SC '13 “Birds of a Feather (BoF)” Final Report on G8 HPC PROJECTS

Abstract

There have been six, G8-funded three-year exascale research projects in progress since 2011. Their objective has been to prepare key scientific grand challenges from the Climate, Fusion Energy, Seismology, and Bio-molecular scientific domains for the exascale. The SC’13 BoF presented the status of the G8 international HPC research program, including funding plans for a new phase of the program beyond 2014. Representatives from the associated international agencies presented the funding landscape, and scientists from the current exascale projects presented their project highlights. This BoF provided the HPC community with a “snapshot” of the G8 program from the perspectives of current exascale research projects as well as the G8 international funding agencies.

Background

Initiated in 2011, the purpose of the G8 extreme scale HPC program has been to prepare scientific applications in several key disciplines - Climate, Fusion Energy, Seismology, and Bio-molecular science - for the exascale computing era. Building on the success of the previous G8 Exascale projects workshop held in conjunction with SC’12, the goal of the SC’13 BoF was to bring together the six current G8 funded international exascale projects and representatives from the international funding agencies supporting G8 HPC research to enable information to be provided about the status of the current research activities (2011-2014) and the prospects for new funding opportunities in the future beyond 2014.

Birds of a Feather (BoF) Meeting at SC’13

International science agency representatives for the G8 countries, the current G8 project researchers, and the general HPC community participated in a well-attended BoF meeting at SC’13. The BoF session of 90 minutes duration was carried out as follows:

Part I:

Key members from the current international exascale projects (2011-2014) highlighted new advances and experiences that included succinct summaries of the associated science, software, and technology challenges. Topics addressed included: (1) how the major exascale scientific challenges in each domain were being met; (2) what were some of the “lessons learned,” regarding the process and methodology for preparing large application codes for the exascale and some of the unexpected hurdles that have been encountered; and (3) what new discoveries and strategies have emerged. Dr. William Tang of Princeton University coordinated these presentations which were collected and included in this SC’13 BoF Report (see attached PDF file of G8 project presentations: W.Tang_G8-BOF_SC’13.pdf). He also announced that Princeton University will host the G8 international agencies review of the final reports from the current international exascale projects at a meeting to be held in Princeton, New Jersey on June 12-13, 2014.

Part II:

Dr. Jean-Yves Berthou of the National Agency for Research in France [Agence Nationale de la Recherche (ANR)] spoke on behalf of the international science agencies (France, United States, United Kingdom, Russia, Germany, Japan, and Canada) that are currently engaged and plan to continue to participate in the G8 extreme scale HPC program. He presented the future funding landscape and collaborative research opportunities beyond 2014 for the next G8 "Big Data and Extreme Computing (BDEC)" program. This information is contained in Dr. Berthou's presentation which is also included in this SC'13 BoF Report (see attached PDF file of G8 agencies presentation: J.Berthou_G8-BOF_SC'13.pdf).

Overall, the combination of presentations from the projects and the funding agencies -- including associated Q&A discussions with the BoF attendees -- provided a valuable forum for the dissemination of knowledge about the G8 extreme scale program to the wider SC'13 audience. It accordingly enabled the HPC community to learn about upcoming G8 Big Data and Extreme Computing R&D opportunities and to interact with scientists that actually carried out the research sponsored by the G8 during the first phase (2011-2014) of this program. In doing so, it achieved the primary goals of the BoF which included:

(i) enabling the general SC'13 audience to have a clearer understanding of the exciting collaborative research being done in these international G8 projects;

(ii) providing a venue for the exchange of valuable information between on-going G8 projects -- such as discoveries, best practices, and challenges; and

(iii) informing all attendees about what G8-sponsored funding is currently planned for extending current projects and for starting new projects.

In view of the fact that a new phase of the G8-supported extreme scale international HPC R&D will be launched during 2014, this SC'13 BoF proved to be both an informative and a timely event. As such, it is very likely that a BoF meeting on this important and stimulating interdisciplinary HPC subject – that will now encompass "Big Data and Extreme Computing (BDEC)" -- will be requested for SC'14.

SC'13 BOF - G8 Extreme Scale & Big Data Program: Progress on Current Exascale Projects & Future Funding Opportunities

G8 Research Council's Initiative on Multilateral Research Funding: "*Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues*"

November 19, 2013

William Tang
Princeton University and Princeton Plasma Physics Laboratory
Princeton, NJ, USA

OUTLINE

1. Brief Summary Reports from Current G8 Exascale Projects

2. Key Upcoming G8 Event:

   G8 Exascale Projects Final Review Meeting in Princeton, NJ – June 12-13, 2014 focusing on Final Reports from the current six G8 Exascale Projects

3. G8 Heads of Research Councils (HORCs) Plans for Multilateral Research Funding for "BDEC" R&D:

➔ *Presentation today by Jean-Yves Berthou (ANR, France) on behalf of the international agencies regarding the upcoming G8 "Big Data and Extreme Computing (BDEC)" Program*

OUTLINE

I. Current Situation Analysis:

- Current 6 G8 projects have served as ***"pilot projects" that motivate***:

(1) continuing G8 support for harvesting greater productivity in a more mature project phase in "Big Data & Extreme Computing (BDEC)" after the initial 3 years period (2011-2014); and

(2) launching possible G8 support for a larger portfolio that includes new collaborative international "BDEC" projects.

- *Substantive achievements:* – setting up international collaborative centers including initiation of access to HPC facilities, hiring of early-career, post-PhD scientists , & significant progress on research objectives → ***highlighted in brief summary presentations from the 6 current G8 projects***

II. Upcoming G8 Activity:

➔ G8 Exascale Projects Meeting @ Princeton University, Princeton, NJ, USA on June 12-13, 2014 with focus on ***Final Review of the 6 current G8 Exascale Projects***

III. Update on G8 Heads of Research Councils (HORCs) Plans for Multilateral Research Funding for "BDEC" R&D:

→ *Presentation by Jean-Yves Berthou, Director ICT Dept., ANR (France)*

G8 Exascale Software Projects (2011- 2014)

- "Enabling Climate Simulation @ Extreme Scale" (ECS) – US, Japan, France, Canada, Spain

FRANCK CAPELLO

- "Climate Analytics on Distributed Exascale Data Archives" (ExArch) UK, US, France, Germany, Canada, Italy

SEBASTIEN DENVIL

- "Icosahedral-Grid Models for Exascale Earth System Simulations" (ICOMEX) – Japan, UK, France, Germany, Russia

JULIEN KUNKIL

- "Nuclear Fusion Simulations @ Exascale" (NuFuSE) – UK, US, Germany, Japan, France, Russia

WILLIAM TANG

- "Modeling Earthquakes and Earth's Interior based on Exascale Simulations of Seismic Wave Propagation" (Seismic Imaging) – US, Canada, France

MATTHIEU LEFEBVRE

- "Using Next-Generation Computers & Algorithms for Modeling Dynamics of Large Bio-molecular Systems" (INGENIOUS) -- Japan, UK, France, Germany, Russia

WILLIAM TANG (on behalf of Makoto Taiji)

G8 ECS: Enabling Climate Simulation at Extreme Scale

Project organization and computer science challenges

Team: **F. Cappello** (Lead PI, INRIA,), M. Snir (ANL, UIUC),

- G. Bosilca (UTK), L. Giraud (INRIA), S. Matsuoka (Titech), M. Sato (U. Tsukuba), F. Wolf (GRS), A. Weaver (U. Victoria), (BSC), D. Wuebbles (UIUC), J. Labarta (BSC), R. Loft and J. Denis (NCAR)
- Gathering climate scientists, climate code developers and computer science researchers

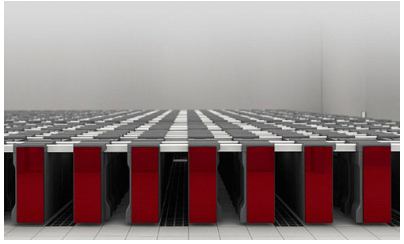
Target codes: CESM (North America) and NICAM (Japan)

Key research topics:

- **Scalability:** Performance tools & models, load balancing, com/comp overlap
- **Node level performance:** Heterogeneous nodes (GPUs), performance tools & models, tasks based parallelism, latency hiding,
- **Resilience:** natural resilience of computational kernel, proportional checkpoint/restart

Target Systems:

- K Computer, BlueGene P/Q, Blue Waters, Tsubame 2



G8 ECS: Enabling Climate Simulation at Extreme Scale

Climate simulation challenges at Exascale

Challenges in climate simulation:

- Decrease uncertainties and improve accuracy

Exascale use case:

- Simulate the past 2000 years and compare with proxy data
- Decadale prediction, Regional prediction

Use case requirements:

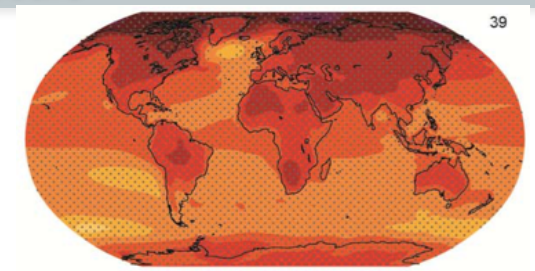
- Increase the resolution significantly, run ensembles and incorporate more components.

→ Need much larger runs

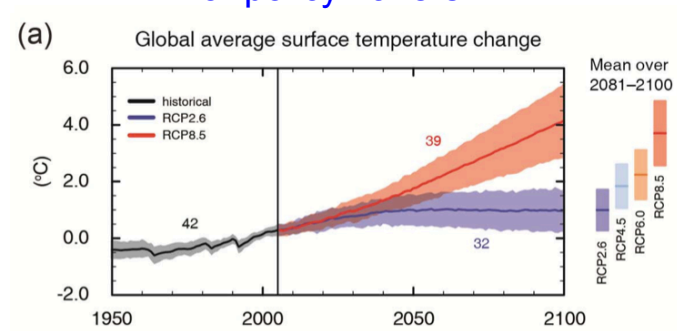
G8 ECS Objectives:

– **Understand what will be the major obstacles that the climate community will face at Exascale**

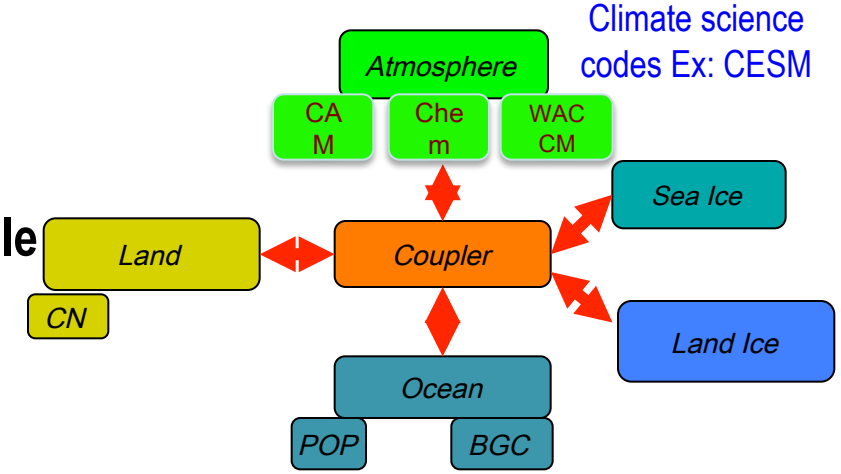
– **Propose and evaluate possible mitigations**



2013 IPCC report for policymakers

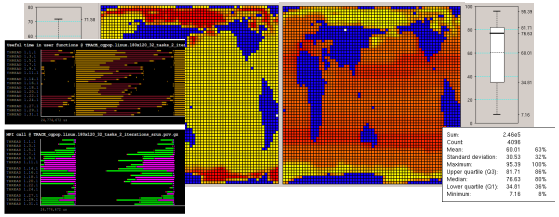


Climate science codes Ex: CESM



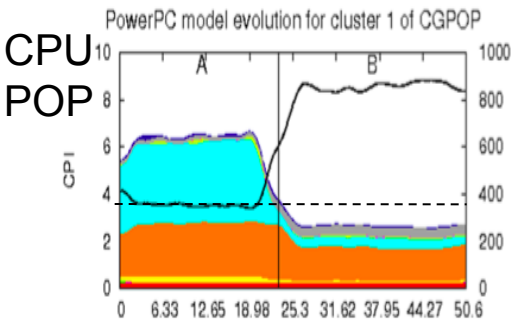
G8 ECS: Enabling Climate Simulation at Extreme Scale
Unexpected Hurdles and Lessons learned

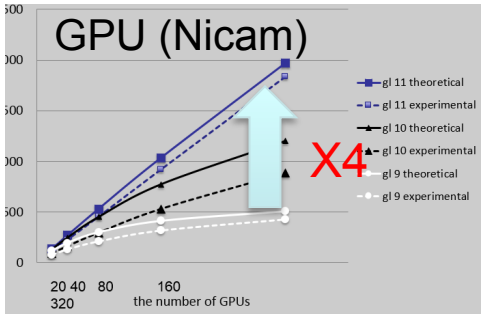
Outstanding contributions:



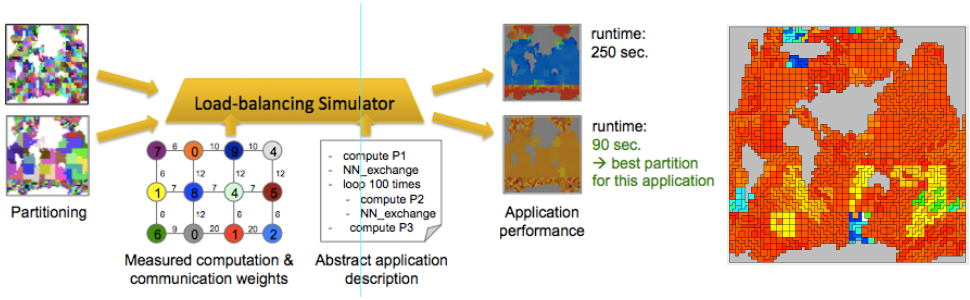
1) **Diagnostic**: where to look for perf. Improvements
   Perf tools: Scalasca (GRS) and Paraver (BSC) are essential

2) **Improved node level performance** Ex: heterogeneous nodes (CPU and GPUs)

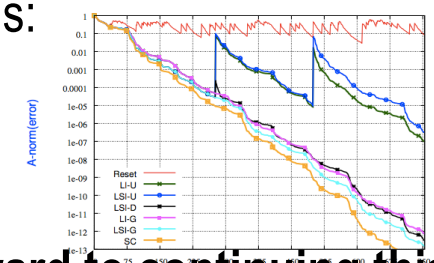


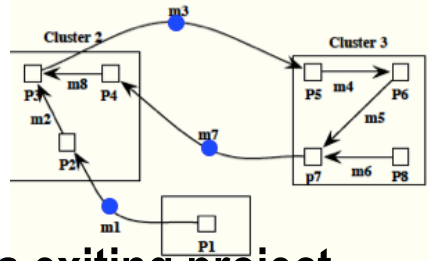


3) **Improved scalability:** New Static load balancing simulator and new space filling curve algorithm



4) **Improved resiliency** for large scale executions:
   New resilient numerical methods, new fault checkpoint/restart for proportional recovery





Very good progresses: the team is looking forward to continuing this exiting project

ExArch: Exascale Analytics on Distributed Archives

The ExArch project seeks to develop a framework for the scientific interpretation of multi-model ensembles at the peta- and exascale. Specifically, a framework for evaluating the imminent Climate Model Intercomparison Project, Phase 5 (CMIP5) archive, which will be largest of its kind ever assembled in this domain and the Coordinated Regional Downscaling experiment (CORDEX), which will push even beyond CMIP5 in resolution, albeit on the regional scale.

- Web processing services Query
- syntax Common
- information model
- Processing operators
- Scientific diagnostics

UCLA

Institut Pierre Simon Laplace

DKRZ

UNIVERSITY OF TORONTO

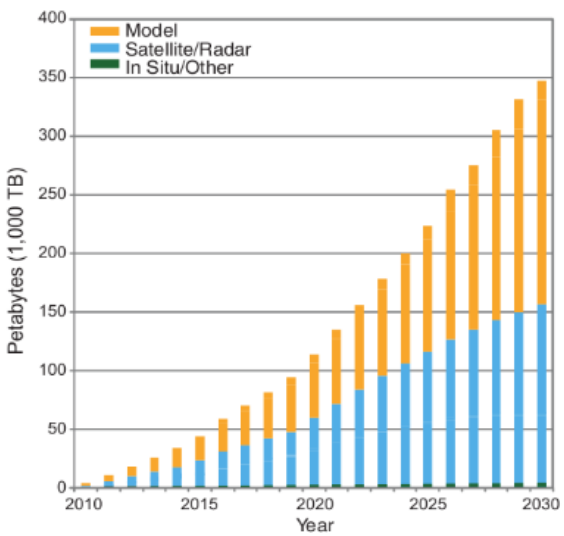
Princeton University

enes European Network for Earth System Modelling

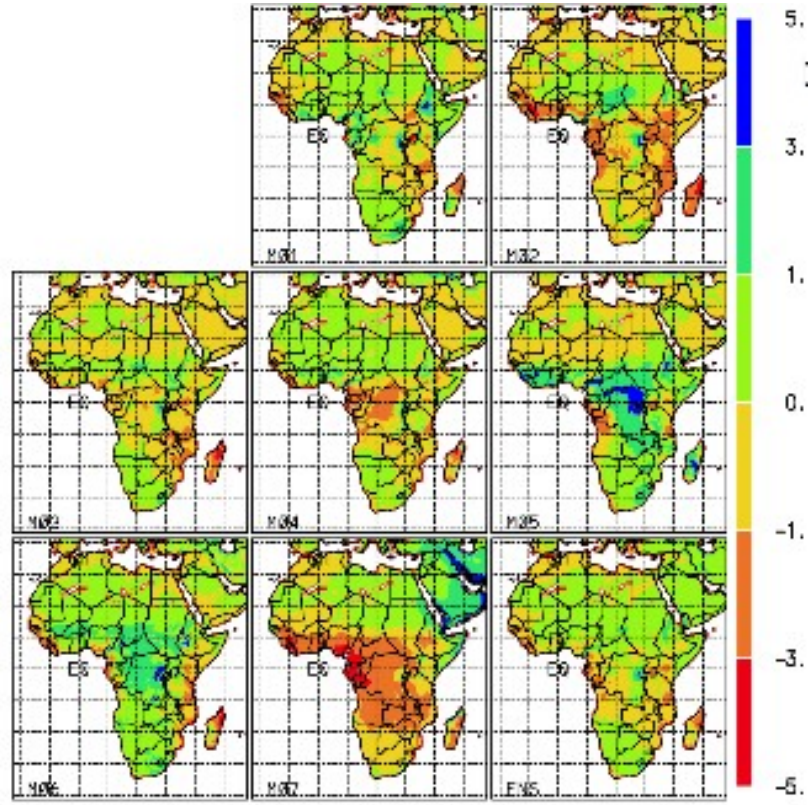
Centro Euro-Mediterraneo per i Cambiamenti Climatici

ExArch: Scientific Applications

Climate data volumes are reaching exabyte-scale within the decade. ExArch is defining and developing climate diagnostics for the distributed CMIP5 archive: bringing analysis to data.



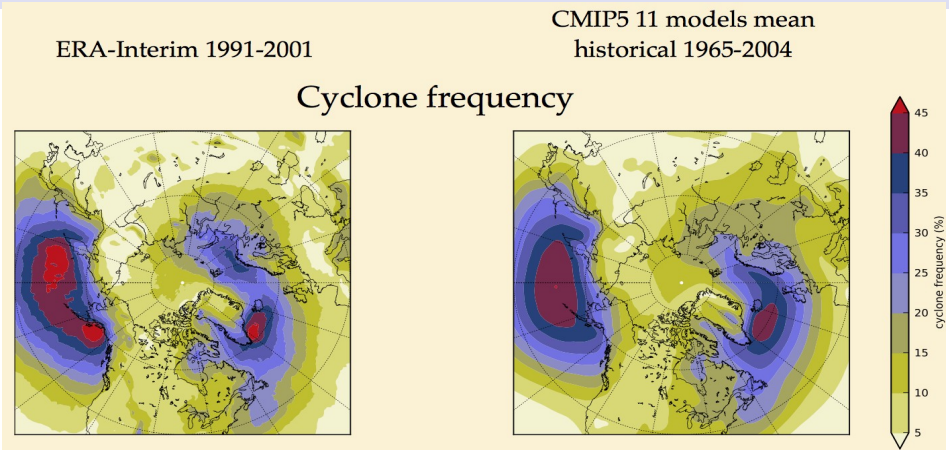
From Overpeck et al 2011.



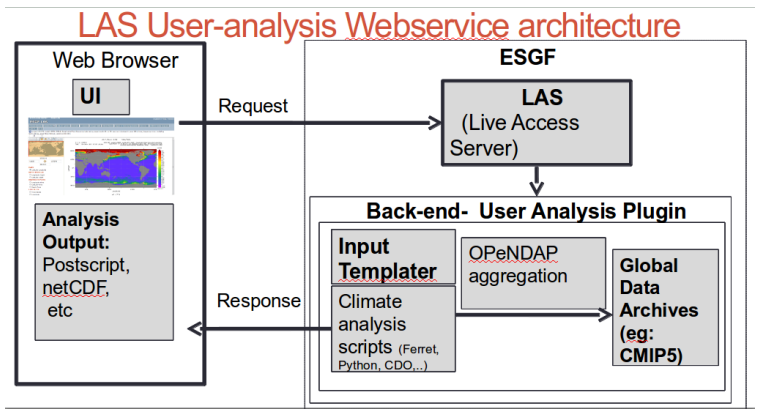
Model biases in the CORDEX-Africa hindcast study (Kim et al. 2013, Clim. Dyn.

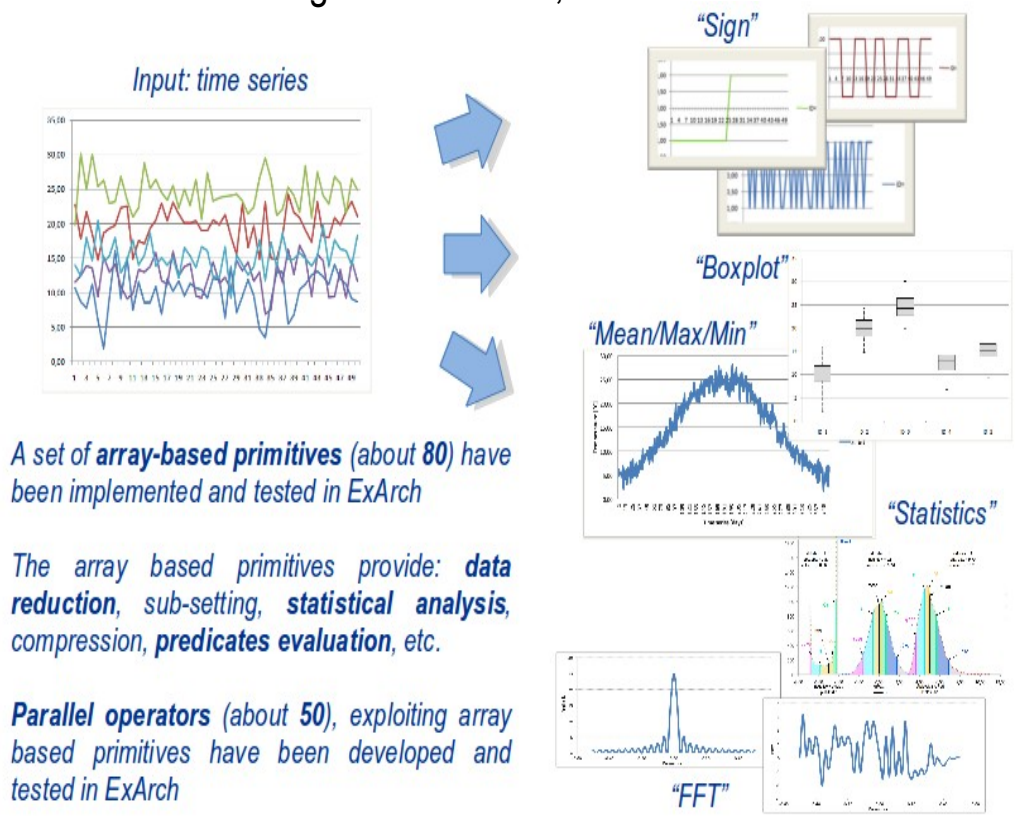
ExArch: T echnical Infrastructure

- Leverages Earth System Grid Federation (ESGF), ES-DOC provenance metadata, OGC Web Processing Services, etc.
- Community-developed climate diagnostics.



From forthcoming ExArch article, BAMS 2014.





S. Fiore, A. D'Anca, C. Palazzo, Ian T. Foster, Dean N. Williams, Giovanni Aloisio, "Ophidia: Toward Big Data Analytics for eScience", ICCS 2013, June 5-7, 2013 Barcelona, Spain, Procedia Computer

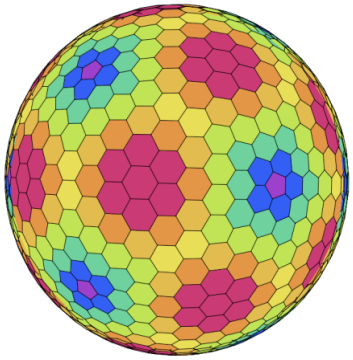
- From Radhakrishnan et al, AGU 2012.

G8 ICOMEX: ICOsahedral-grid Models for Exascale Earth System Simulations [Japan, UK, France, Germany, Russia]

→ Lead PI: **Günther Zängl**, Deutscher Wetterdienst, Germany

Objective: Prepare 4 advanced Earth system models (ESMs) based on icosahedral grids – *with differences in terms of numerics and grid structures*

- NICAM, Structured hexagonal A-grid
- ICON, Unstructured triangular C-grid
- MPAS, Unstructured hexagonal C-grid
- DYNAMICO, Structured hexagonal C-grid

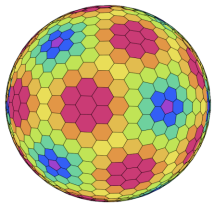


- Exascale computing required
- Icosahedral grids are believed to be well suited because of relatively uniform mesh size

→ Basic strategy

- Address selected key problems on the way to exascale and derive generic solutions
- Work packages focus on the optimization of computational performance and parallelization of I/O
- They are complemented by an overarching WP involving a regular model intercomparison exercise on K computer

G8 ICOMEX: Progress and problems



- Intercomparison and evaluation of models

  → *Porting the model codes to K computer turned out to be difficult*

  - *Non-standard software stack (e.g. MPI library)*
  - *Initially, remote memory access did not work*
  - *OpenMP is not supported. Using the available auto-parallelization requires code refactoring at a level that is not feasible for the non-Japanese groups*

  → *Thus, only a limited performance comparison could be conducted so far*

- Improving CPU-level computational efficiency

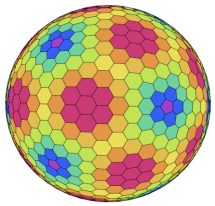
  → *Abstract model description scheme*

  - Prototype implementation available that allows adapting the memory layout to a given computing platform
  - For the ICON dynamical core, changing the memory layout from (cells, levels, blocks) to (levels, cells, blocks) yields a speedup between 11% and 17% on IBM Power 6 and Intel Westmere

  → *Assess potential of using GPUs*

  - Uses DYNAMICO code as work base; OpenACC directives will be considered first

G8 ICOMEX: Progress and problems



- Implicit solvers for massively parallel computing platforms

  → *Multigrid Helmholtz solver avoids global communication*

  → *First results indicate competitive computational performance and scaling*

- Parallel I/O and internal postprocessing

  → *I/O benchmarking and optimization*

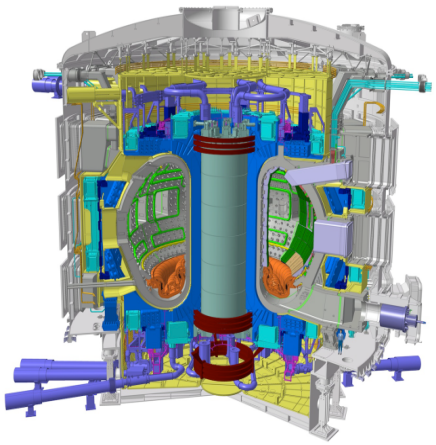
  - Benchmarking revealed performance degradation due to interactions between high-level I/O libraries and file system
    - A patch circumventing the NetCDF cache speeds up serial write by a factor of 3
    - MPI-IO layer on DKRZ supercomputer (IBM Power 6) required major performance fix
    - Embarrassingly parallel output (one file per task) continues to be fastest (A patch for HDF5 has been developed in the WP)
  - A generic performance optimized interface is needed to reduce optimization effort!

    → *Parallel internal postprocessing*

  - As a first step, a second-order accurate, conservative, scalable and efficient remapping scheme for arbitrary grids has been developed and successfully tested

G8 NuFuSE: Nuclear Fusion Simulations @ Exascale
[UK, US, Germany, Japan, France, Russia]

- **Objectives**: ***(toward goal of delivering Fusion as viable energy source)***



→ Deliver *high fidelity predictive capability for addressing burning plasma issues in ITER.*
→ Develop needed software to utilize *computing at extreme scale* to address this challenge.
→ Demonstrate effective cross-disciplinary research & cultivate a *new generation of fusion scientists* with multi-disciplinary expertise.

- **Four focus areas:**

Plasma Physics

- *Large scale simulation codes capable of new physics discoveries enabled by productive use of modern extreme scale supercomputers.*
- *Interdisciplinary ("co-design") with CS & Applied Math to help ensure code efficiency & scalability when deployed on modern low-memory HPC systems.*

Edge Physics

- *Improve conventional approaches for dealing with complex geometries and associated resolution issues.*
- *Investigate alternative simulation technologies to deal with most challenging spatial simulation requirements.*

Fusion Materials Physics

- *Address challenge of high temporal and spatial demands via simulations spanning "ab-initio" to reactor lifetime.*
- *Introduce new functionality to deal with "rare event" simulation & address scaling issues of current material codes.*

Computer Science/Applied Mathematics

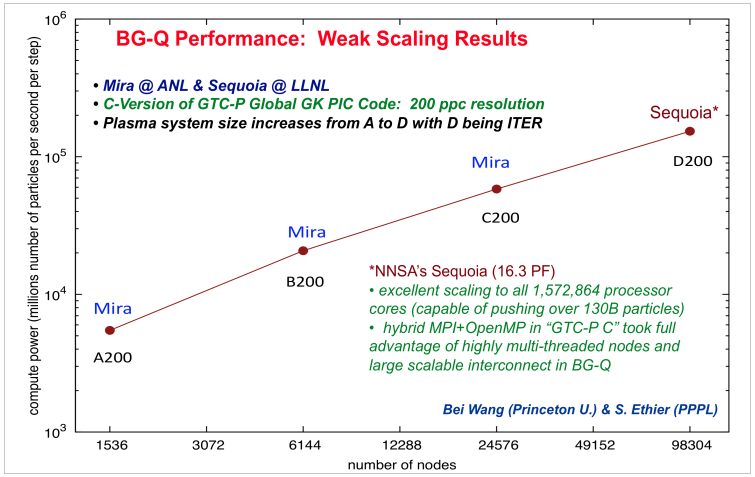
- *Develop algorithms and software technology to enable development of new codes and/or modernization of existing software to enable effective use of path to extreme scale architectures.*
- *Utilize new programming languages or simulation techniques to enable optimization and portability of this project's codes in the three physics areas.*

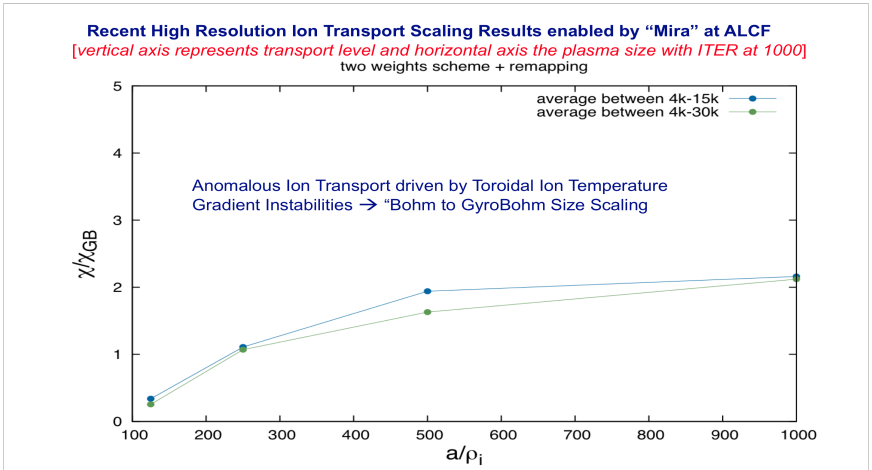
cea | epcc | IPP Max-Planck-Institut für Plasmaphysik | JÜLICH FORSCHUNGSZENTRUM | PPPL PRINCETON PLASMA PHYSICS LABORATORY

Nu-FuSE Progress Highlights http:// www.nu-fuse.com

- **New Fusion Physics Results:**

(1) Unprecedented high-resolution, long duration simulations of ITER-scale plasmas using new version of GTC-P code on most powerful multi-PF BG-Q systems worldwide ("Mira" @ ALCF and "Sequoia @ LLNL) produced *important new physics results that previous estimates (over past decade) for improvement of confinement with increasing plasma size* ***actually*** *exhibits a much more gradual "rollover" transition with magnitude of transport reduced by a factor of two.* [(i) Nov. 16 HPC wire article: http://www.hpcwire.com/2013/11/16/sc13-research-highlight-extreme-scale-plasma-turbulence-simulation/ ; (ii) Nov. 19 IDC HPC Innovation Excellence Award; and (iii) Nov. 20 SC'13 oral paper by ***Bei Wang,*** Nov. 20].





(2) New simulations with improved DFT (density functional theory) codes for modelling paramagnetic materials produced *new insights into defect energies for austenitic materials .*

Nu-FuSE Progress Highlights http:// www.nu-fuse.com

- **Advances in Software Tools Testing/Development/Implementation:**
  - Explored possible use of XcalableMP (XMP) and XMP-Dev capability on a number of NuFuSE codes *[featured at 2-days G8 NuFuSE Post-Doc Workshop in Edinburgh (March, 2012)]*
  - Explored MDMP for alternative parallelization functionality
  - GPU version of GTC-P code developed and being improved (in collaboration with LBNL team)
  - Developed and optimised *PEPC-F mesh-free simulation code* to enable extreme scale edge simulations on low-memory systems such as BG/Q
- **HPC resources access**
  - Project access to HELIOS (1.5 PFlop/s BullX B510 system) → *9.6 million core hours*
  - Access to (i) **partner systems** → *MIRA & JUQUEEN BG/Q; HECToR Cray XE6; HA-PACS GPGPU; K-COMPUTER; …* & (ii) **external systems** → *SEQUOIA BG/Q; TITAN & TH1-A GPGPU; STAMPEDE, TH-2 INTEL-MIC; …*
- **Outreach, Training, and Dissemination**
  - EASC2013 conference (Exascale Applications and Software Conference) → *sponsored & organized new Exascale Conference, 130 attendees, 3 day program*
  - Training and Meetings on HPC & Science → *educate post-doc members (e.g., Bei Wang)*

G8 Seismic Imaging: Modeling Earthquakes and Earth's Interior based on Exascale Simulations of Seismic Wave Propagation [US, Canada, France]

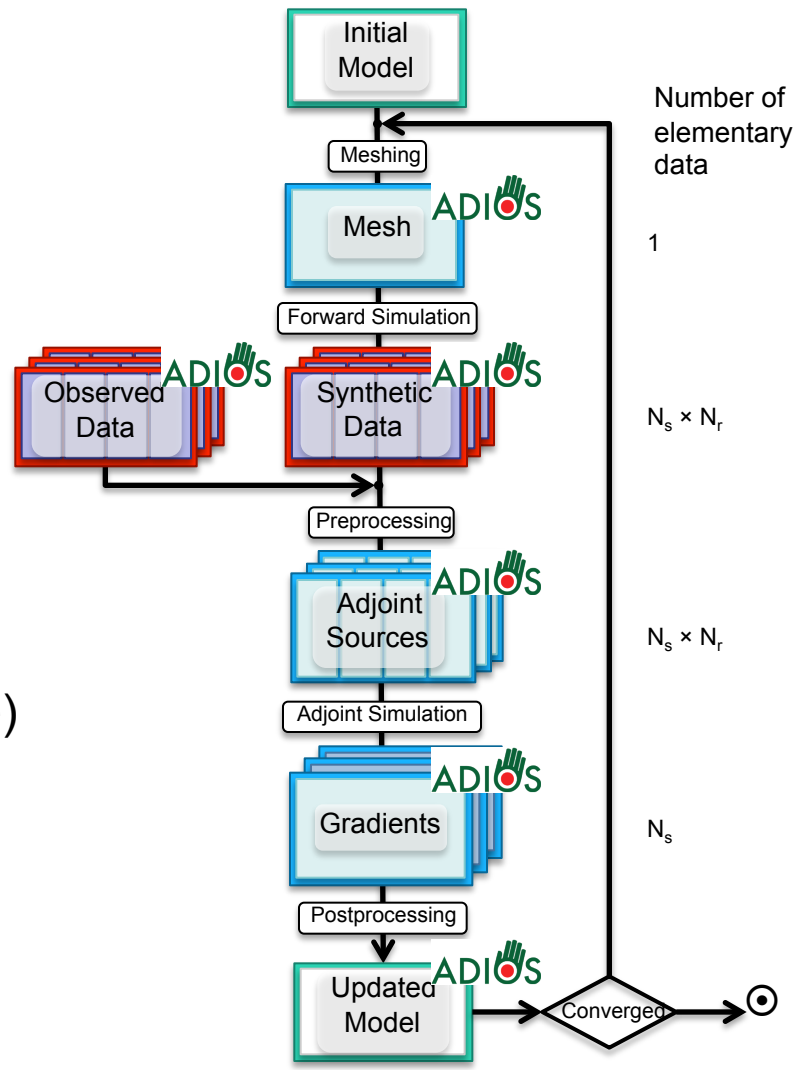
- Team
  - **Jeroen Tromp** (Main PI, Princeton University)
  - Dimitri Komatitsch (Marseille, France)
  - Qinya Liu (University of Toronto, Canada)
- Objectives:
  - Accelerate progress toward global seismic imaging
    - → spectral-element and adjoint methods
    - → forward modeling @ unprecedented speeds, scales, & accuracy
    - → Scaling the adjoint tomography workflow to a large number of earthquakes

  -- *Positive implications for near real-time simulations & hazard assessment*
- Research Progress:
  - GPU computing results for studies of seismic wave propagation
  - "Big Data" issues are tackled with ADIOS, a parallel I/O library
  - First global tomographic imaging results obtained

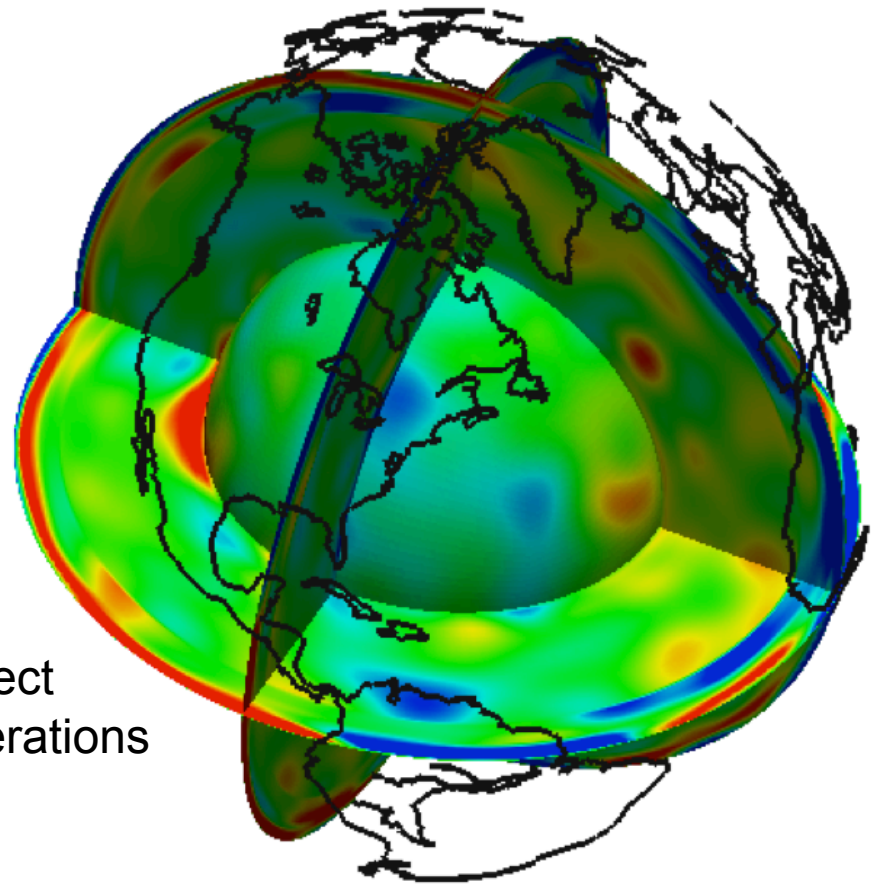
G8 Seismic Imaging: Adjoint Based Seimic Workflow and "Big Data"

- Computational Data
  - Mesh related variables
  - Accelerate mesher and solver I/O
  - Write up to 16.9 GB/s on Titan (~70%)
  - VisIt reader in progress

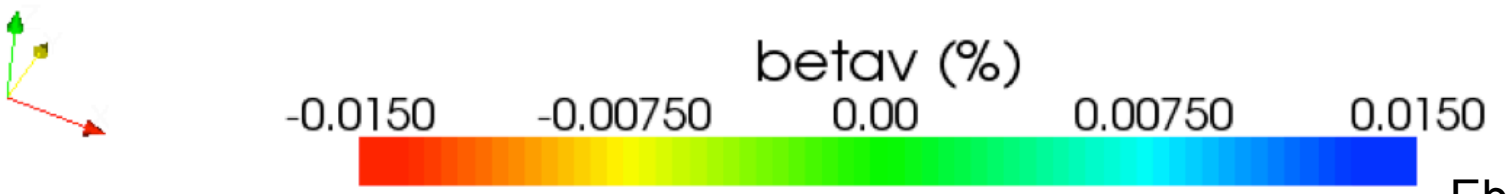
- Seismic Data
  - Legacy Seismic Data Format
    - Lack of flexibility (fixed header / size)
    - Hard to parallelize
  - ASDF
    - Adaptable Seismic Data Format
    - Take advantage of metadata
    - Easily parallelizable



G8 Seismic Imaging: Global Tomography – Model Evolution



Perturbation with respect
To 1D model after 3 iterations



Ebru Bozdag

G8 INGENIOUS: Using Next-Generation Computers & Algorithms for Modeling Dynamics of Large Bio-molecular Systems [Japan, UK, France, Germany, Russia]

- Team: **Makoto Taiji (Main PI, RIKEN, QBiC ACIS, Japan), et al.**

Societal challenge: computational modelling of large bio-molecular systems (e.g. proteins) in water (crucial for biomedical applications)

Solution: combining molecular dynamics with continuum models (explicit, local, easy to parallelise, memory efficient)

- Research Progress:

Developed a conceptually new hybrid framework that smoothly combines fully atomistic (MD) regions with fully continuum (hydrodynamics)

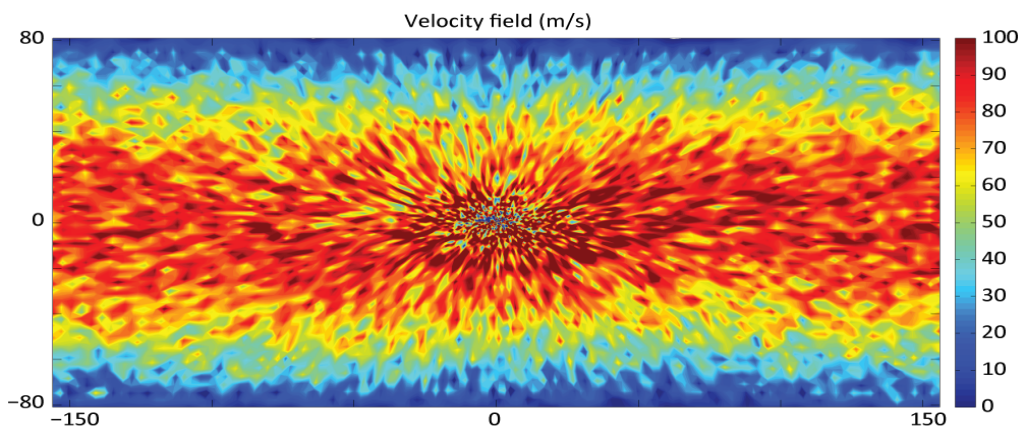
-- Atomistic: high performance MD (MDGRAPE-4)

-- Continuum: Fluctuating Hydrodynamics (Landau-Lifshitz 1958)

Journal Publication to appear in *Philosophical Transactions of the Royal Society A*

"Multi-scale Systems in Fluids and Soft Matter: Approaches, Numerics, & Applications"

TARDIS = Time Asynchronous Relative Dimension In Space

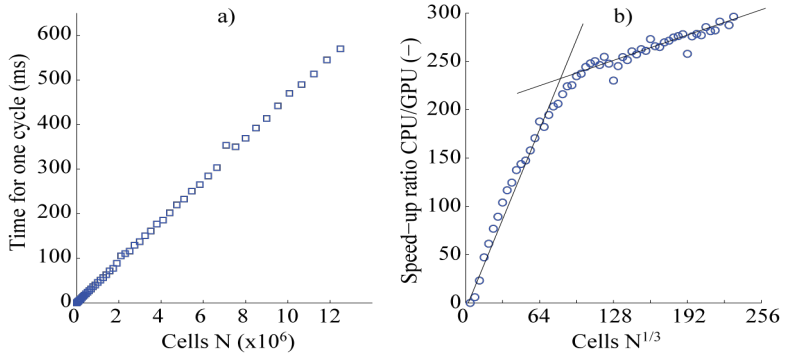


Resolving Brownian fluctuations within a Stokes channel flow

- "Meshless" zoom-in function for the regions of interest
- Space and time rescaling to achieve required resolution in the zoomed area
- Solving with a method preserving macroscopic conservation laws
- Markesteijn and Karabasov, *J. Comp. Phys.* 2013

Scalability of FHD solver with NVidia Tesla C2075 GPU

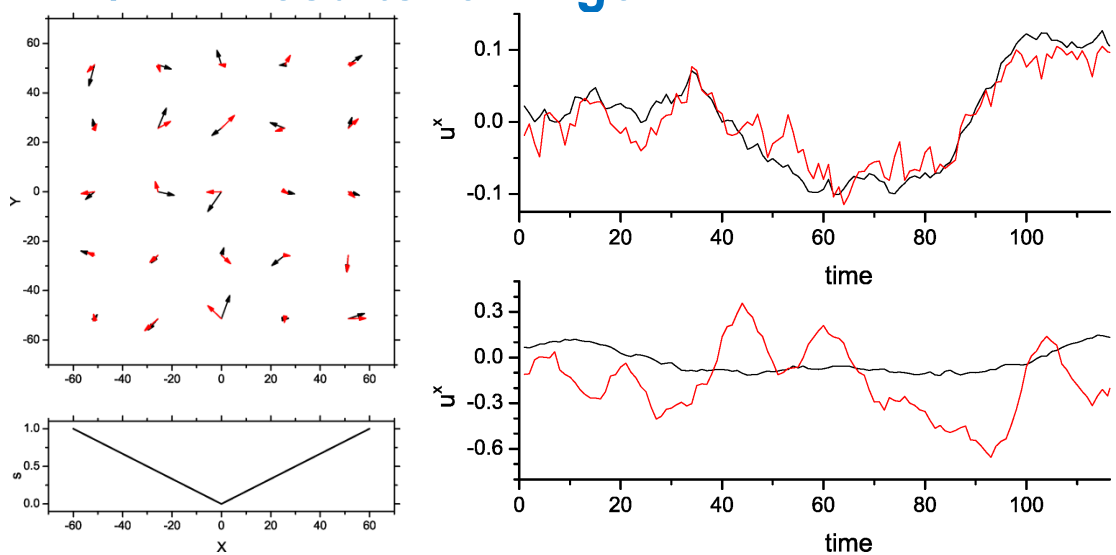
G8 INGENIOUS



- a) Amount of time one cycle takes on GPU versus number of cells (N)
- b) Ratio between time taken to execute one cycle on CPU versus that on GPU versus the number of cells in one direction of the cubed domain
- Markesteijn et al. 2013 (under review)

Hybrid MD/FHD results for Argon

- **Left top**: HD velocities (black) and MD velocities averaged over the cell (red)
- **Left bottom**: the "zoom in" function: HD in the middle, MD at the left and right edges
- **Right top**: MD velocities follow HD in the "HD" region
- **Bottom**: MD velocities are independent in the "MD" region



Bottlenecks and lessons learned: *efficient multi-time-space algorithms are required*

Accelerated Molecular Simulation for Multi-scale Simulations

- **Multi-scale approach combining MD and CFD**

  MD part requires comparable speed with continuum simulations with longer timestep

  Fast MD simulations of small systems are required

  Strong scaling problem

- **Special-purpose computer for MD simulation :**

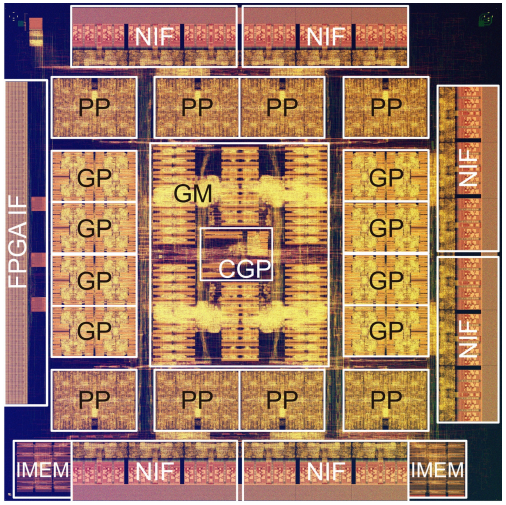
  MDGRAPE-4

  – System-on-Chip based approach for fast MD simulations

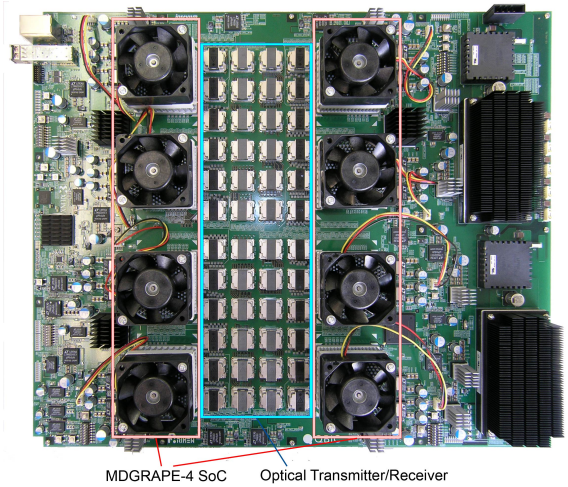
  – Integrates processor cores, networks, and dedicated pipelines

  – 1.3 PFLOPS/512-chip system scale up to ~ 10^5 atoms

  – <u>Completion</u> : *expected by first half of 2014*



MDGRAPE-4 SoC Image



MDGRAPE-4 System Board

G8 INGENIOUS

OUTLINE

1. Brief Summary Reports from Current G8 Exascale Projects

2. Key Upcoming G8 Event:

   G8 Exascale Projects Final Review Meeting in Princeton, NJ – June 12-13, 2014 focusing on Final Reports from the current six G8 Exascale Projects

3. G8 Heads of Research Councils (HORCs) Plans for Multilateral Research Funding for "BDEC" R&D:

➔ *Presentation **now** by Jean-Yves Berthou (ANR, France) on behalf of the international agencies regarding the upcoming G8 "Big Data and Extreme Computing (BDEC)" Program*

SC'13 BOF - G8 Extreme Scale & Big Data Program: Progress on Current Exascale Projects & Future Funding Opportunities

Associated partner:

Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues

Jean-Yves Berthou, *French National Research Agency*

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G8 Research Councils Initiative on Multilateral Research Funding

- G8 Heads of Research Councils (HORCs) meeting in Kyoto, Japan, in May 2008: Proposal for a **multilateral funding activity**:
  - Multilateral research projects can address global challenges in ways that are beyond the capacity of national or bilateral activities.
  - The G8 HORCs framework provides the unique opportunity to pilot a new modality for conducting international research.
- Goals: supporting **excellent** and **interdisciplinary** research on topics of **global relevance** best tackled through a multinational approach.
- Research topics defined separately for each call.
- 7 Funding Agencies: NSERC (Canada), ANR (France), DFG (Germany), JSPS (Japan), RFBR (Russia), RCUK (UK), NSF (USA).
- Principles:
  - A common call text with selection criteria predefined together
  - A **multinational peer review** process in 2 stages (pre-proposals and full proposals)
  - Consortia consisting of partners from at least 3 of the participating countries.
  - **National funding** according to normal terms and conditions for national project funding.
  - Funding meant for **collaborative research**, not merely for networking, mobility or communication.

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G8HORCS calls planned

- 2011 : *Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues*
- 2012 : *Interdisciplinary Programme on Material Efficiency – A First Step towards Sustainable Manufacturing*
- 2013 : *Interdisciplinary Programme on Coastal vulnerability & Fresh water security* – Belmont Forum (IGFA - International Group of Funding Agencies for Global Change Research)

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Preparing HPC Codes and Software for Exascale Computing: Early results of the G8 Exascale Projects

G8 Exascale workshop – November 2012

1. Share the early results of these 6 projects and their impact on science
2. Explore common lessons learned in terms of Exascale research
3. Present early feedback on this innovative multinational collaborative pilot program
4. Discuss between funding agencies, PIs and the Exascale community related to the G8 tool: call, award management, cooperation between partners, consortium management

Funding Organizations

- The Natural Sciences and Engineering Research Council of Canada (NSERC)
- The French National Research Agency (ANR)
- The German Research Foundation (DFG)
- The Japan Society for the Promotion of Science (JSPS)
- The Russian Foundation for Basic Research (RFBR)
- The Research Councils of the United Kingdom (RCUK)
- The U.S. National Science Foundation (NSF)

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First Feedbacks:

- Worldwide Collaborations

A unique opportunity to enable collaborations between 3 to 6 different countries (4 projects with 5 or 6 countries):

  - making improvement available in all these countries while usual international collaborations are bilateral or regional ones (EC, US, Asia),
  - enabling international comparison of great value, leading to some of the most important recent advances in some of the scientific fields funded
  - transforming the frontiers , fostering international collaboration, speeding-up the research
  - enabling a mix of top world researchers to collaborate

- Education and training: involving an average 10 students / project, providing them a unique opportunity to collaborate and be trained by the best worldwide researchers in the field
- Enabling the access to top worldwide facilities, HPC computers and Big Data.
  - ECS : BLueWaters (NCSA), Intrepid (ANL), K computer (Riken), Tsubame2(Titech), Jugene (PRACE), Marenostrum2 (BSC)
  - NuFuse: BG-Q (DOE-SC's"Mira"@ALCF & NNSA's "Sequoia" at LLNL), K-Computer (Riken), Jugene (JSC); Titan (OLCF); TH 1-A and initial access to TH-2 (China).

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First Feedbacks:

Interest of non G8 countries:

- NCAR and Spain joined the ECS project, China joined Nu-Fuse project.

Interest of companies:

- The SEISMIC IMAGING project has initiated a collaboration with Intel and IBM.

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First Feedbacks:

- Projects :

research engaged need to continue beyond the 3 years project

- NFOs:

management burden not sustainable for some agencies (Canada)

- All :
  - One call does not make sense, need 5 years visibility at least
  - very little amount of money
  - Need to find way to make sustainable, long term, multi-lateral collaborations

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ICT scientific programme manager/directors from NSF/ DFG/ANR proposition to the G8 HORCs, May 2013

The way forward…..G8 HORCs Pilot call as a seed

take over by scientific departments/ boards

1. Follow up call : " *Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues*"
2. 2011 G8 Exascale call: final projects review, June 12-13, 2014 in Princeton University, Princeton, NJ, USA.

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ICT scientific programme manager/directors from NSF/ DFG/ANR proposition to the G8 HORCs, May 2013

A follow-up call, "Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues"

1. A "two-threads " approach
2. Enabling some existing G8 Exascale projects to propose a second phase
3. Also open for new proposals
   - Participation à la carte to 1 and/or 2
   - Open to new countries out of G8

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

Scientific Perimeter

"This international program aims at supporting collaborations between experts in research areas related to ***global challenges*** *and developers of* ***future computing and data platforms****, so that they can together address the relevant needs of the research community during the early design stages of emerging new computing systems.*

The program will support ***interdisciplinary projects*** *targeting the exploration and development of* ***open source algorithms and data operations that are resilient, sustainable and scalable to Big Data and Extreme Computing for application solutions to socially relevant global scale issues****. It is only through the close cooperation of computing specialists with global scale issues specialists,* ***including related humanity and social scientists*** *where appropriate, that future high performance computing and Big Data systems can successfully be applied to tackle essential challenges for mankind in the 21st century."*

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

Major evaluation criteria:

- Scientific quality and innovativeness of the joint research plan
- Sound project management, methodological approach, feasibility and appropriateness of the joint research plan
- Added value to be expected from the research collaboration
- Balanced cooperation
- Competence and expertise of teams and complementarities of consortium (interdisciplinary / inclusion of all necessary expertise)
- Appropriateness of resources and funding requested
- Expected impacts: e.g. scientific, technological, economic, societal
- Opportunities for early career researchers

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

Funding organizations

ANR DFG EPSRC Pioneering research and skills NSF RFBR RUSSIAN FOUNDATION FOR BASIC RESEARCH

DFG will only funds Follow-up Proposal: "built on the results of a project funded by the first "*G8-Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues*" call. It must address an extension of the initially funded topic of research. Its consortium must be as close as possible to the one of the initially funded project. It is allowed to change the Leading PI. Each modification must be justified."

Associated partner: JSPS 日本学術振興会 Japan Society for the Promotion of Science

"JSPS is collaborating with the Group of Program Coordinators but follows its own evaluation process. JSPS will provide funding opportunity in parallel with the Joint Call. JSPS will deliver the confirmation of budget directly to the Group of Program Coordinators during the evaluation process. "

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

Agenda

T0
Publication of the "Call for Proposal"

T0+3months
Pre-Proposal submission deadline

T0+5months
s Invitation to submit Full Proposal

T0+7months
Full Proposal submission deadline

T0+11months
Official Funding Decision

- It is expected to fund approximately 4-8 consortia
- Total approximate budget : 10 million € over three years.
- Funding can be provided for projects lasting three years.
- Each consortium must consist of at least one academic participant from a minimum of 3 different countries represented by the participating Funding Organizations.
- More than one partner from each country is possible in each consortium. However, consortia should aim for a balanced geographical contribution to the research project.

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

Participation of applicants from countries not represented by any of the Funding Organizations (including JSPS)

"A proposal **may include applicants from countries not represented by any of the Funding Organizations**. In this case they will have to secure their own budget:

- The **Preliminary Proposal** must integrate a document describing the status of acquiring their budget needed for achieving the contribution to the proposal.
- **Full proposals** that include PIs from countries not represented by any of the Funding Organizations must contain **an alternative scenario** addressing the consequences for the proposal of an unsecured budget, including but not limited to, the consequences of their possible withdrawal from the proposal consortium.
- Applicants from countries not represented by any of the Funding Organizations will have to provide a confirmation related to the acquisition of their budget at the latest **one month prior to the final review**. The Associate Partner Organizations will provide directly the outcome of its own evaluation process.
- Such applicants **cannot act as leading PI** of a proposal.

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Call secretariat:

ANR: Mouna.ESSABBAH@agencerecherche.fr

Members of the Group of Program Coordinators

DFG: marcus.wilms@dfg.de
NSF: dkatz@nsf.gov (Daniel S. Katz)
ANR: Jean-yves.berthou@agencerecherche.fr, Mouna.Essabbah@agencerecherche.fr
EPSRC: Jane.Nicholson@epsrc.ac.uk, Susan.Morrell@epsrc.ac.uk, Daniel.Emmerson@epsrc.ac.uk
RFBR: a.sharov@rfbr.ru (Alexander Sharov), ysorokot@rfbr.ru (Yaroslav Sorokotyaga)
DOE: William.Harrod@science.doe.gov

Associated partner:

JSPS: kiyoshi-saito@jsps.go.jp

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Interdisciplinary Program on Application Software towards Extreme Computing and Big Data for Global Scale Issues

RFBR support letter

RUSSIAN FOUNDATION FOR BASIC RESEARCH

Leninsky pr., 32A, Moscow, GSP-1,119991
Ph.: (495) 952-58-47, fax: (495) 938-19-31
http://www.rfbr.ru

08.11.2013 № 1157-Д/16

Ref. _____ Dated _____

November 8, 2013

Dr. Jean-Yves Berthou
Director
ICT Department
Agence Nationale de la Recherche (ANR)
and the international agency representatives for the G8 "Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues"

Dear Dr. Berthou,

We regret not to be in a position to join you and our colleagues from the G8 research councils at their meeting during the 2013 Supercomputing Conference on November 18th. Nevertheless, we would like to re-emphasize herewith the RFBR strong support – which has of course been communicated to you in our previous discussions -- for the continuation beyond its initial 3-year period of the excellent program on "Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues."

In consideration of the exascale systems with acceptable levels of power consumption that are being planned for the near future, it is clear that computing at scale will fundamentally change many aspects of computations that impacts key areas of societal importance. This includes significant challenges associated with scaling, resiliency, result validation, and programmability – as well as "big-data discovery" challenges and opportunities.

We believe that the G8 program in "Big Data and Extreme Computing (BDEC)" will enable continuation of the excellent productivity of the existing projects as well as providing opportunities for worthy new projects. The Russian Foundation for Basic Research (RFBR) strongly supports the G8 "BDEC" Program and believes that it is very important to continue this international collaborative research into the future.

Sincerely,

Dr. Alexander N. Sharov

Head, International Relations Department,

Russian Foundation for Basic Research (RFBR)