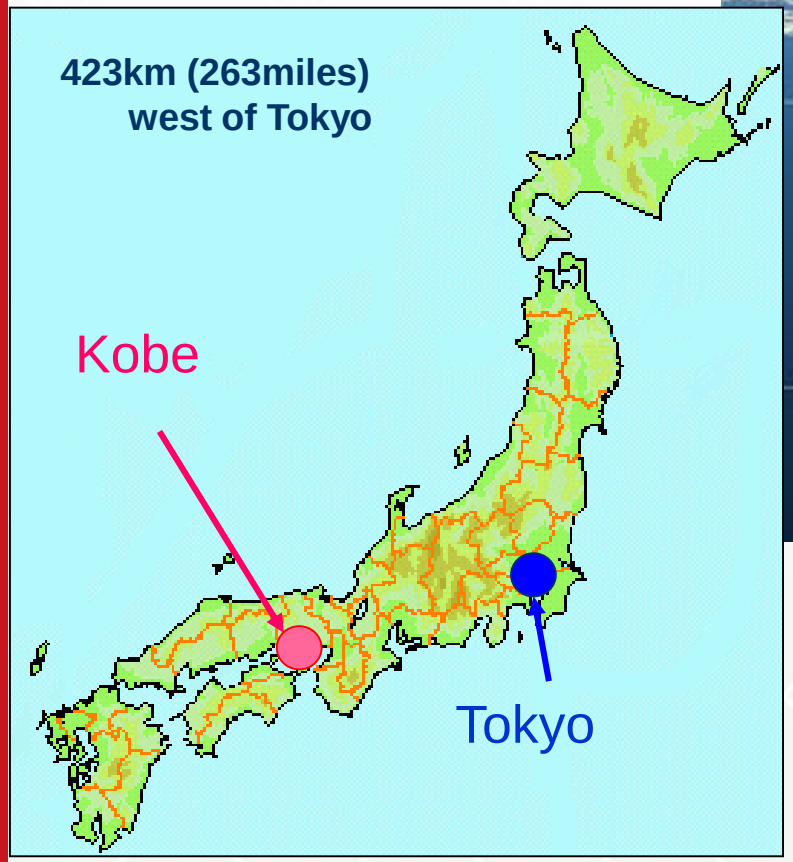
28 June 2015
International HPC Summer School
Ljubljana, Slovenia

RIKEN AICS Overview

(Coordinator 2016: Toshiyuki Imamura)
RIKEN AICS

Computer simulations create the future

Site of AICS and K computer

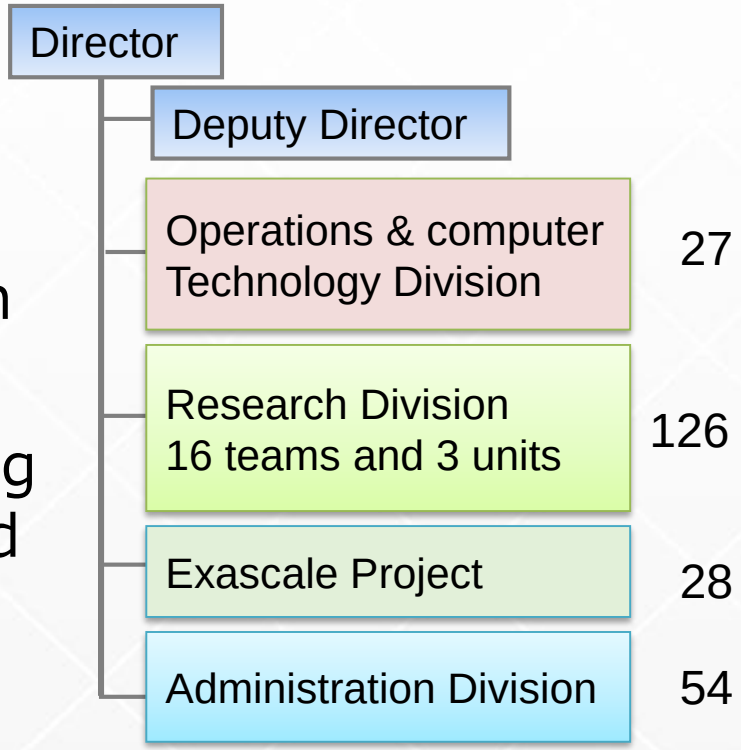


RIKEN
Advanced Institute for Computational Science

Advanced Institute for Computational Science (AICS)

Computer simulations create the future

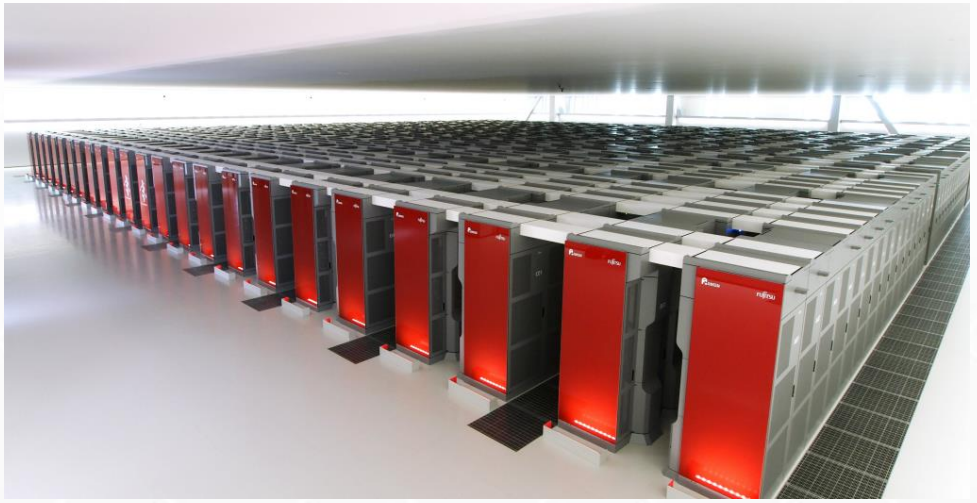
- **Foundation : July 2010**
- **Missions :**
  - Operation of K computer for research including industry applications
  - Leading edge research through strong collaborations between computer and computational scientists
  - Development of Japan's future strategy for computational science, including 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. 1 in Jun. 2014, Jul. & Nov. 2015
  - No. 2 in Nov. 2014
- **HPCG rankings**
  - No. 2 in Nov. 2014, Jun. & Nov. 2015

versatile performance for a wide spectrum of computing needs



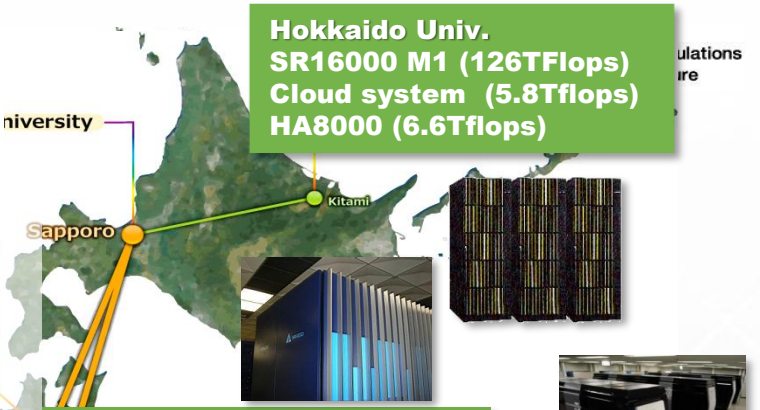
Real application performance on K

Name	Area	# of nodes	Performance
NICAM	Global climate	81,920	1.05PF (10%)
Seism3D	Earthquake	82,944	2.02PF (19%)
PHASE	Material	82,944	2.12PF (20%)
RSDFT	Material	82,944	5.84PF (55%)
FrontFlow/Blue	Flow analysis	82,944	0.64PF (6%)
LatticeQCD	Particle physics	82,944	1.59PF (15%)

HPCI

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



Tohoku Univ.
NEC SX-ACE(282Tflops)
NEC LX-406Re-2(31.3Tflops)

Kyoto Univ.
CRAY XE6 (51.2Tflops)
CRAY XC30 (90Tflops)
CRAY XC30 with MIC (300Tflops)

NII
(Authentication Authority)

Univ. of Tsukuba
COMA(PACS-IX)
(22.4Tflops)

RIKEN AICS
K computer (10 Pflops, 4PB)

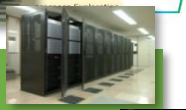
Univ. of Tokyo
FX10 (177.4Tflops)

ISM
SGI UV2000 (49.2Tflops)

Nagoya Univ.
CX400(470.6Tflops)
FX10(90.8Tflops)

JAMSTEC
SX-9E (104.8Tflops)

Kyushu Univ.
FX10(90.8Tflops)
CX400(88.4Tflops)



Tokyo Instiute of Technology
Tsubame 2.5 (1.6 Pflops)

Osaka Univ.
SX-ACE (423Tflops)
Express5800/53Xh (16.6Tflops)
Large-scale Visualization (28.1Tflops)

Total 13.5Pflops

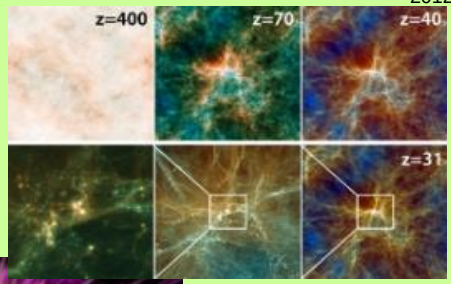
Some recent results from the K computer

RIKEN AICS Computer simulations create the future

Fundamental science

2012/11/17

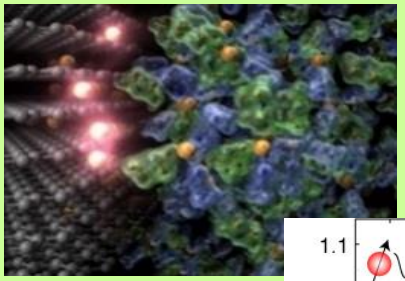
Dark matter with $2x10^{12}$ particles Gordon Bell 2012



Supernova explosion through neutrino heating

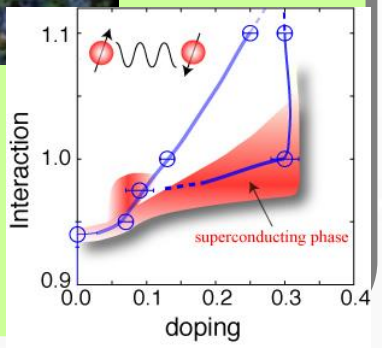
Materials& Energy

2014/03/30
2014/03/27



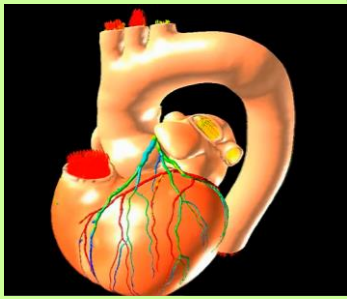
Fast Charging mechanism of Lithium Ion battery

Charge-fluctuation origin of iron-based superconductors



Life sciences

Artificial heart and blood flow



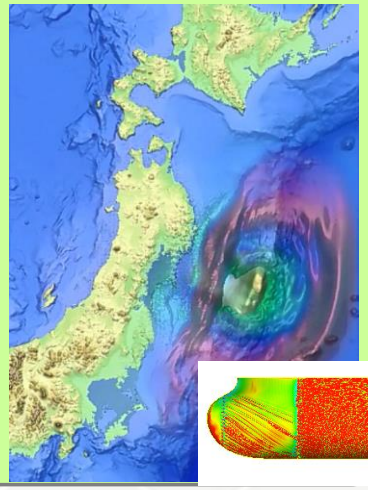
High thruput docking simulation for drug design

Neuronal simulation with 10^13 neurons

Disaster prevention

2013/10/18

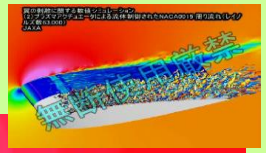
Cloud resolving NICAM runwith less than 1km mesh

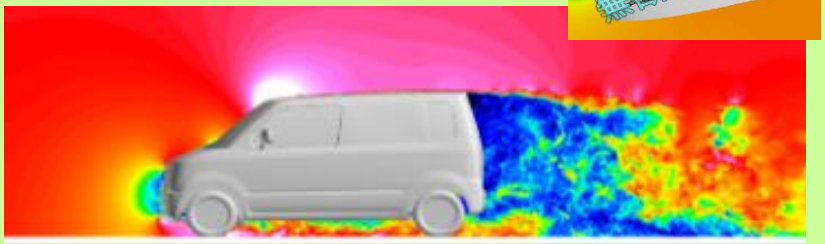


Coupled earth quake-plate dynamics-tsunami simulation

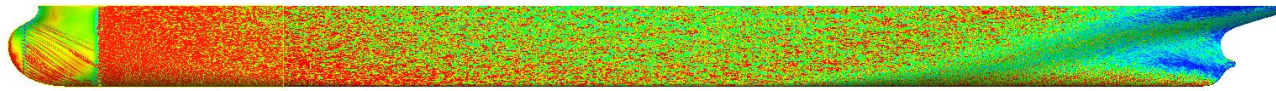
Engineering

Large-scale aerodynamics simulation for accelerated vehicle design





Fluid flow simulation accelerates design of transport vehicles

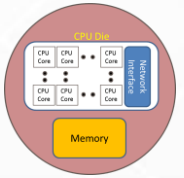


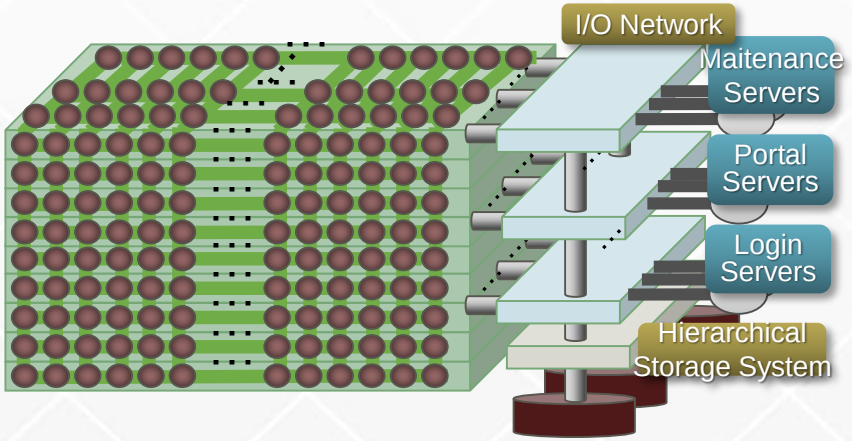
Flagship2020 Project

Flagship2020 Project

Computer simulations create the future

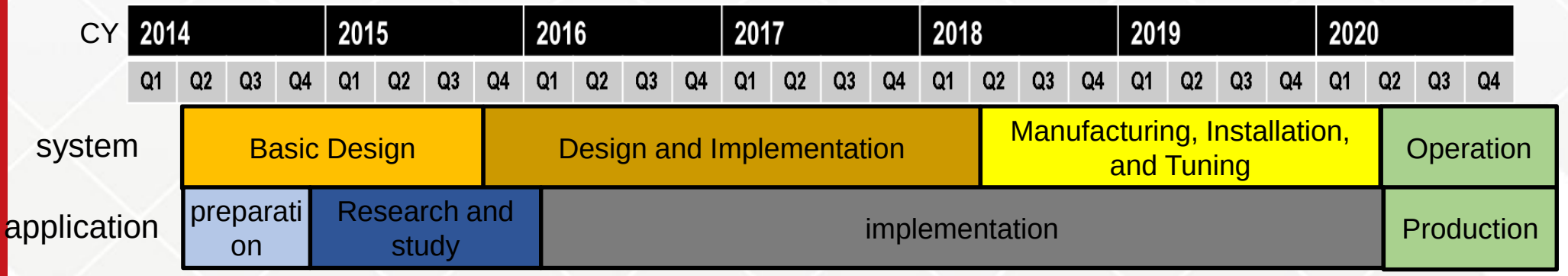
- **Missions**
  - Develop the next Japanese national flagship supercomputer, Post K
  - Simultaneously develop a wide range of HPC applications, to run on Post K, in order to solve social and science issues
- **Budget**
  - 110 Billion JPY(about 0.91 Billion USD in case of 120 JPY/$)
  - including research, development and acquisition, and application development
- **Hardware and System Software**





RIKEN AICS is in charge of development

Fujitsu is vendor partner

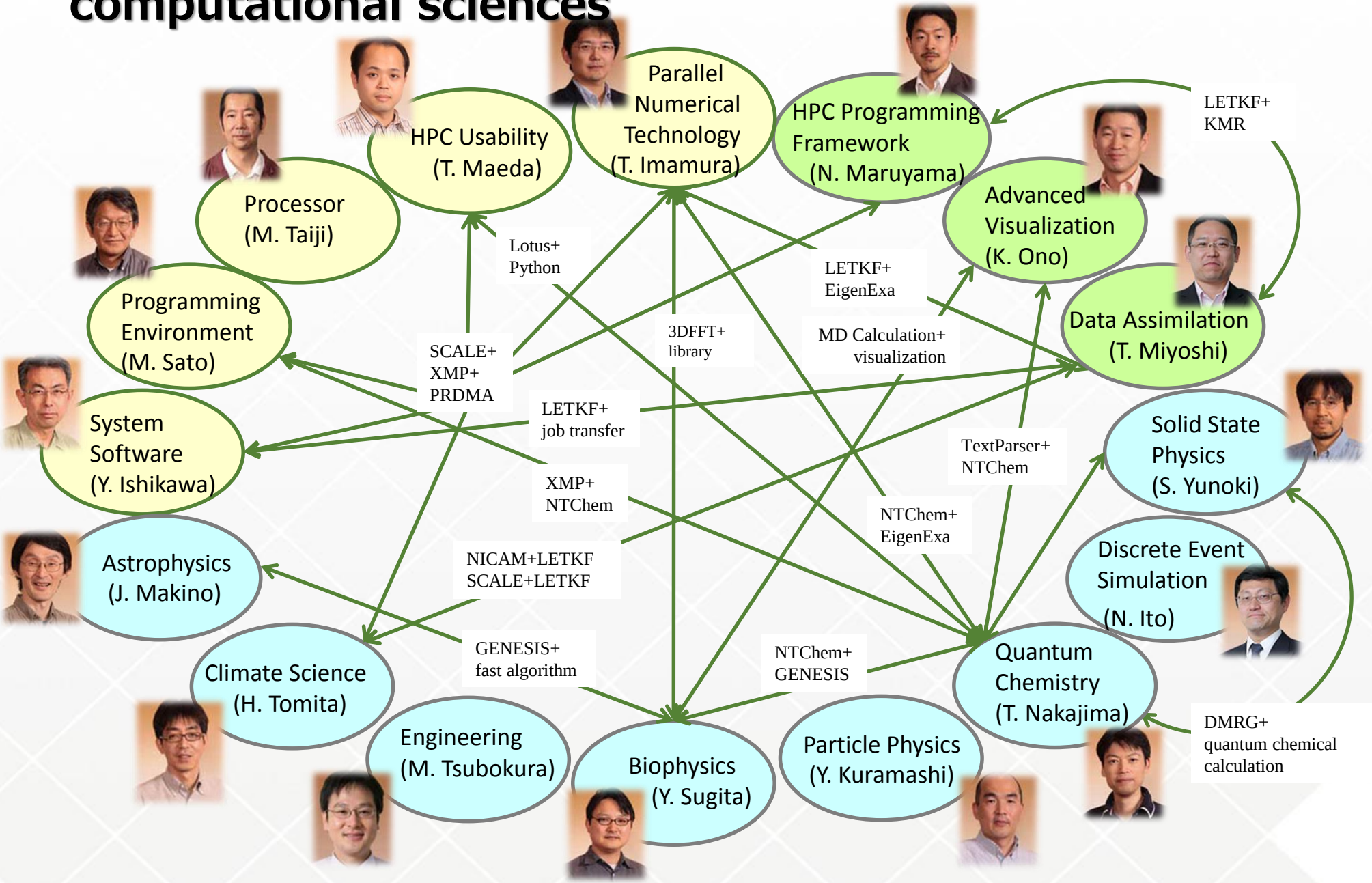


International Collaborations & Human Resource Development

Research opportunities at RIKEN AICS

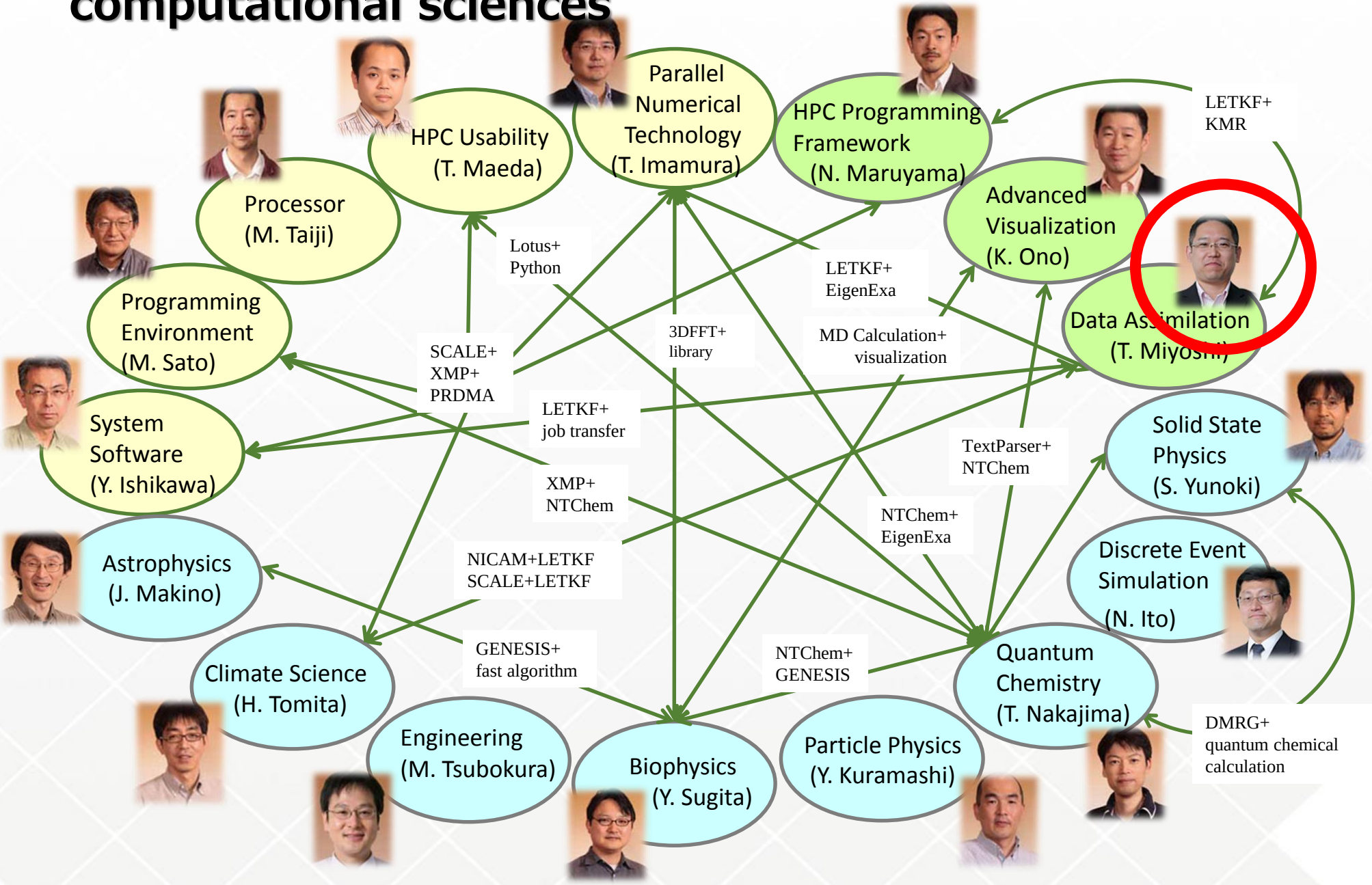
Working across computer and computational sciences

RIKEN AICS Computer simulations create the future



Working across computer and computational sciences

RIKEN AICS Computer simulations create the future



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.
  - 31projects 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.)

Computer simulations create the future

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

XSEDE

Extreme Science and Engineering Discovery Environment

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

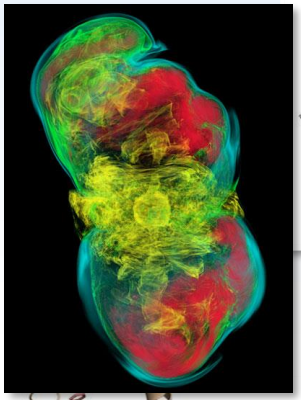
XSEDE's Vision:

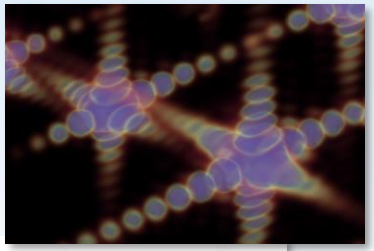
a world of digitally enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing advanced computing resources and sharing data to tackle society's grand challenges.

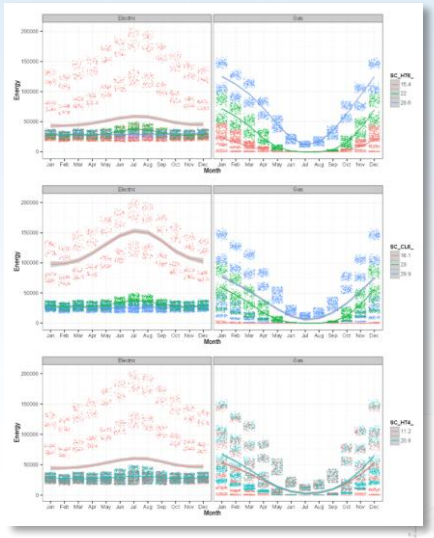
XSEDE's Mission:

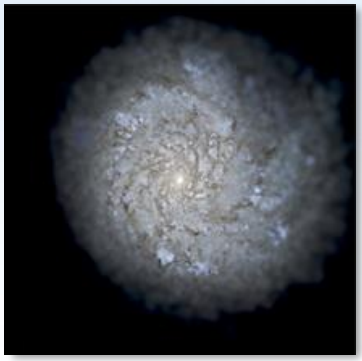
to enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research by coordinating and adding value to the leading cyberinfrastructure resources funded by the NSF and other agencies.

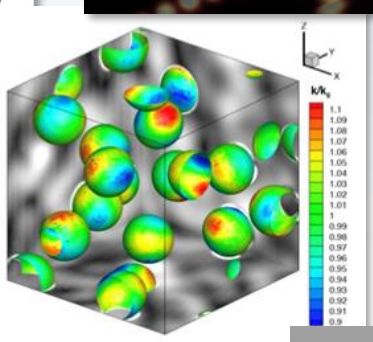
Vision/Mission: Enable Realizing Best Science

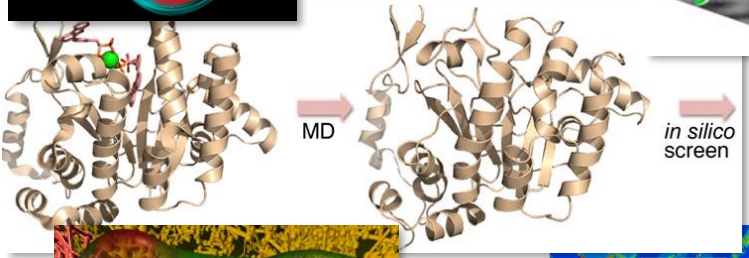


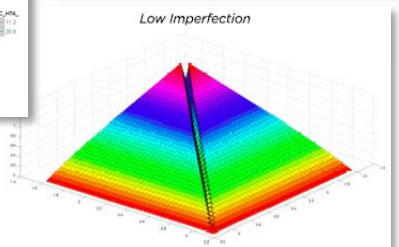


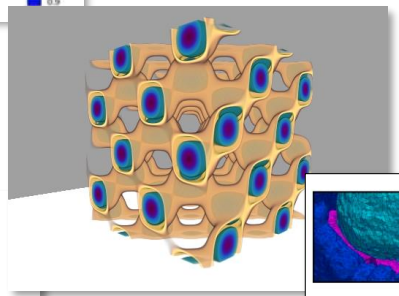


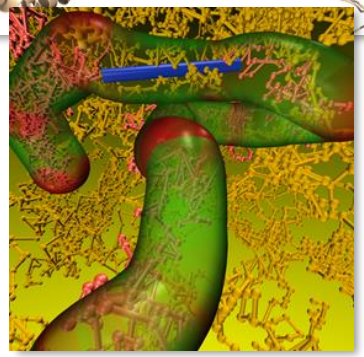


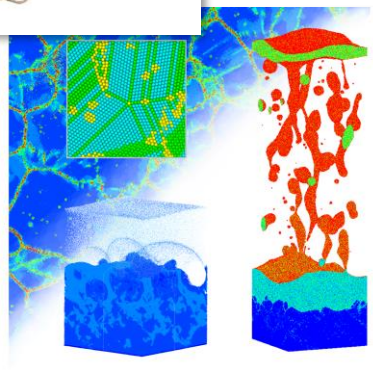


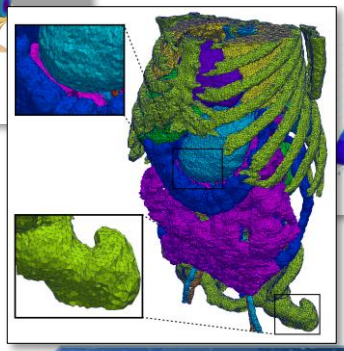


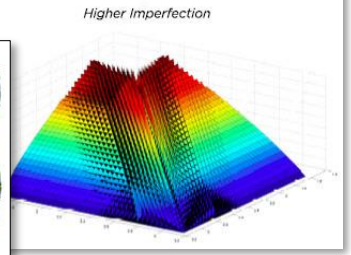












XSEDE Factoids: high order bits

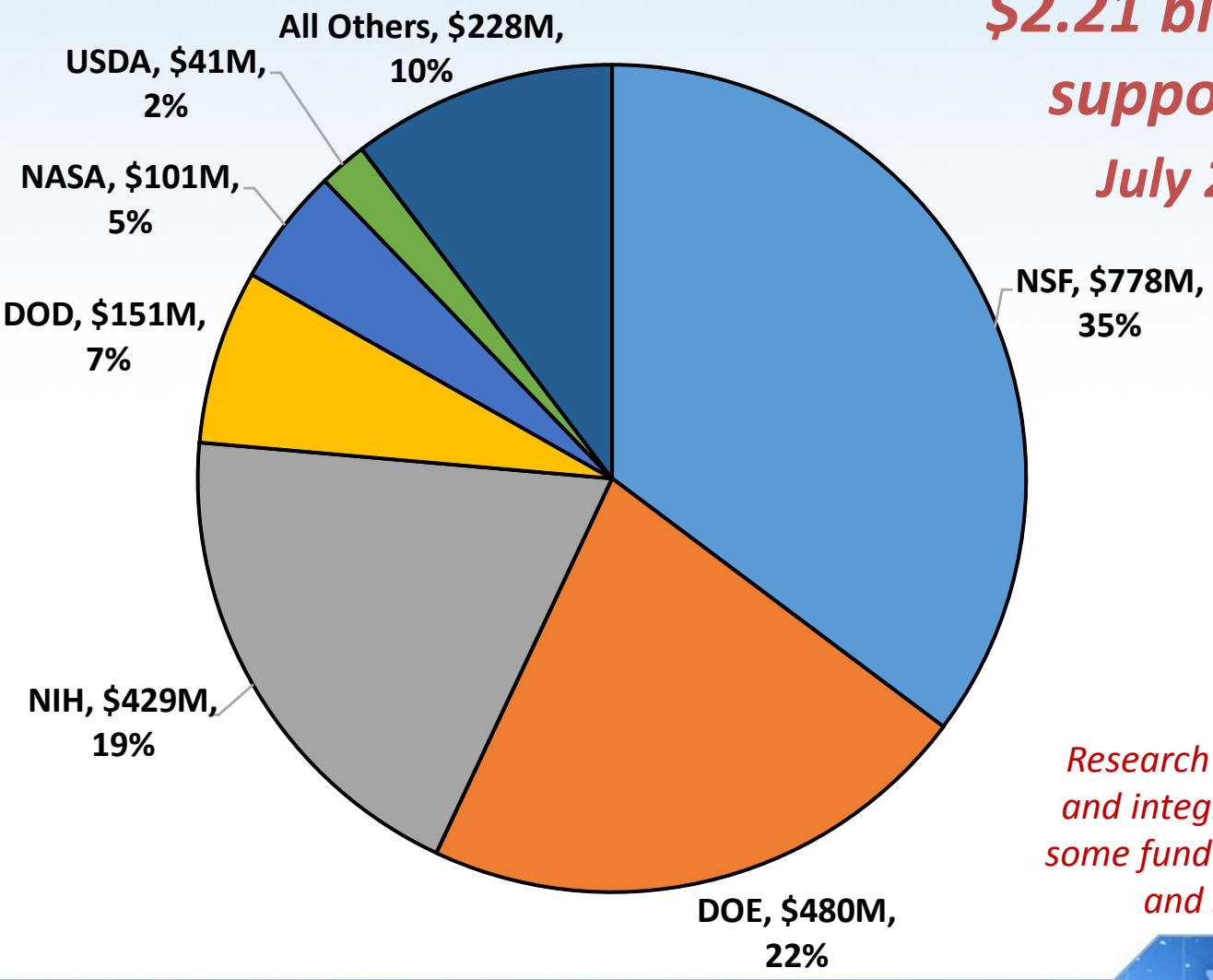
- 5 year, US$121M project
  - plus US$9M, 5 year Technology Investigation Service
    - separate award from NSF
  - in process of obtaining a new award for an additional 5 years
- No funding for major hardware
  - coordination, support and creating a national/international cyberinfrastructure
  - coordinate 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

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

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

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

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

Questions?

Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
XSEDE
Extreme Science and Engineering
Discovery Environment