Global Simulation of Plasma Microturbulence at the Petascale and Beyond

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“A Presentation of Mira’s First Science”

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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 minute’s worth of fuel in 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 by need for large-scale energy storage nor for long-distance energy transmission

- **Fusion is complementary to other attractive energy sources**
Progress in Magnetic Fusion Energy (MFE) Research

Data from Tokamak Experiments Worldwide

Fusion Power

Megawatts

1,000

100

10

Kilowatts

1,000

100

10

Watts

1,000

100

10

Milliwatts

1,000

100

10

Years

1975

1985

1995

2005

2020

10MW

16MW

500MW

ITER

TFTR (U.S.)

JET (EUROPE)
ITER Goal: Demonstration of the Scientific and Technological Feasibility of Fusion Power

• **ITER** is an ~$20B facility located in France & involving 7 governments representing over half of world’s population
  ➔ dramatic next-step for Magnetic Fusion Energy (MFE) producing a sustained burning plasma
  -- Today: 10 MW(th) for 1 second with gain ~1
  -- **ITER**: 500 MW(th) for >400 seconds with gain >10

• **“DEMO”** will be demonstration fusion reactor after **ITER**
  -- 2500 MW(th) continuous with gain >25, in a device of similar size and field as **ITER**

• Ongoing R&D programs worldwide [experiments, theory, computation, and technology] essential to provide growing knowledge base for **ITER** operation targeted for ~ 2020

➢ **Realistic HPC-enabled simulations required to cost-effectively plan, “steer,” & harvest key information from expensive (~$1M/long-pulse) **ITER** shots**
Magnetically confined plasmas in a tokamak are complex and require HPC analysis.

- **B field line**: Represents the magnetic field lines within the tokamak.
- **Magnetic surface**: The boundary within which the plasma is confined.
- **Larmor radius \( \rho_L \)**: Describes the radius of the circular path a particle follows in a magnetic field.
- **Particle trajectory**: The path a particle follows within the tokamak.
- **Trapped particles**
- **Passing particles**
- **\( \nabla B \) and curvature drifts**: Refers to the divergence of the magnetic field and its effects on particle motion.
- **Helical torsion (rotational transform)**: A key aspect in confining plasma particles within the tokamak.
Modern HPC-enabled simulations open opportunities for “transformational” science to accelerate understanding in fusion energy research

Though equations are well-known (Boltzmann-Maxwell), the problem is a physics grand challenge

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q}{m}[E + \mathbf{v} \times \mathbf{B}] \cdot \nabla_v f = C(f) + S(f)
\]

- Seven dimensional equation of motion in phase space, \( f(x, v, t) \) for each species and 2 coupled vector fields
- Extreme range of time scales – wall equilibration/electron cyclotron \( O(10^{14}) \)
- Wide range of spatial scales – machine radius/electron gyroradius \( O(10^4) \)
- Extreme anisotropy – mean free path in magnetic field parallel/perpendicular \( O(10^8) \)
- Intrinsic nonlinearity (e.g. plasma distributions generate significant E and B fields through Maxwell’s equations)
- Sensitivity to geometric details

Advanced simulations required to address grand challenges in plasma science
FES Needs to be Prepared to Exploit Local Concurrency to Take Advantage of Most Powerful Supercomputing Systems in 21\textsuperscript{st} Century (e.g., U.S.'s Blue-Gene-Q & Titan, Japan's Fujitsu-K, China's Tianhe-1A, ...)

- Multi-core Era: A new paradigm in computing
- Massively Parallel Era: USA, Japan, Europe
- Vector Era: USA, Japan
Particle Simulation of the Boltzmann-Maxwell System

• The Boltzmann equation (Nonlinear PDE in Lagrangian coordinates):
\[
\frac{dF}{dt} = \frac{\partial F}{\partial t} + \mathbf{v} \cdot \frac{\partial F}{\partial \mathbf{x}} + \left( \mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \cdot \frac{\partial F}{\partial \mathbf{v}} = C(F).
\]

• “Particle Pushing” (Linear ODE’s)
\[
\frac{dx_j}{dt} = v_j, \quad \frac{dv_j}{dt} = \frac{q}{m} \left( \mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right)_x.
\]

• Klimontovich-Dupree representation,
\[
F = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j) \delta(\mathbf{v} - \mathbf{v}_j),
\]

• Poisson’s Equation: (Linear PDE in Eulerian coordinates (lab frame))
\[
\nabla^2 \phi = -4\pi \sum_{\alpha} q_\alpha \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_{\alpha j})
\]

• Ampere’s Law and Faraday’s Law [Linear PDE’s in Eulerian coordinates (lab frame)]
Particle-in-Cell Simulations

• Early attempts [Buneman (1959); Dawson (1962)]

• Finite-Size Particles and Particle-in-Cell Simulation [Dawson et al. (1968) and Birdsell et al. (1968)]
  - Coulomb potential is modified for a finite size particle due to Debye shielding
  - no need to satisfy \(1/(n \lambda_D^3) \ll 1\)

• Number of calculations for N particles
  - \(N^2\) for direct interactions and \(N\) for PIC

• Collisions are treated as sub-grid phenomena via Monte-Carlo methods [Shanny, Dawson & Greene (1976)]
Gyrokinetic Particle Simulation

Ref. [W. W. Lee, PF ('83); JCP ('87)]

- Gyrophase-averaged Vlasov-Maxwell equations for low frequency microinstabilities.

- Spiral motion of a charged particle is modified as a rotating charged ring subject to guiding center electric and magnetic drift motion as well as parallel acceleration -- *speeds up computations* by 3 to 6 orders of magnitude in time steps and 2 to 3 orders in spatial resolution.
Basic Particle-in-Cell Method

- Charged particles sample distribution function
- Interactions occur on a grid with the forces determined by gradient of electrostatic potential (calculated from deposited charges)
- Grid resolution dictated by Debye length (“finite-sized” particles) up to gyro-radius scale

Specific PIC Operations:
- “SCATTER”, or deposit, charges as “nearest neighbors” on the grid
- Solve Poisson Equation for potential
- “GATHER” forces (gradient of potential) on each particle
- Move particles (PUSH)
- Repeat…
Microturbulence in Fusion Plasmas – Mission Importance: Fusion reactor size & cost determined by balance between loss processes & self-heating rates

• “Scientific Discovery” - Transition to favorable scaling of confinement produced in simulations for ITER-size plasmas
  - $a/\rho_i = 400$ (JET, largest present lab experiment) through
  - $a/\rho_i = 1000$ (ITER, ignition experiment)

• Multi-TF simulations using GTC global PIC code [Z. Lin, et al, 2002] deployed a billion particles, 125M spatial grid points; 7000 time steps @ NERSC ⇒ 1st ITER-scale simulation with ion gyroradius resolution

• Understanding physics of plasma size scaling demands much greater computational resources + improved algorithms [radial domain decomposition, hybrid (MPI+Open MP) language, ..] & modern diagnostics

⇒ Excellent Scalability of Global PIC Codes on modern HPC platforms enables much greater resolution/physics fidelity to improve understanding

⇒ BUT - further improvements for efficient usage of current LCF’s demands code re-write featuring modern CS/AM methods addressing locality, low-memory-per-core, …..

⇒ ESP & INCITE GTC-P Projects on BG-Q @ ALCF
**Performance Speed Up Comparison Results**

(IBM BG-Q vs. BG-P)

<table>
<thead>
<tr>
<th>M0180 ppc =100</th>
<th>Our test</th>
<th>ANL</th>
<th>IBM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed up per node (Q/P ratio)</td>
<td>10.7</td>
<td>10.7</td>
<td>11.2</td>
</tr>
</tbody>
</table>

Speed up per node *comparison with ALCF and IBM results* for “M0180” problem size (i.e., 180 grid-points in radial direction) *using GTC-P code*

→ Test Case for phase-space resolution with particles/cell (ppc) =100 for 100 time-steps
→ “Time to Solution” improvement from *BG-Q hardware*
  • 4X (core) 2X (frequency) 2X (SIMD) = 16 (“theoretical”)
Features of new “GTCP-C” Code

• “GTCP-C” code based on a greatly optimized version of the C-version of the original GTC code (introduced at SC 2011)
  • “C” (instead of usual Fortran) to best incorporate CS community advances in multi-threading for low-memory-per-core systems

• Key additional level of domain decomposition introduced into radial dimension ➔ essential for efficiently carrying out simulations on large-scale plasmas such as ITER
  • Alleviates grid memory requirement issue for large size plasma simulation
  • Improves locality

• Multiple levels of parallelism
  • 2D domain decomposition (toroidal and radial dimensions)
  • Particle decomposition in each domain
  • Multi-threaded, shared memory parallelism implemented with loop-level OpenMP directives

• Improvements over GTCP-FORTRAN code
  • Remove PETSc library for carrying out Poisson field solve
    • Significantly improves code portability to various LCF’s
    • Introduces loop level parallelism in the Poisson solve

 ➔ Overall Software Improvement gives another 50% gain in “Time to Solution”
Reference Fortran Version of GTC-P

(\textit{includes} radial domain decomposition)

![Bar chart showing wall-clock time per step (s) for different node counts and tasks.]

Run on BG-Q (16 cores/node)

- A: 128 nodes
- B: 512 nodes
- C: 2048 nodes
- D: 8192 nodes (ITER size)

Tasks: charge, push, shift, poisson, field, smooth
Optimized C Version of GTC-P [“GTC-P C”]

Wall-clock time per step (s)

Run on BG-Q (16 cores/node)

- **Charge**
- **Push**
- **Shift**
- **Poisson**
- **Field**
- **Smooth**

Nodes ➔

A: 128
B: 512
C: 2048
D: 8192 (ITER size)
Comparative Performance for PIC Operations

Case “D” for ITER Plasma Size

**Mira** 1MPI/
64 OpenMP
[16 cores w/each launching 4 threads]

**Hopper** 4MPI/
6 OpenMP
[Intel design -- avoid NUMA effects]

**Edison** 2MPI/
8 OpenMP
[avoid NUMA effects]
Strong Scaling Study of GTCP-C on Mira

D (ITER-scale) Problem for 100 Time Steps

- 64-way toroidal partitioning on all numerical experiments
- BG/Q (Mira) system -- use 4 processes/node, 16 threads/process

<table>
<thead>
<tr>
<th>Radial partitions</th>
<th>Time on Mira</th>
<th>Ideal</th>
<th>“Eff” (efficiency)</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>527.5</td>
<td>527.5</td>
<td>100%</td>
</tr>
<tr>
<td>64</td>
<td>265.1</td>
<td>263.8</td>
<td>99%</td>
</tr>
<tr>
<td>128</td>
<td>137.1</td>
<td>131.9</td>
<td>96%</td>
</tr>
<tr>
<td>256</td>
<td>72.6</td>
<td>65.9</td>
<td>91%</td>
</tr>
<tr>
<td>512</td>
<td>41.4</td>
<td>33</td>
<td>80%</td>
</tr>
</tbody>
</table>
Weak Scaling Study of GTCP-C on Mira

- GTCP-C Titan points beyond 8192 nodes (dashed line) are extrapolated
- 32768 nodes represents 2/3 of Mira BG-Q system
K-Computer Performance: Weak Scaling Results

- **Fujitsu-K Computer @ RIKEN AICS, Kobe, Japan**
- **C-Version of GTC-P Global GK PIC Code: 200 ppc resolution**
- **Plasma system size increases from A to D with D being ITER**

![Graph showing weak scaling results for GTC-P C.](https://example.com/graph.png)

*Takenori Shimosaka (RIKEN) & Bei Wang (Princeton U.)*
BG-Q Performance: Weak Scaling Results

- **Mira @ ANL & Sequoia @ LLNL**
- **C-Version of GTC-P Global GK PIC Code**: 200 ppc resolution
- **Plasma system size increases from A to D with D being ITER**

- Excellent scaling to all 1,572,864 processor cores (capable of pushing over 130B particles)
- Hybrid MPI+OpenMP in “GTC-P C” took full advantage of highly multi-threaded nodes and large scalable interconnect in BG-Q

*Bei Wang (Princeton U.) & S. Ethier (PPPL)*
Particle Resolution (ppc) Convergence Study
GTC-P C Code for ITER (D-size) Case on BG-Q

Time History of Thermal Diffusivity from ITG Instability
Time History of ITG-driven Thermal Diffusivity (with & without collisions)

→ higher heat flux in NL saturated state (as expected) in presence of collisional dissipation
Summary: Programming Model Challenges in Moving toward Extreme Scales

• **Locality:** Need to improve data locality (e.g., by sorting particles according to their positions on grid)
  -- due to physical limitations, moving data between, and even within, modern microchips is more time-consuming than performing computations!
  -- scientific codes often use data structures that are easy to implement quickly but limit flexibility and scalability in the long run

• **Latency:** Further exploration of highly multi-threaded algorithms to address memory latency motivated, e.g., by positive results from present studies

• **Flops vs. Memory:** Need to utilize Flops (cheap) to better utilize Memory (limited & expensive to access)

• **Advanced Architectures:** Need more “demo-apps” that deploy innovative algorithms within modern science codes on low memory per core architectures – (e.g, BG/Q, Fujitsu-K, Titan, Tianhe-1A, .....
  -- multi-threading within nodes, maximizes locality while minimizing communications
  -- large future simulations (PIC ➞ very high-resolution (ppc) production runs for long-duration in large-plasma-size scaling studies)

Encouraging performance achieved with “GTC-P C” code on BG/Q (Mira & Sequoia), on Fujitsu-K Computer (Japan), and also CPU part of Titan (OLCF)