Computational Challenges in Large-Scale Gyrokinetic Particle-in-Cell Simulations of Fusion Plasmas

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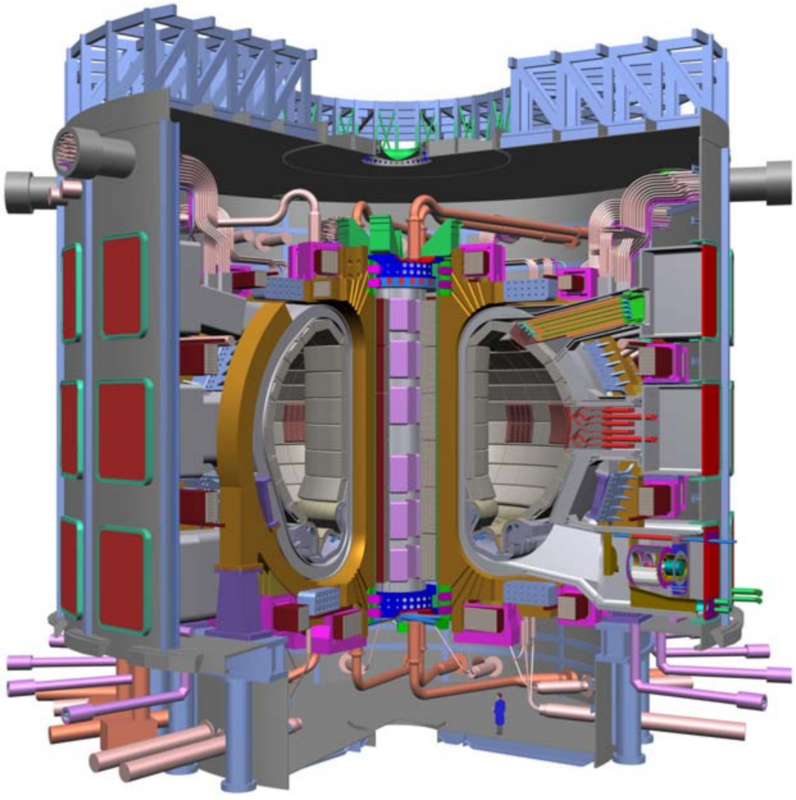
Turbulent Transport in Burning Plasmas.

Motivation: Importance of studying (micro-)turbulence in fusion plasmas

- **Turbulence is believed to be the 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.
- **Critical for ITER, the largest fusion project ever attempted.**



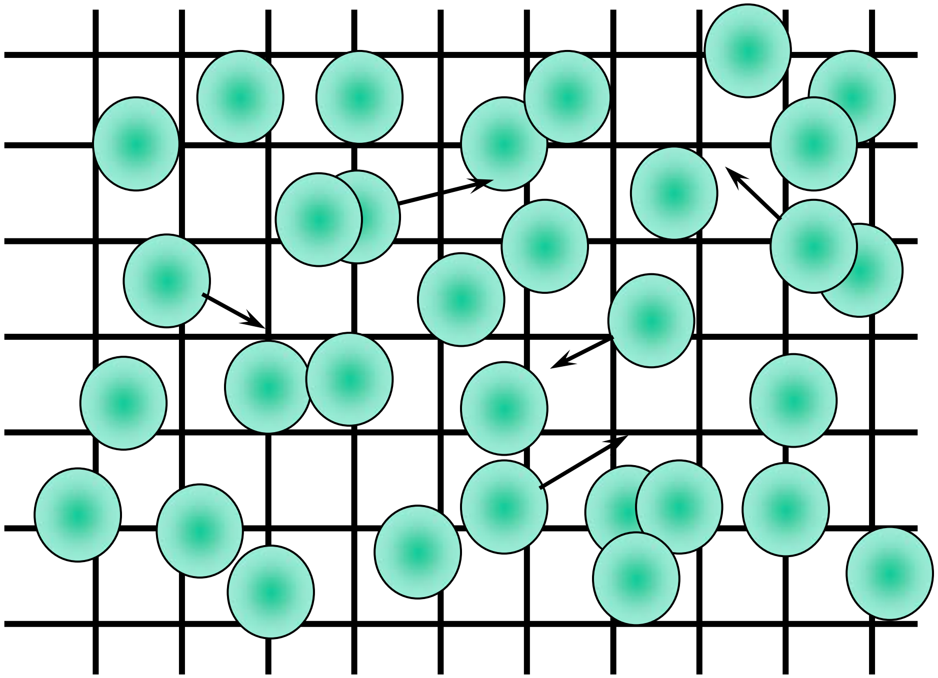
ITER fusion reactor being built in France. Largest device ever. International collaboration.

Best/only way to study plasma turbulence: Large-scale simulations

- 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.
- Requires kinetic treatment using large-scale simulations.
- **The Particle-in-Cell method is well-suited for this type of calculation, and is very scalable.**

Particle-in-cell (PIC) method

- Particles sample distribution function in phase space.
- The particles interact via a grid, on which the potential is calculated from deposited charges.

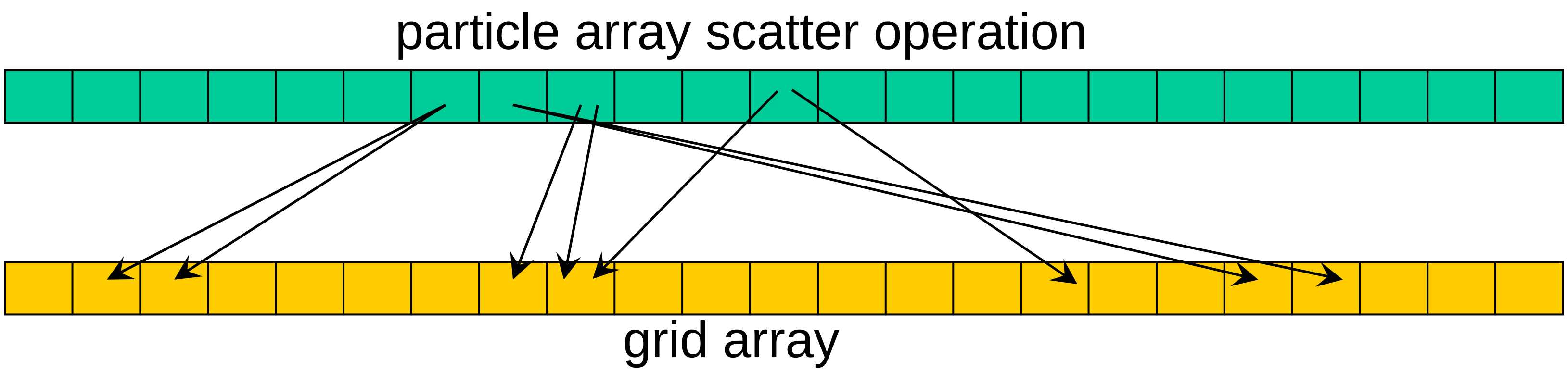


The PIC Steps

- **"SCATTER", or deposit, charges on the grid (nearest neighbors)**
- **Solve Poisson equation**
- **"GATHER" forces on each particle from potential**
- **Move particles (PUSH)**
- **Repeat…**

Main optimization challenge for PIC

- “Gather-Scatter” operation in PIC codes
  - The particles are randomly distributed in the simulation volume (grid).
  - Particle charge deposition on the grid leads to indirect addressing in memory
  - Not cache friendly (relatively low percentage of peak).
  - Need to be tuned differently depending on the architecture.



Possible improvements of gather/scatter performance

- The Cray XMT well-suited to handle gather/scatters
  - A large number of threads could hide memory latency?
  - What about the order in reduction operations?
- SIMD/vectorization works well for the “push” phase (gather) but requires local copies of the grid for the charge deposition (scatter phase).
  - Our application, GTC, reached 24% of peak on the Earth Simulator
  - But uses a lot of memory
- Sorting the particles to improve locality is also a possibility but is it really worth it?

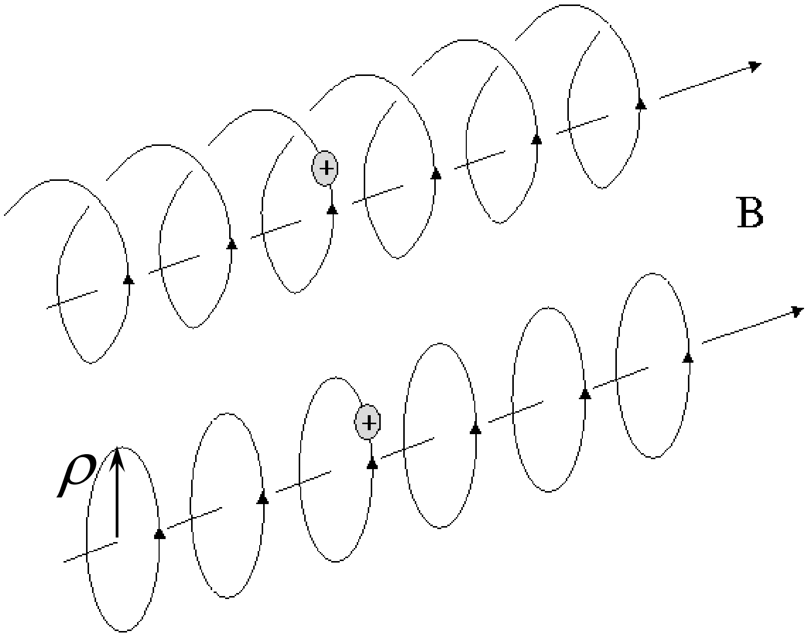
Gyrokinetic approximation for low frequency modes

- Gyrokinetic ordering →

$$\frac{\omega}{\Omega} \sim \frac{\rho}{L} \sim \frac{e\phi}{T} \sim k_{//}\rho << 1$$

$$k_{\perp}\rho \sim 1$$

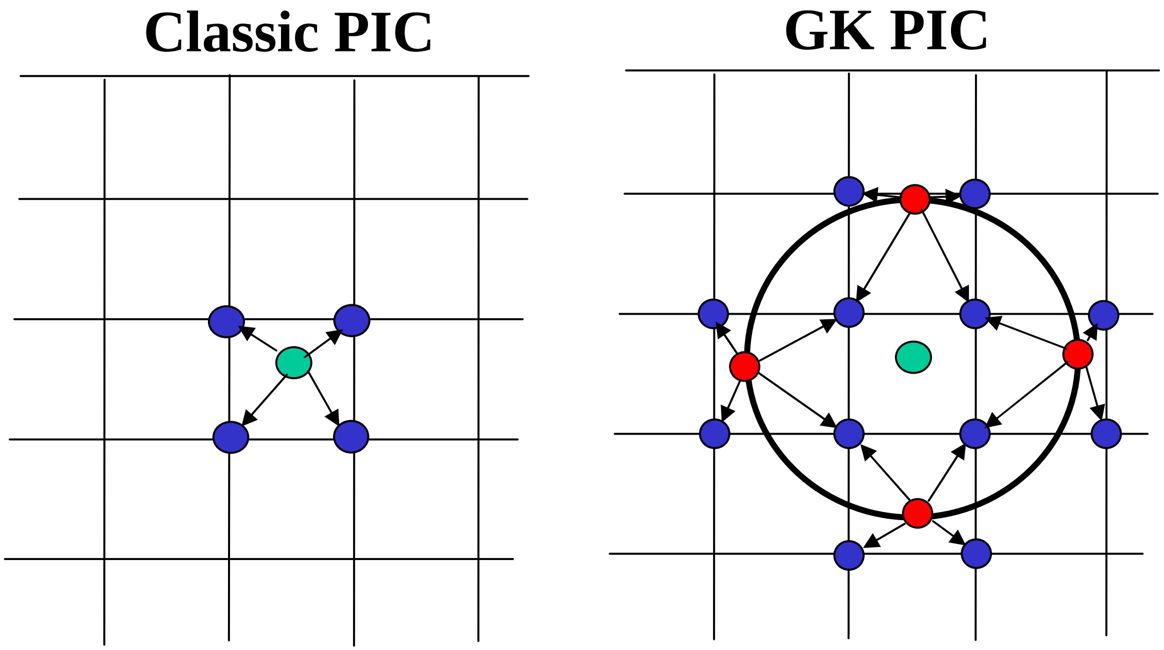
- Gyro-motion: guiding center drifts + charged ring
  - Parallel to B: mirror force, magnetically trapped
  - Perpendicular: E x B, polarization, gradient, and curvature drifts
- Gyrophase-averaged **5D** gyrokinetic equation
  - Suppress plasma oscillation and gyro-motion
  - Larger time step and grid size, smaller number of particles



Gyrokinetic PIC: point particles replaced by “charged rings”

The radius of each ring changes with local magnetic field strength and particle velocity.

Charge Deposition Step (SCATTER operation)



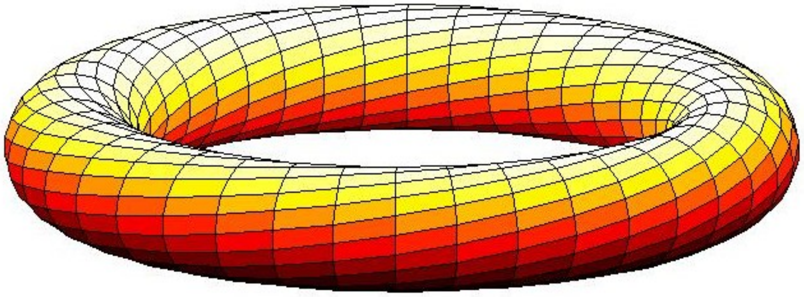
4-Point Average
(W.W. Lee)

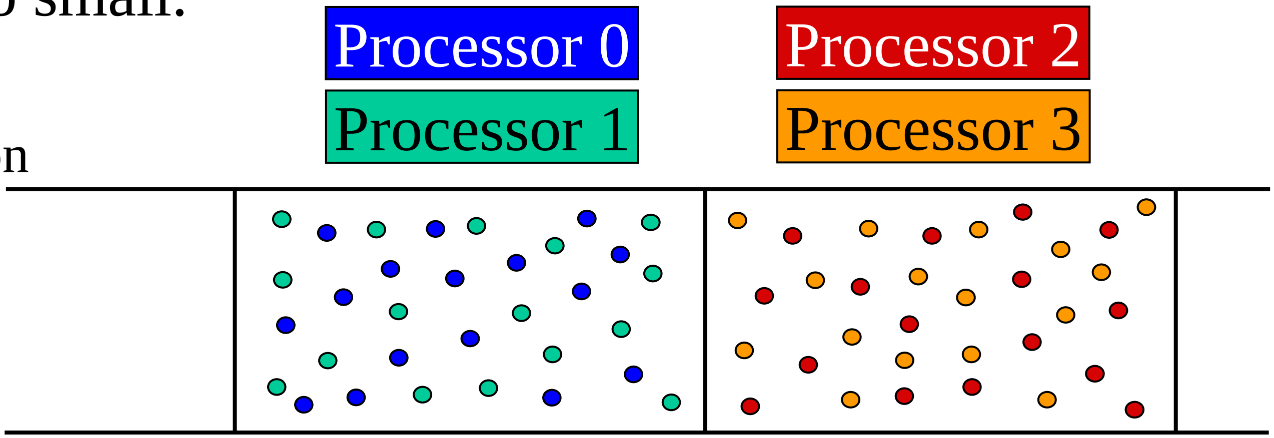
Solving the Maxwell equations on the grid

- All PIC codes need to solve the Poisson equation
- Many codes use FFTs to solve the equation spectrally
  - Easy and straightforward.
  - Requires AlltoAll communications (transpose) for multi-dimensional FFTs = very intensive.
  - Will it scale to very large number of processors?
- Other codes, including GTC, solve the equation in real space
  - A popular library to handle this is PETSc
  - Can switch solvers, pre-conditioners, use multi-grid, etc
  - Will it continue to scale as well?
- Fortunately, the gyrokinetic Poisson equation is only 2D

Parallel model for PIC: Domain decomposition + particle distribution

- Domain decomposition:
  - 3D grid (with its particles) divided between MPI processes.
- Particle distribution method
  - The particles in a toroidal section a equally divided between several MPI processes
- Particles randomly distributed between processors within a toroidal domain.
- Domains cannot be too small.
- GTC:
  - Toroidal decomposition
  - Particle distribution
  - Radial decomposition





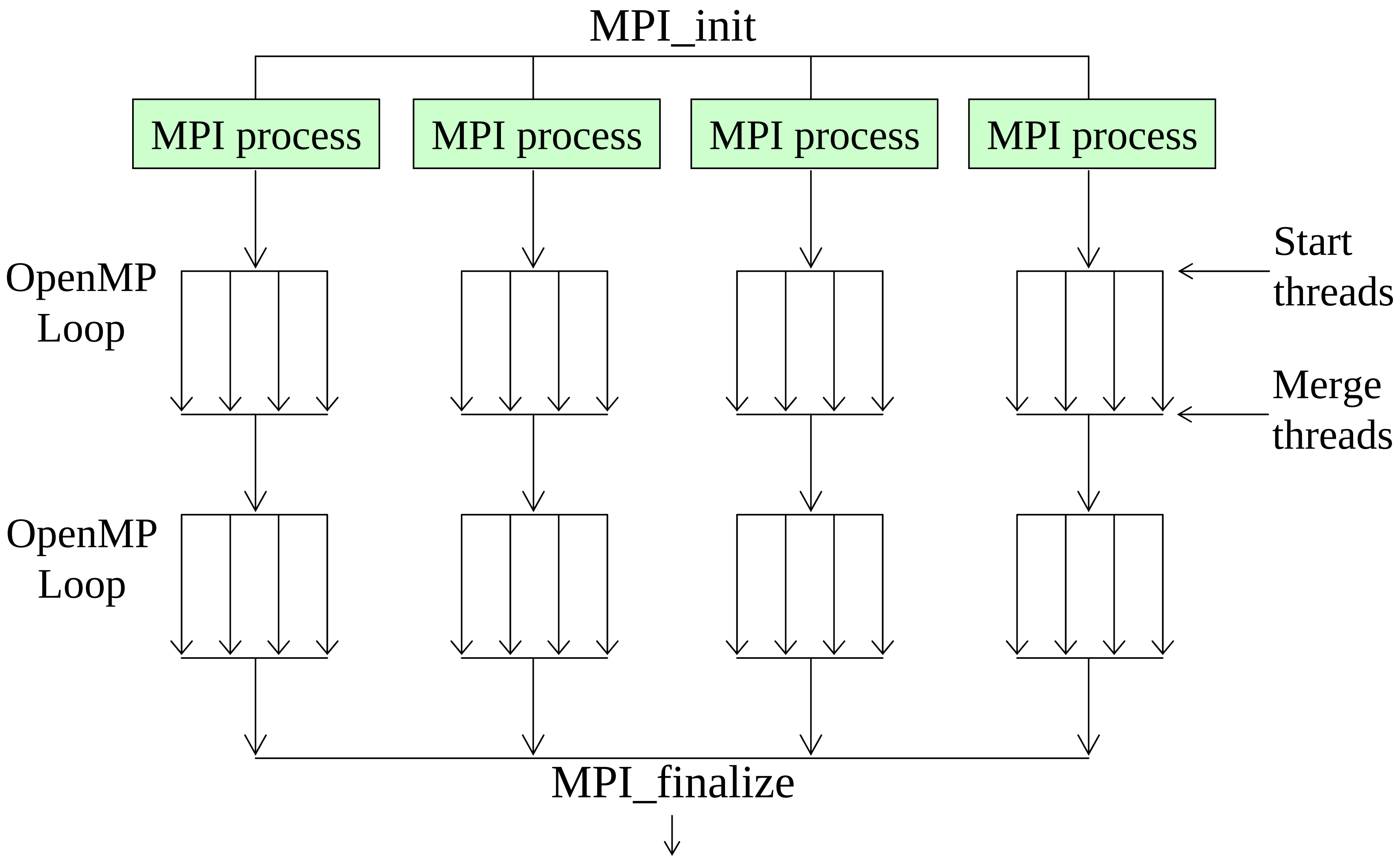
Processor 0

Processor 1

Processor 2

Processor 3

Hybrid MPI-OpenMP loop-level parallelism in GTC



MPI_init

MPI process

MPI process

MPI process

MPI process

OpenMP Loop

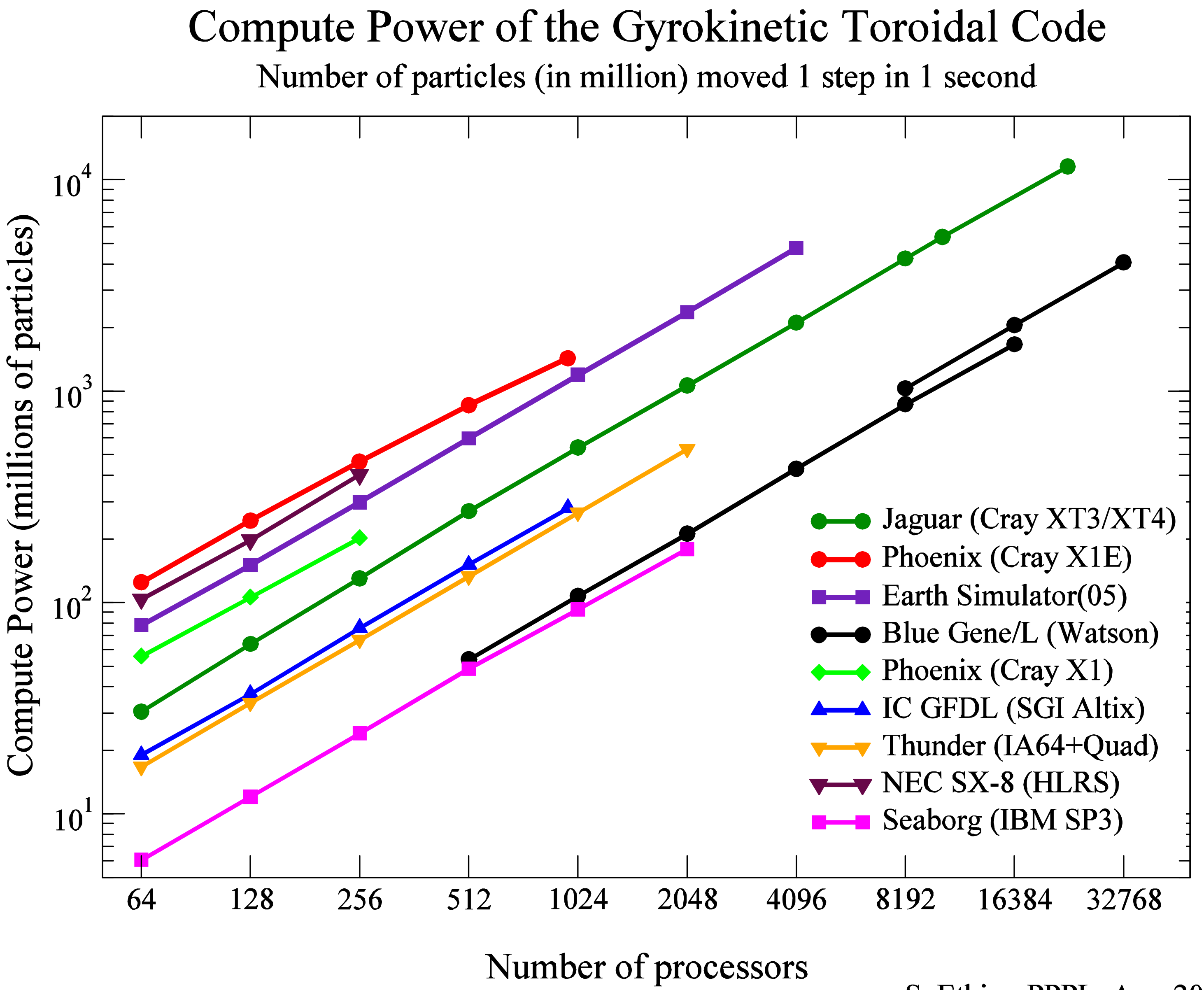
Start threads

Merge threads

OpenMP Loop

MPI_finalize

Great particle scaling for GTC…



S. Ethier, PPPL, Apr. 2007

New challenges for scaling

- Having both kinetic ions and kinetic electrons in the same simulation creates true multi-scale calculation
  - The electrons are much faster than the ions.
  - Need to “sub-cycle” the electrons, i.e. push the electrons several steps between each ion step.
  - The electrons can cross several grid cell in a single sub-step, which creates new challenges for parallel scaling.
  - Equations for the fields are much more difficult to solve.
  - Requires much higher resolution grid = more grid points.
- Fully electromagnetic kinetic simulations for fusion plasmas are very challenging
  - Ultimate goal for “gyrokinetic MHD”.

Concluding remarks

- Improving the performance of the gather/scatter algorithm in PIC codes is key.
- Fast and scalable solvers are required to handle the fully electromagnetic system.
- For gyrokinetic MHD simulations, we will need to run the codes for considerably more time steps, which requires more particles.
- How far can we push the current parallel model?
- How can the new architectures help?