G8 Exascale Software Applications: Fusion Energy

International Exascale Software Project (IESP) Workshop

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Context: G8 Exascale Software Applications Awards
Source: Irene Qualters, NSF Program Director for Cyberinfrastructure

- “Enabling Climate Simulation @ Extreme Scale” – US, Japan, France, Canada, Spain

- “Icosahedral-Grid Models for Exascale Earth System Simulations” – Japan, UK, France, Germany, Russia

- “Nuclear Fusion Simulations @ Exascale” – UK, US, Germany, Japan, France, Russia

- “Using Next-Generation Computers & Algorithms for Modelling Dynamics of Large Biomolecular Systems” – Japan, UK, France, Germany, Russia

- “Modeling Earthquakes and Earth's Interior based upon Exascale Simulations of Seismic Wave Propagation” – US, Canada, France

- “ExArch: Climate Analytics on Distributed Exascale Data Archives” – UK, US, France, Germany, Canada, Italy
Fusion: an Attractive Energy Source

• Abundant fuel, available to all nations
  – Deuterium and lithium easily available for millions of years
• Environmental advantages
  – No carbon emissions, short-lived radioactivity
• Cannot “blow up or melt down,” resistant to terrorist attack
  – Less than a minute’s worth of fuel in the chamber
• Low risk of nuclear materials proliferation
  – No fissile materials required
• Compact relative to solar, wind and biomass
  – Modest land usage
• Not subject to daily, seasonal or regional weather variation; no requirement for local CO₂ sequestration
  – Not limited in its application by need for large-scale energy storage nor for long-distance energy transmission
• Fusion is complementary to other attractive energy sources
Fusion Energy: Burning plasmas are self-heated and self-organized systems

Deuterium-Tritium Fusion Reaction

Plasma self-heating

Energy Multiplication
About 450:1

\[ D^+ + T^+ \rightarrow ^4\text{He}^{++} (3.5 \text{ MeV}) + n^0 (14.1 \text{ MeV}) \]
Progress in Magnetic Fusion Research

Data from Tokamak Experiments Worldwide

Fusion Power

Megawatts

Kilowatts

Watts

Milliwatts

Years


TFTR (U.S.)

JET (EUROPE)

ITER

10MW

16MW

500MW
ITER Goal: Demonstration of the Scientific and Technological Feasibility of Fusion Power

- **ITER is a dramatic next-step for Fusion:**

  -- **Today:** 10 MW(th) for 1 second with gain ~1
  -- **ITER:** 500 MW(th) for >400 seconds with gain >10

- Many of the technologies used in ITER will be the same as those required in a power plant but additional R&D will be needed

  -- “DEMO”: 2500 MW(th) continuous with gain >25, in a device of similar size and field as ITER
    * Higher power density
    * Efficient continuous operation

- Strong R&D programs are required to support ITER and leverage its results.

  -- Experiments, theory, *computation*, and technology that support, supplement and benefit from ITER
G8 Exascale Project: Fusion Energy Sciences
Some Criteria for Consideration

(1) **Demonstrated need for Exascale**

-- leading FES application codes currently utilize, e.g., Leadership Class Facilities (LCF’s) at ORNL (Cray XT5) and ANL (IBM-BGP), demonstrating scalability of key physics with increased computing capability

(2) **Significant Scientific Impact:** Identified: (i) “Grand Challenges in FES & Computing @ Extreme Scale (DoE Report, March 2010); and (ii) “Opportunities & Challenges of Exascale Computing – DoE Advanced Scientific Computing Advisory Committee Report (Fall, 2010)

*Priority Research Directions:*

- high physics fidelity predictive simulation capability for multi-physics, multi-scale FES dynamics
- ITER/burning plasmas physics simulation capability

(3) **Productive Pathway (over 10 years) to Exploitation of Exascale**

-- demonstrated ability to carry out confinement simulations (e.g., turbulence-driven transport) of higher physics fidelity with access to increased computational capability
Exascale Application Domain: Fusion Energy Science
(Figure courtesy of D. Keyes)

“Big Copper”

Physics Priority Research Directions (PRD’s)

Mathematical Formulations

Scalable Algorithms

Data Analysis, Mgt., Visualization

Programming Models, Tools, Frameworks

“Big Iron”
The petascale challenge of simulating magnetic confinement fusion experiments

• **The goal**: predictive simulation of fusion experiments at all time and spatial scales

• **The reality**: currently need at least 4 levels of codes to treat this extremely complex multiscale physics.
Elements of Fusion System Integrated Model

- Sawtooth Region ($q < 1$)
- Core confinement Region
- Magnetic Islands
- Edge Pedestal Region
- Scrape-off Layer
- Vacuum/Wall/Conductors/Antenna
G8 Research Council’s Initiative on Multilateral Research Funding
“NuFUSE” (Nuclear Fusion Simulations @ Exascale)

- **UK** -- Graeme Ackland (Univ. of Edinburgh) – Lead PI (Lead for Plasma Materials Physics) – EPCC, Edinburgh*
- **USA** -- William Tang (Princeton University/PPPL) – Co-PI (Lead for Plasma Physics) – ALCF, Argonne*
- **France** -- Xavier Garbet (CEA, Cadarache) – Plasma Physics
- **Germany** -- Detlev Reiter (Juelich) – Co-PI (Lead for Edge Physics) – JSC, Juelich*
  & Frank Jenko (IPP, Garching) – Plasma Physics
- **Japan** -- Taisuke Boku (Tsukuba University) – Co-PI (Lead for Computation) – CCS, Tsukuba*
- **Russia** -- Boris Chetveruskin (Keldish Institute of Applied Math) – Edge Physics – IHEP, Moscow*

*Supercomputing Centres involved in the NuFUSE Project

**NOTE:** G8 funding process still in progress in some countries

> 1st “Face-to-Face” NuFUSE Project Meeting to be scheduled
Importance of Turbulence in Fusion Plasmas

- Turbulence is believed to be primary mechanism for cross-field transport in magnetically confined plasmas:
  - Size and cost of a fusion reactor determined by particle and energy confinement time and fusion self-heating

- Plasma turbulence is a complex nonlinear phenomenon:
  - Large time and spatial scale separations similar to fluid turbulence.
  - Self-consistent electromagnetic fields: many-body problem
  - Strong nonlinear wave-particle interactions: kinetic effects.
  - Importance of plasma spatial inhomogeneities, coupled with complex confining magnetic fields, as drivers for microinstabilities and the ensuing plasma turbulence.
LCF-enabled simulations provide new insights into nature of plasma turbulence

- Teraflops-to-petaflops computing power have accelerated progress in understanding heat losses caused by plasma turbulence

- Multi-scale simulations accounting for fully global 3D geometric complexity of problem (spanning micro and meso scales) have been carried out on DOE-SC Leadership Computing Facilities

- Excellent Scalability of Global PIC Codes enabled by strong ASCR-FES collaboration in SciDAC projects

- Exascale-level production runs are needed to enable running codes with even higher physics fidelity and more comprehensive & realistic integrated dynamics

  e.g. -- Current petascale-level production runs on ORNL’s Jaguar LCF require 24M CPU hours (100,000 cores × 240 hours)

**Mission Importance:**
Fusion reactor size and cost are determined by balance between loss processes and self-heating rates
Scaling of 2D Domain Decomposition on IBM BG-P System

Particle + grid scaling study of GTCP on Intrepid (IBM BG/P)

Number of particles moved 1 step in 1 second

- Weak scaling of grid and particles
- ITER-size device (131 million grid points)
- D3D-size device (8.2 million grid points)

ITER-size simulation with only 512 MB/core!

S. Ethier, PPPL, Sep. 2009
Some PIC Challenges in Moving toward Exascale

**Locality**: Need to improve data locality (e.g., by sorting particles according to their positions on grid)
-- basic gather-scatter PIC algorithm expends too much time accessing random numbers in a large grid array

**Latency**: Need to explore highly multi-threaded algorithms to address memory latency

**Flops vs. Memory**: Need to utilize Flops (cheap) to better utilize Memory (limited & expensive to access)
-- redo some calculations instead of storing results that are reused somewhere else in the code (e.g. particle-grid positions).

**Emerging Architectures**: Need to deploy innovative algorithms within modern codes that demonstrably deliver new science on GPU and GPU-CPU hybrid systems
-- multi-threading within nodes, maximizing locality while minimizing communications, etc.

**Large Future Simulations**: Need to likely work with >10 billion grid points and over 100 trillion particles!!