Global Simulation of Plasma Microturbulence at the Petascale and Beyond

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Early Science Program Principal Investigators Meeting
"A Presentation of Mira's First Science"

Argonne Leadership Computing Facility
Argonne National Laboratory
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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 CO_2 sequestration**
  - → Not limited by need for large-scale energy storage nor for long-distance energy transmission
- **Fusion is complementary to other attractive energy sources**

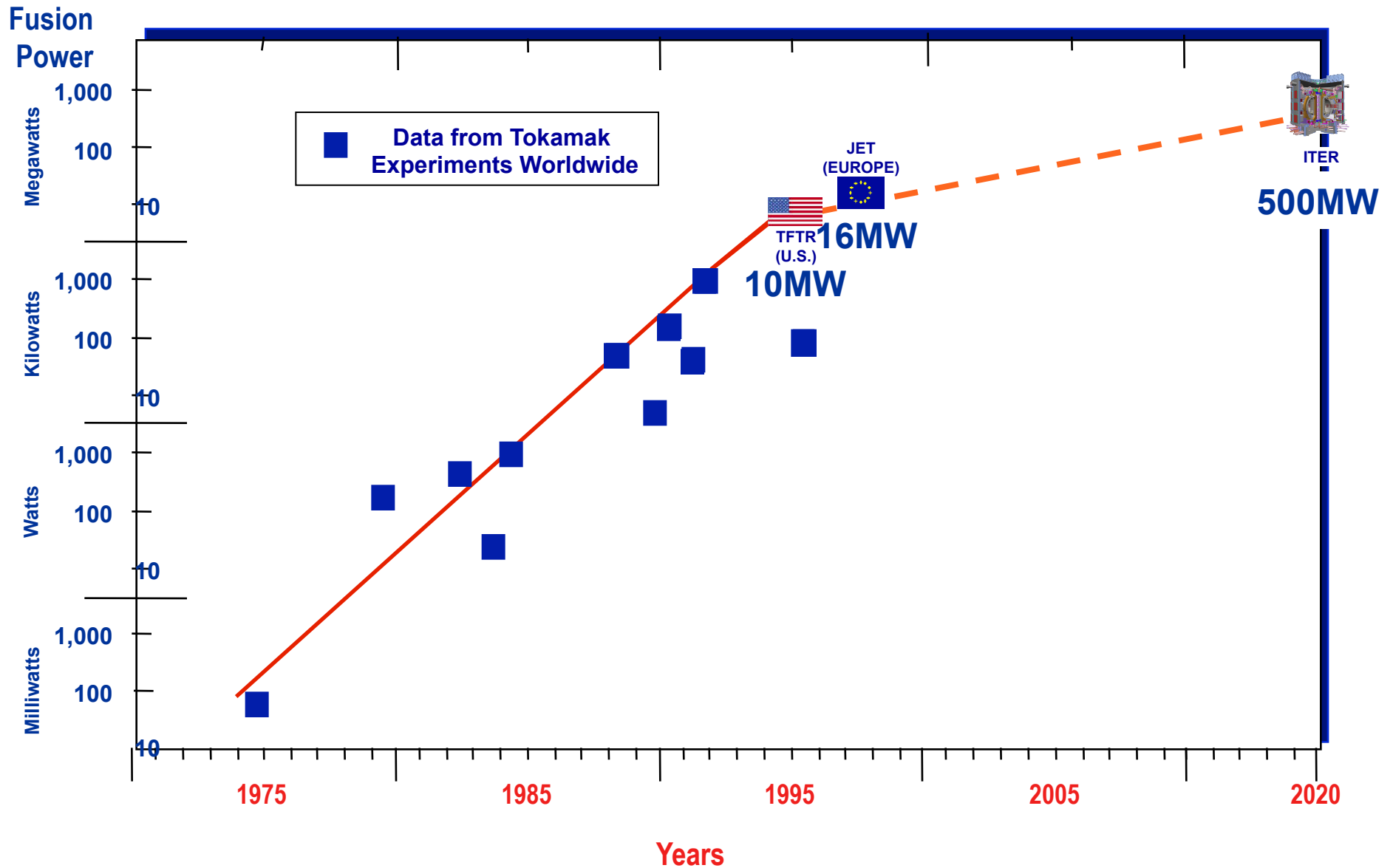**Fusion Energy:** *Burning plasmas are self-heated and self-organized systems*

Deuterium-Tritium Fusion Reaction

Plasma self-heating
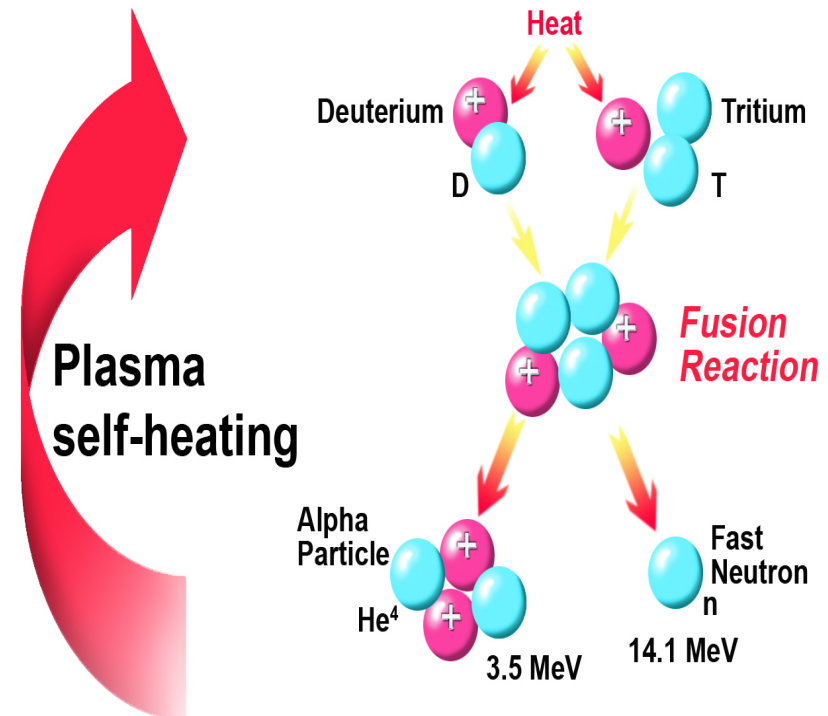
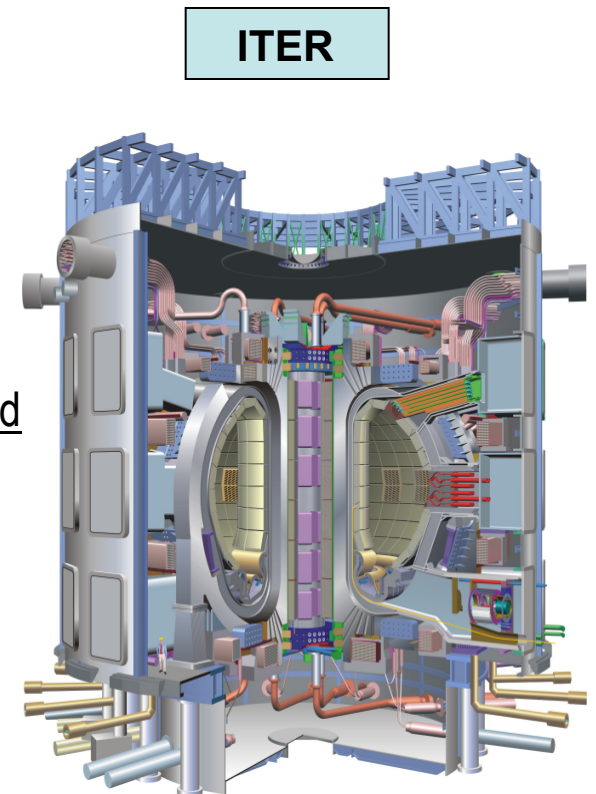*Energy Multiplication About 450:1*

$$D^+ + T^+ \rightarrow {}^4He^{++} (3.5\ MeV) + n^0 (14.1\ MeV)$$

Progress in Magnetic Fusion Energy (MFE) Research

Fusion Power

Megawatts
- 1,000
- 100
- 10

Kilowatts
- 1,000
- 100
- 10

Watts
- 1,000
- 100
- 10

Milliwatts
- 1,000
- 100
- 10

Data from Tokamak Experiments Worldwide

TFTR (U.S.) 10MW

JET (EUROPE) 16MW

ITER 500MW

Years
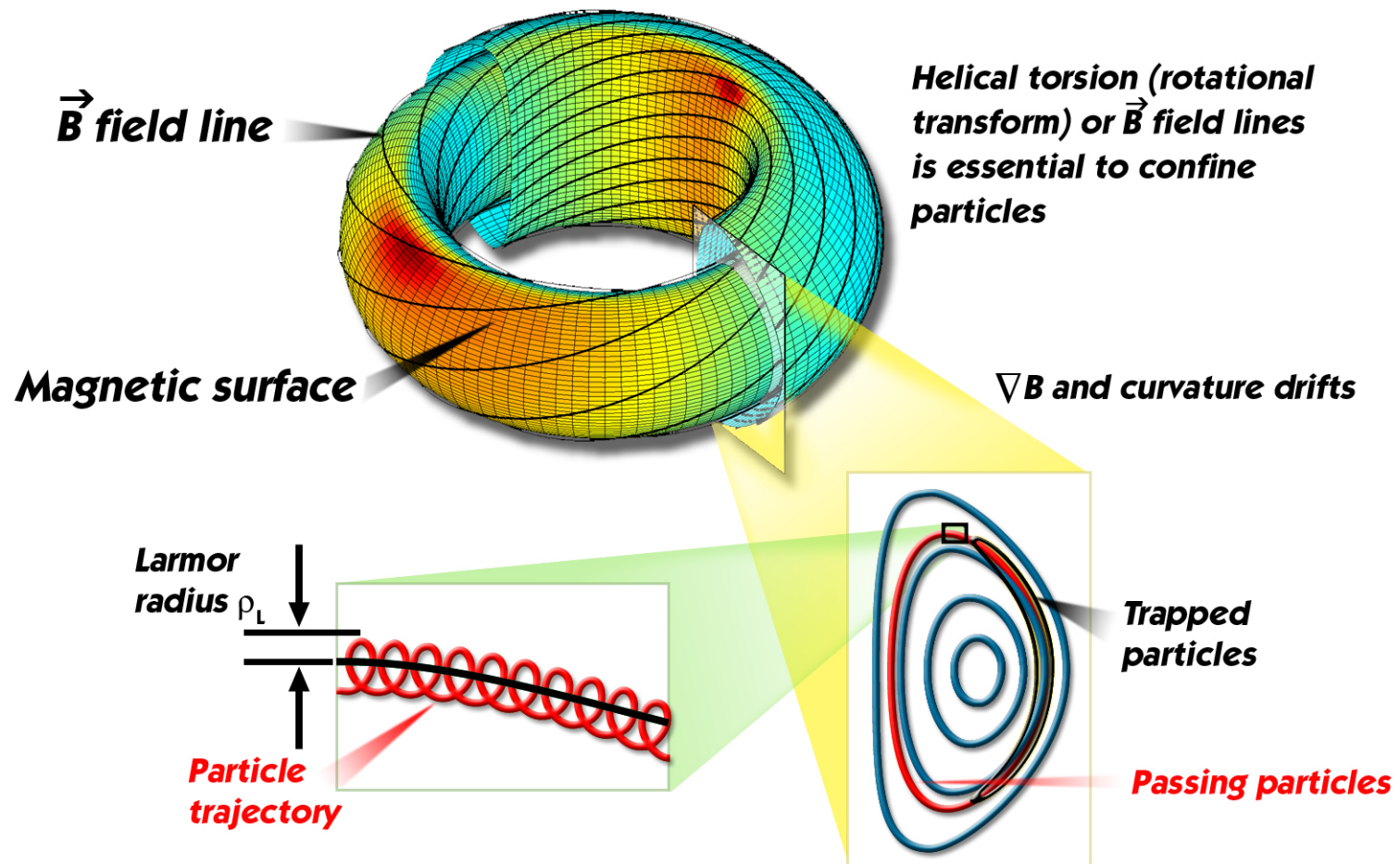- 1975
- 1985
- 1995
- 2005
- 2020

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*

ITER

Magnetically confined plasmas in a tokamak are complex and require HPC analysis

$\vec{B}$ field line

Magnetic surface

Helical torsion (rotational transform) or $\vec{B}$ field lines is essential to confine particles

∇B and curvature drifts

Larmor radius ρ_L

Particle trajectory

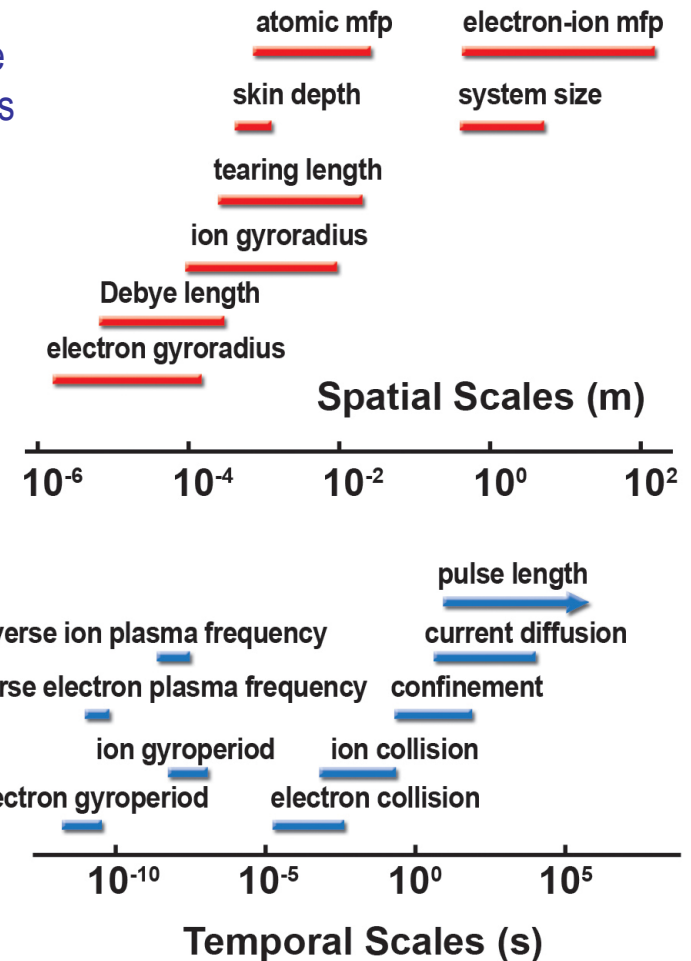**Trapped particles**

Passing particles

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

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q}{m}\left[E + \mathbf{v} \times B\right] \cdot \nabla_{\mathbf{v}} f = C(f) + S(f)$$
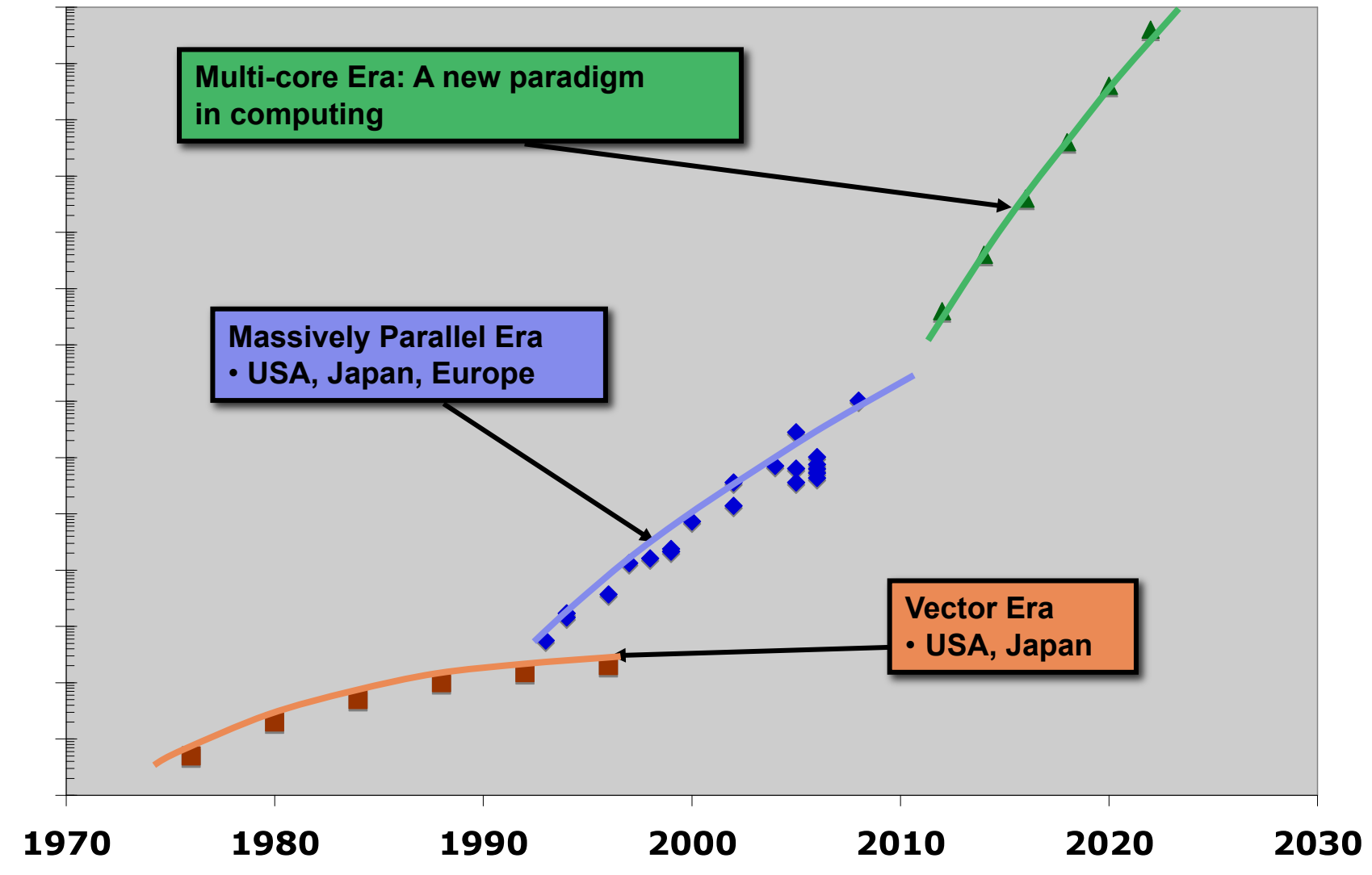
convection in space   convection in velocity space   collisional relaxation   particle sources

- 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*

atomic mfp   electron-ion mfp

skin depth   system size

tearing length

ion gyroradius

Debye length

electron gyroradius

Spatial Scales (m)

10^{-6}	10^{-4}	10^{-2}	10^{0}	10^{2}

pulse length

inverse ion plasma frequency   current diffusion

inverse electron plasma frequency   confinement

ion gyroperiod   ion collision

electron gyroperiod   electron collision

10^{-10}	10^{-5}	10^{0}	10^{5}

Temporal Scales (s)

FES Needs to be Prepared to Exploit *Local Concurrency* to Take Advantage of Most Powerful Supercomputing Systems in 21st 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

1970   1980   1990   2000   2010   2020   2030

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)

$$\frac{d\mathbf{x}_j}{dt} = \mathbf{v}_j, \qquad \frac{d\mathbf{v}_j}{dt} = \frac{q}{m} \left(\mathbf{E} + \frac{1}{c} \mathbf{v}_j \times \mathbf{B} \right)_{\mathbf{x}_j}.$$

- 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 Birdsall et al. (1968)*]

    - Coulomb potential is modified for a finite size particle due to Debye shielding

    - no need to satisfy $1/(n \lambda_D^3) << 1$

• 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)*]
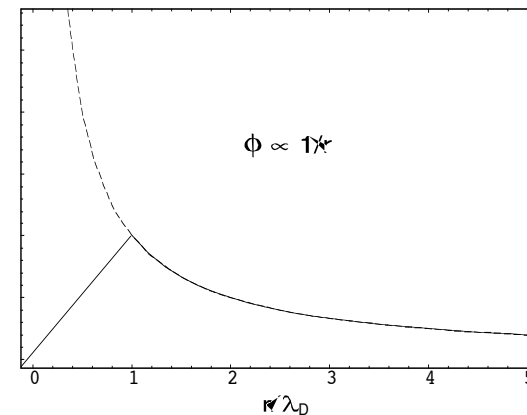
Gyrokinetic Particle Simulation

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
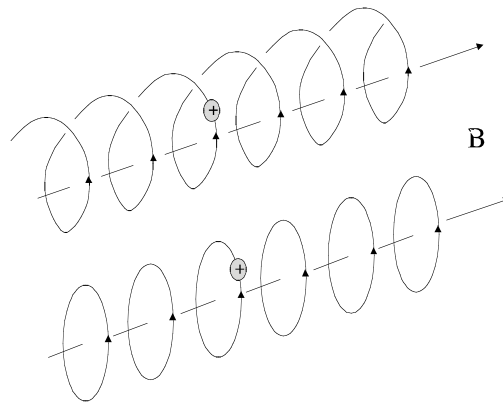
Basic Particle-in-Cell Method

- 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
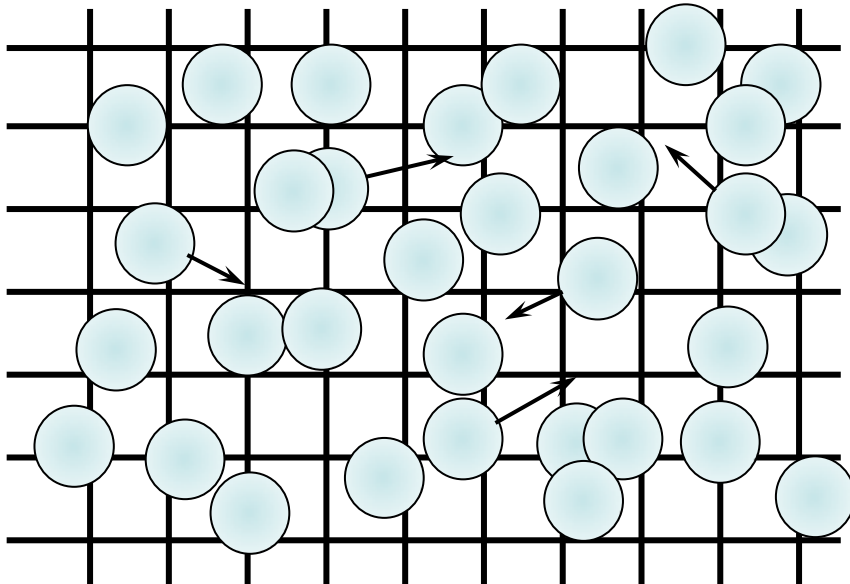
Specific PIC Operations:

- *"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

  ➔ *ESP & INCITE GTC-P Projects on BG-Q @ ALCF*

Good news for ITER!
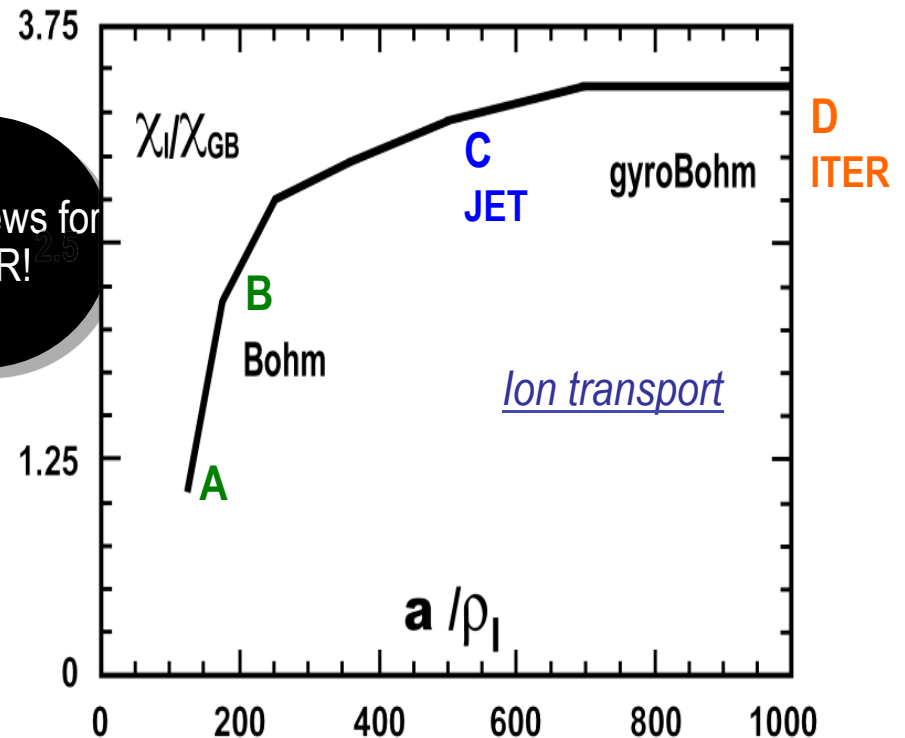
➔ *Excellent Scalability of Global PIC Codes on modern HPC platforms enables much greater resolution/physics fidelity to improve understanding*

➔ *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, ...*

Performance Speed Up Comparison Results
(IBM BG-Q vs. BG-P)

M0180 ppc =100	Our test	ANL	IBM
Speed up per node (Q/P ratio)	10.7	10.7	11.2

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***

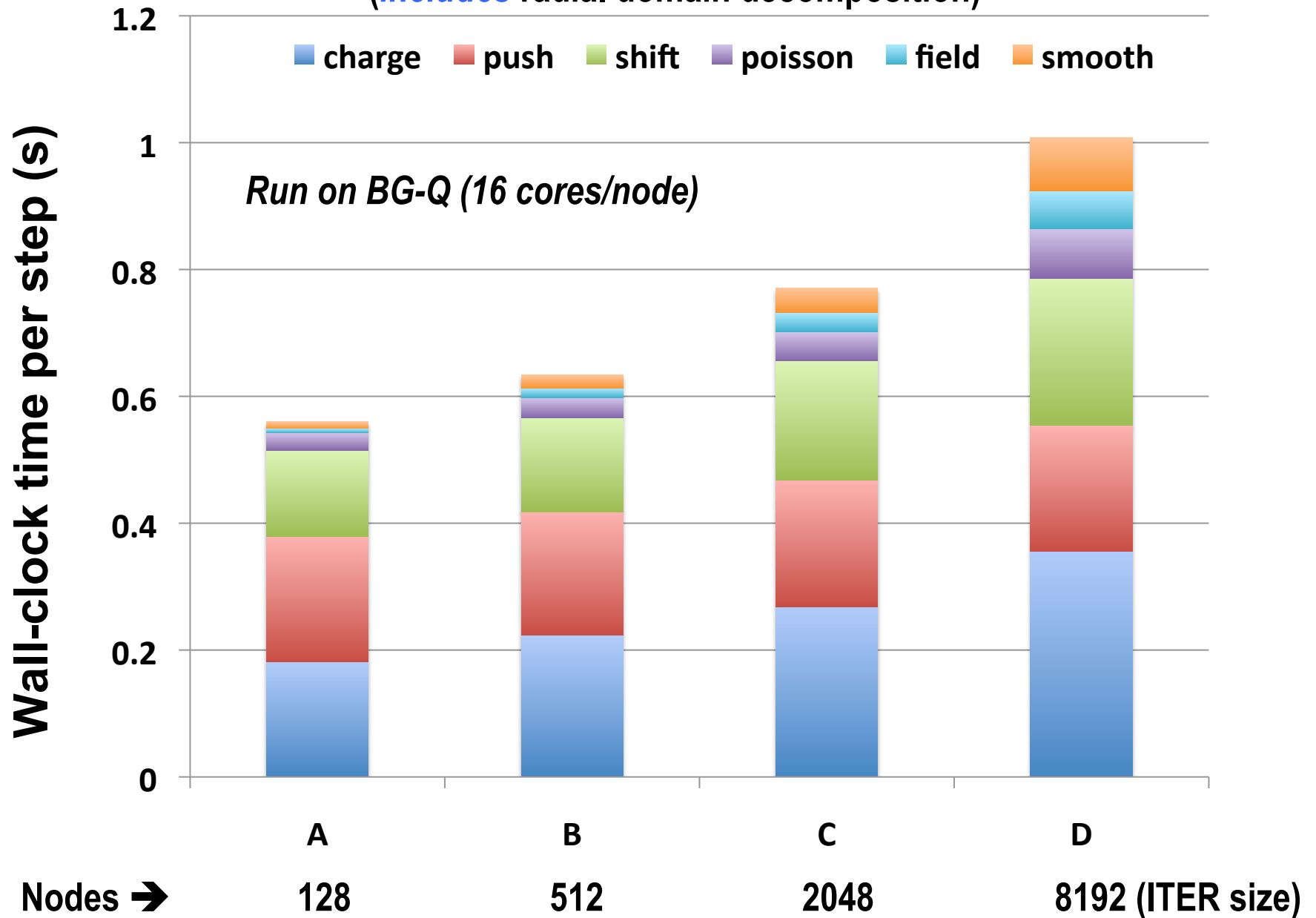- *4X (core) 2X (frequency) 2X (SIMD) = 16 ("theoretical")*

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

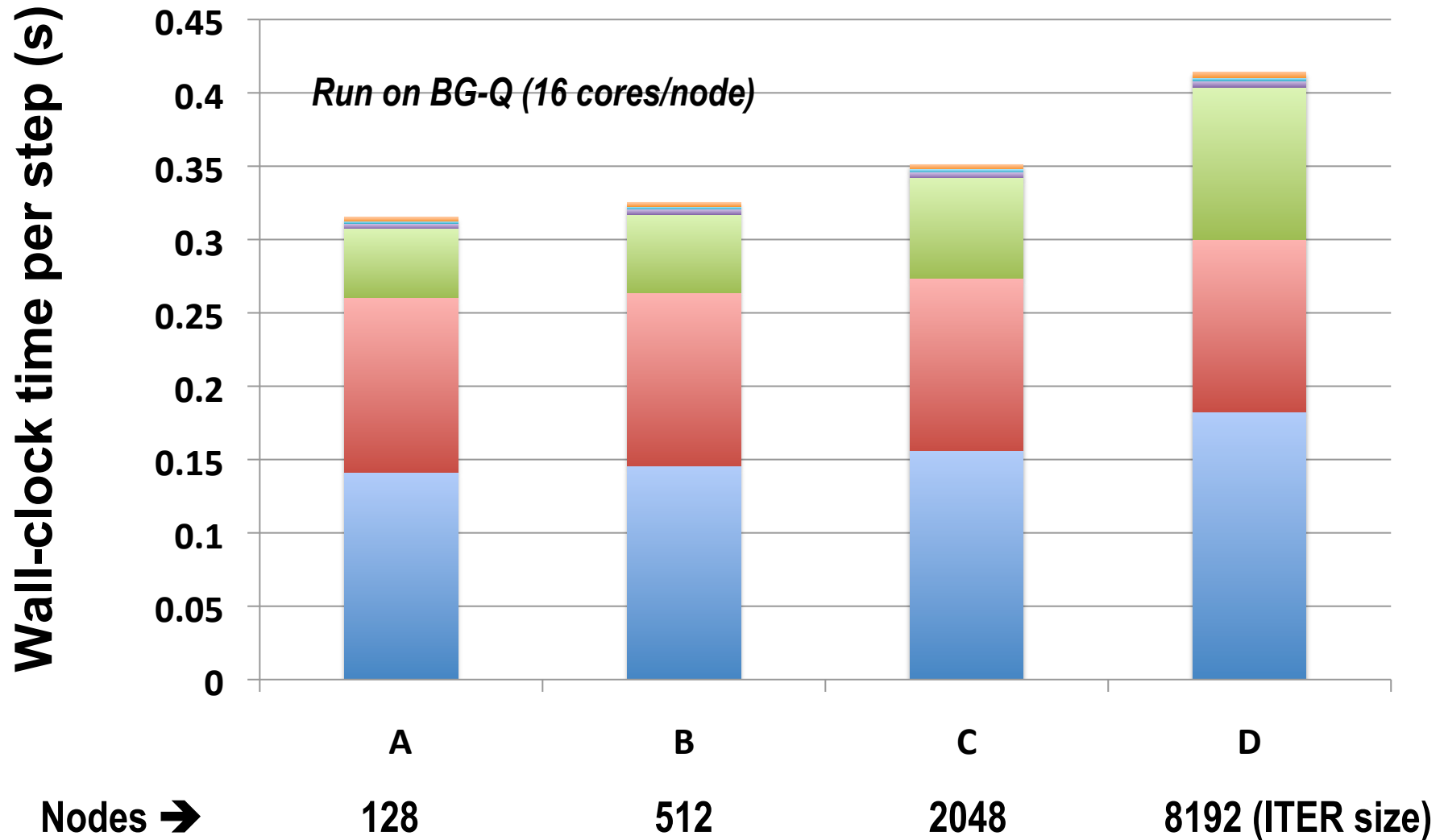 ➔ ***Overall Software Improvement gives another 50% gain in "Time to Solution"***

Reference Fortran Version of GTC-P
(*includes* radial domain decomposition)

legend: charge — push — shift — poisson — field — smooth

Wall-clock time per step (s)

Run on BG-Q (16 cores/node)

Nodes ➜	A	B	C	D
	128	512	2048	8192 (ITER size)

Optimized C Version of GTC-P ["GTC-P C"]

■ charge   ■ push   ■ shift   ■ poisson   ■ field   ■ smooth

Run on BG-Q (16 cores/node)

Wall-clock time per step (s)

	A	B	C	D
Nodes ➜	128	512	2048	8192 (ITER size)

Comparative Performance for PIC Operations

Legend: charge, push, shift, poisson, field, smooth

Case "D" for ITER Plasma Size

Y-axis: Wall-clock time per step (s)
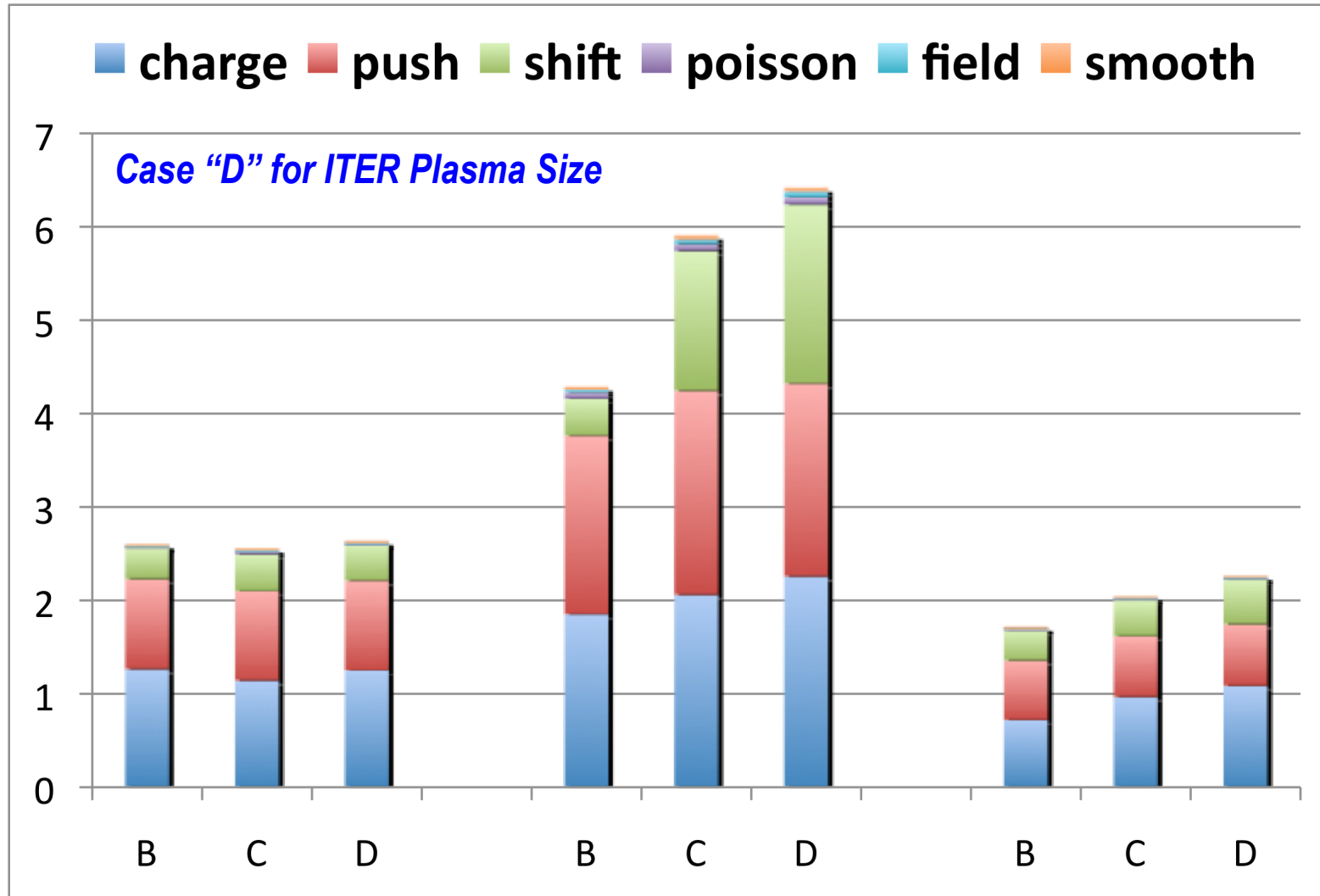
X-axis groups:
Mira 1MPI/ 64 OpenMP [16 cores w/each launching 4 threads] — B, C, D
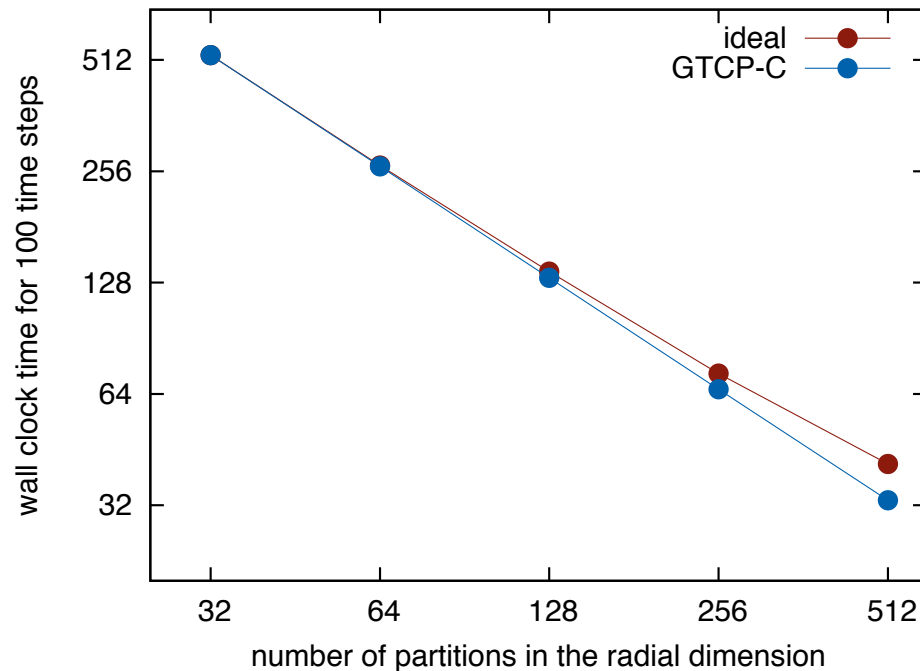*Hopper* 4MPI/ 6 OpenMP [Intel design -- avoid NUMA effects] — B, C, D
Edison 2MPI/ 8 OpenMP [avoid NUMA effects] — B, C, D

Strong Scaling Study of GTCP-C on Mira

D (ITER-scale) Problem for 100 Time Steps

Radial partitions	Time on Mira	Ideal	"Eff" efficiency
32	527.5	527.5	100%
64	265.1	263.8	99%
128	137.1	131.9	96%
256	72.6	65.9	91%
512	41.4	33	80%

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

Weak Scaling Study of GTCP-C on Mira
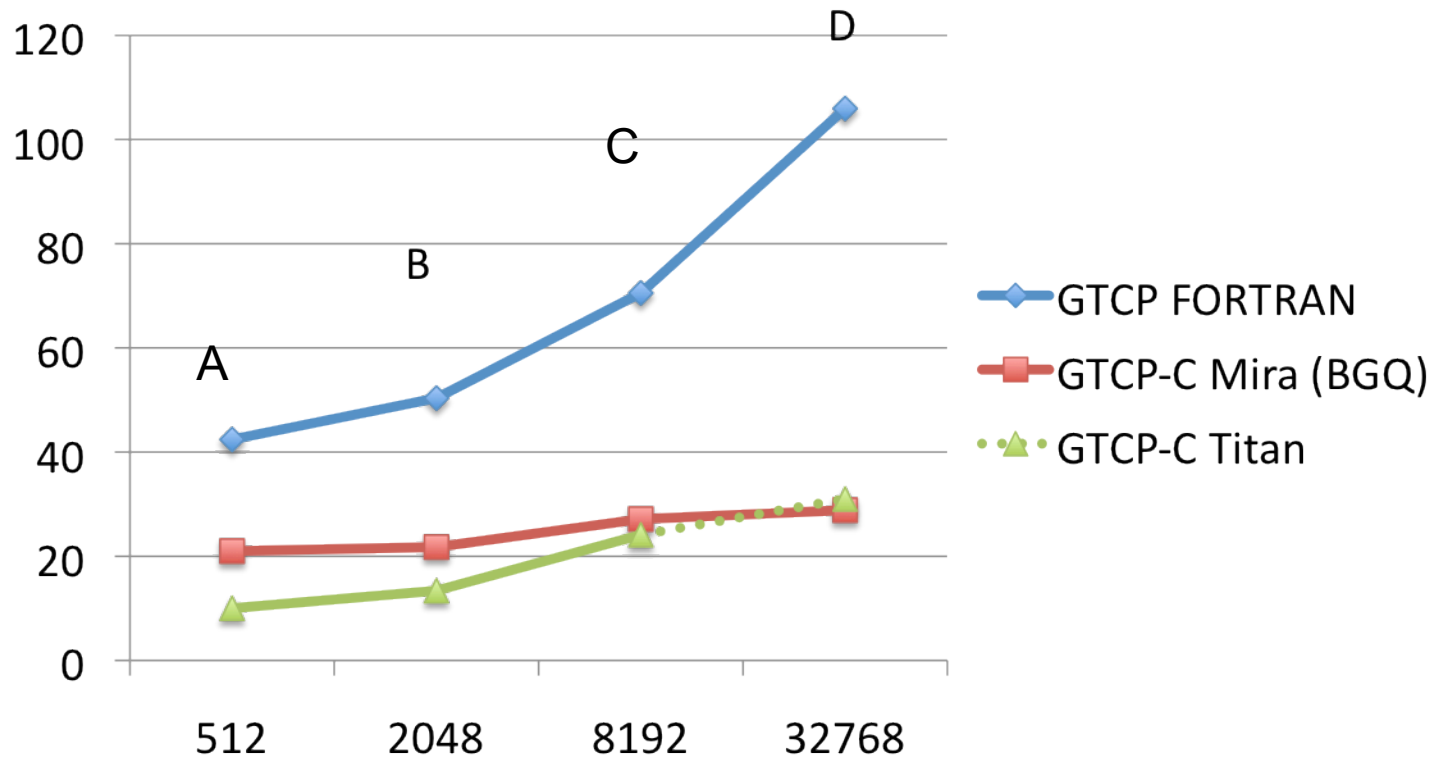
- *GTCP-C Titan points beyond 8192 nodes (dashed line) are <u>extrapolated</u>*

- 32768 nodes represents 2/3 of Mira BG-Q system
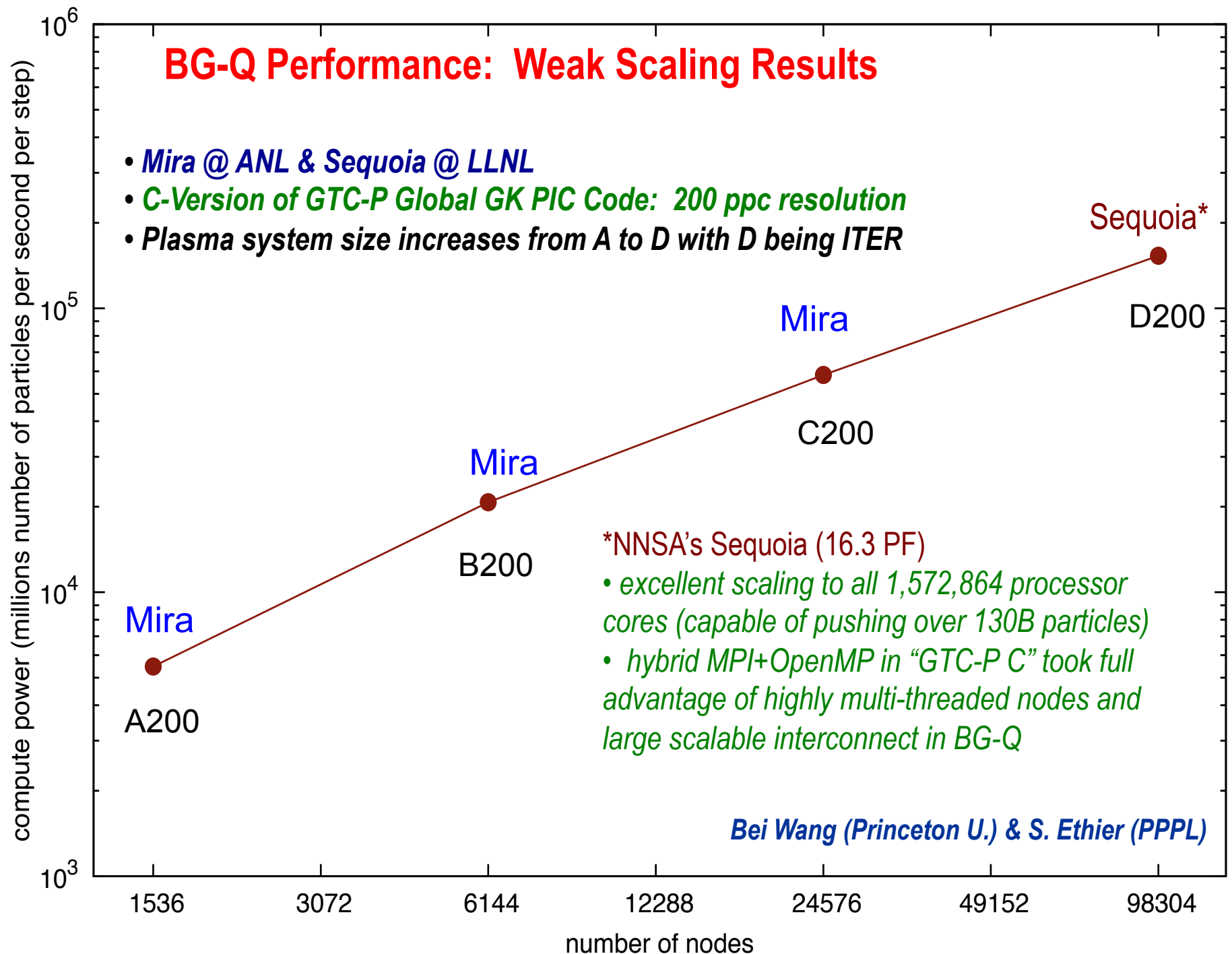
K-Computer Performance: Weak Scaling Results

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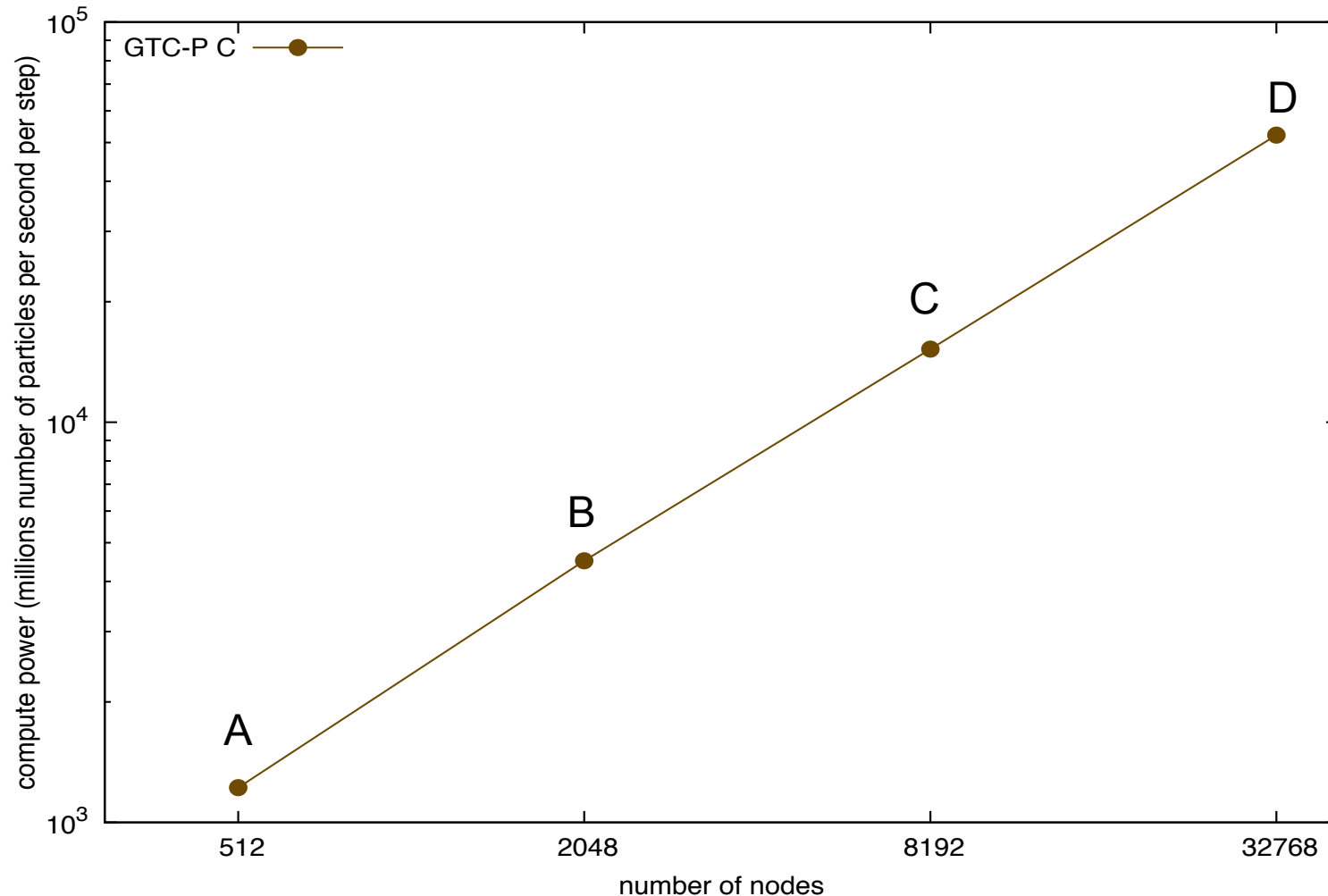
Takenori Shimosaka (RIKEN) & Bei Wang (Princeton U.)
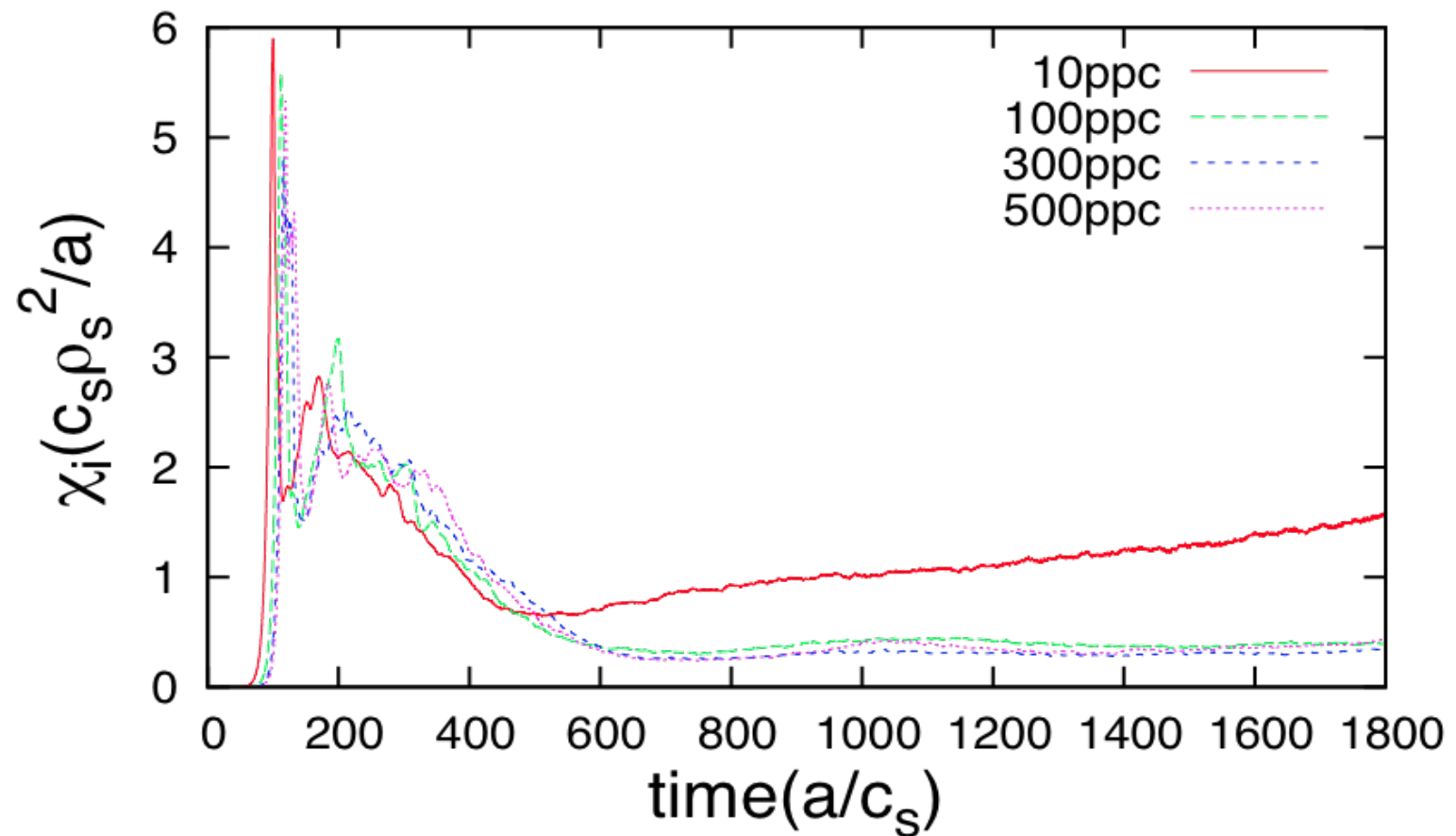
BG-Q Performance: Weak Scaling Results

- *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*

Sequoia*

Mira

Mira

D200

Mira

C200

B200

*NNSA's Sequoia (16.3 PF)
- *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*

A200

Bei Wang (Princeton U.) & S. Ethier (PPPL)

compute power (millions number of particles per second per step)

number of nodes

Influence of Collisions on Thermal Diffusivity: Fokker-Planck Model*

GTC-P C Code for ITER (D-size) Case on BG-Q with 100 ppc

*Ref. S. Ethier, W. M. Tang, R. Walkup, and L. Oliker, IBM Journal of R & D, 52 (1-2) 105-115 (2005)

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

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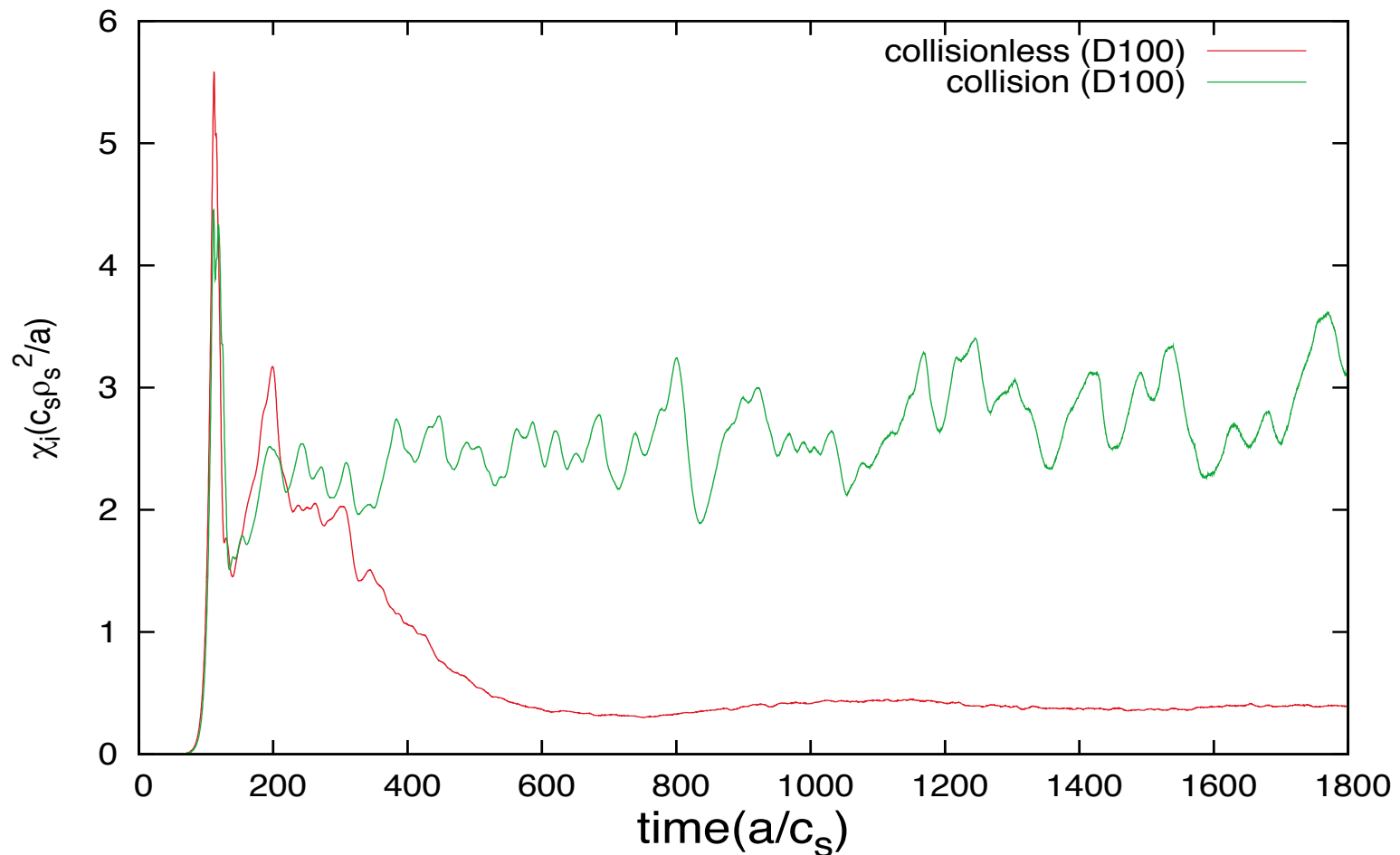
Summary: Programming Model Challenges in Moving toward Extreme Scales

• **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 <u>highly multi-threaded algorithms</u> 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 <u>"demo-apps"</u> 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)