KINETIC PLASMA TURBULENCE SIMULATIONS ON TOP SUPERCOMPUTERS WORLDWIDE

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INTRODUCTION

I. FOCUS: HPC Performance Scalability and Portability with FES as appropriate example application domain

→ *Illustration of domain application that delivers discovery science with good performance scaling, while also helping provide viable metrics on top supercomputing systems such as "portability," "time to solution," & associated "energy to solution"*

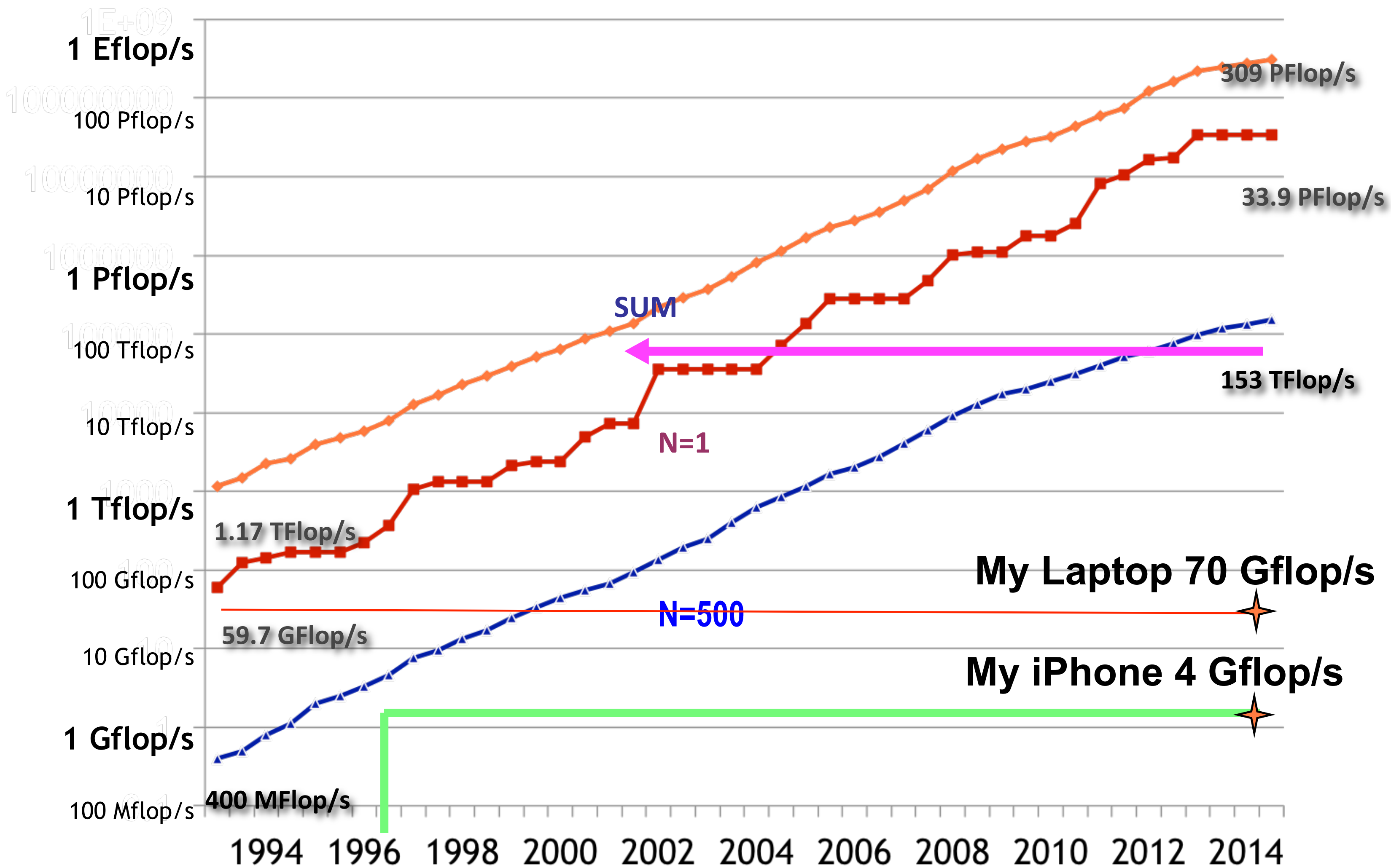
Reference: "Scientific Discovery in Fusion Plasma Turbulence Simulations @ Extreme Scale;" W. Tang, B. Wang, S. Ethier, Computing in Science and Engineering (CiSE), vol. 16. Issue 5, pp.44-52, 2014

II. PHYSICS & COMPUTATIONAL PROGRESS: *Enabled by deployment of innovative algorithms – e.g., using MPI & OpenMP within modern code that delivers new scientific insights on world-class systems → currently: Mira; Sequoia; K-Computer; Titan; Piz Daint; Blue Waters; Stampede;TH-2*

& in near future on: Summit (via CAAR), Cori, Stampede-II, Tsubame 3.0, -----

III. FUTURE: *Ability to utilize computing at exascale & beyond will require algorithmic & solver advances enabled by Applied Mathematics – in an interdisciplinary "Co-Design" type environment together with Computer Science & Extreme-Scale HPC Domain Applications*

Performance Development of HPC over the Last 22 Years from the Top 500 (J. Dongarra)



Applications Impact → *Actual value of extreme Scale HPC to scientific domain applications & industry*

Context: new US Govt. announcement of NATIONAL STRATEGIC COMPUTING INITIATIVE

- ***Practical Considerations:*** **"Better Buy-in" from Science & Industry requires:**
  - Moving beyond **"voracious"** (**more of same - just bigger & faster**) to **"transformational"** (**achievement of major new levels of scientific understanding**)
  - Improving **experimental validation** and **verification** to enhance **realistic predictive capability** of both ***hypothesis-driven*** and ***big-data-driven statistical approaches***
  - Deliver software engineering tools to improve **"time to solution"** and **"energy to solution"**
  - David Keyes (KAUST/Columbia U) → *"Billions of $ of scientific software worldwide hangs in the balance until better algorithms arrive to span the **architecture-applications gap."***

- ***Associated Challenges:***

- ***Hardware complexity***: Heterogeneous multicore; gpu+cpu → Summit; mic+cpu → Aurora

- ***Software challenges***: *Rewriting code focused on data locality*

- ***Applications Imperative:*** ***"Accountability" aspect***

→ ***Need to provide specific examples of impactful scientific and mission advances enabled by progress from terascale to petascale to today's multi-petascale HPC capabilities***

Demonstration of GTC Productivity & Impact → Delivery of Scientific Advances with use of Increasingly Powerful Supercomputing Systems

GTC Simulation	Computer name	PE # used	Speed (TF)	# Particles used	Time steps	Physics Discovery (Publication)
1998	Cray T3E NERSC	10^2	10^{-1}	10^8	10^4	Ion turbulence zonal flow (***Science**, 1998*)
2002	IBM SP NERSC	10^3	10^0	10^9	10^4	Ion transport size scaling (***PRL**, 2002*)
2007	Cray XT3/4 ORNL	10^4	10^2	10^{10}	10^5	Electron turbulence (***PRL**, 2007*); EP transport (***PRL**, 2008*)
2009	Jaguar/Cray XT5 ORNL	10^5	10^3	10^{10}	10^5	Electron transport scaling (***PRL**, 2009*); EP-driven MHD modes
2012 to present	Cray XT5→Titan ORNL Tianhe-1A (China)	10^5	10^4	10^{11}	10^5	Kinetic-MHD (***PRL**, 2012*); Turbulence + EP + MHD TAE Modes (***PRL**, 2013*)
2018 (future)	Path to Exascale HPC Resources	TBD	10^6	10^{12}	10^6	Turbulence + EP + MHD + RF

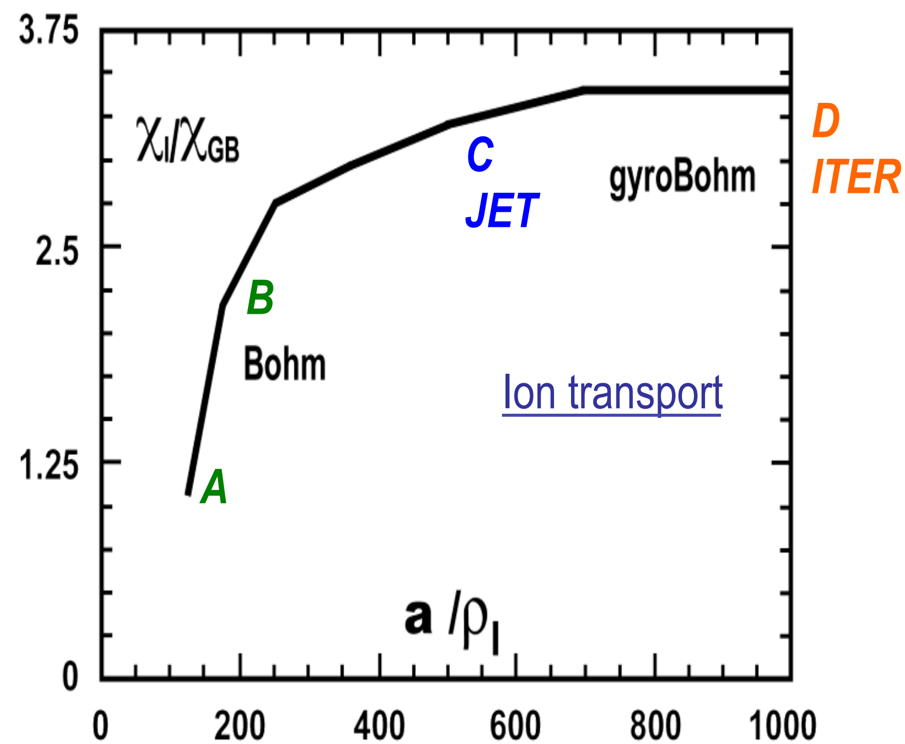
*** GTC is first FES code to deliver production run simulations @ TF in 2002 and PF in 2009

DOE SciDAC Success Story from Fusion Energy Science: PIC Code Simulations of Confinement Loss from Turbulent Transport

- **Mission Importance:** *Fusion reactor size & cost determined by balance between loss processes due to turbulent transport & self-heating rates from fusion reactions*

- **"Scientific Discovery"** - Transition to favorable scaling of confinement for ITER-size plasmas [Good News for ITER!]
  - a/ρ_i = 400 (JET, largest present lab experiment)
  - a/ρ_i = 1000 (ITER, ignition experiment)

  from **Multi-TF** simulations using 3D PIC code [Z. Lin, et al, **2002** ➔ 1st ITER-scale simulation with ion gyroradius resolution with GTC-Code



- **"Co-Design Enabled Advances @multi PF"** → Excellent scalability of 3D PIC Codes on top 7 **multi-PF** supercomputers worldwide

  → enables unprecedented resolution/physics fidelity needed for better understanding of large fusion systems

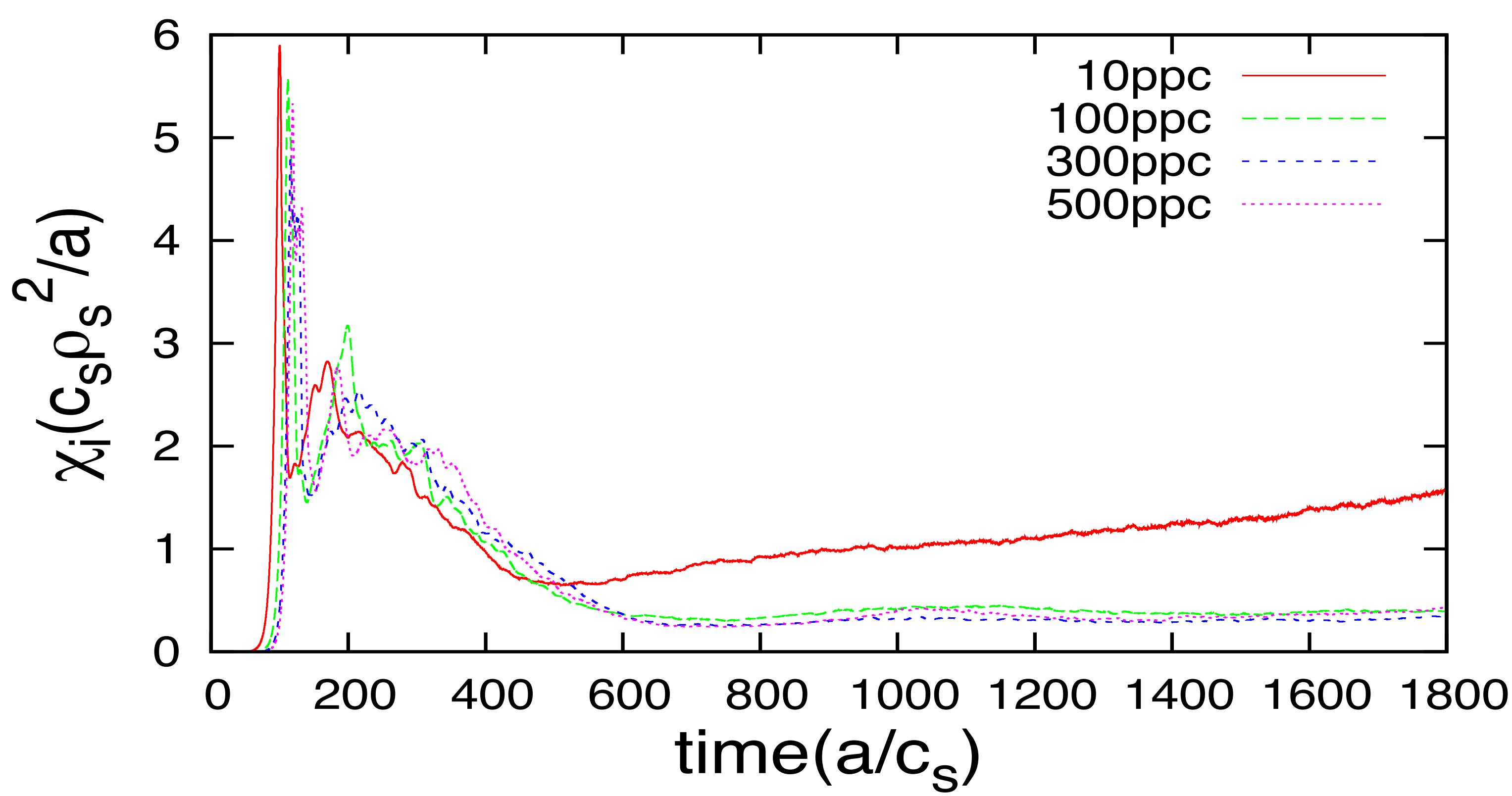
Accelerated progress enabled by SciDAC-based interdisciplinary approach with Computer Science (CS), Applied Math (AM), & Domain Applications

➔ *Recent achievements enabled by SciDAC approach plus "CoDesign" inclusion of Hardware Design*

Particle Resolution (ppc) Convergence Study

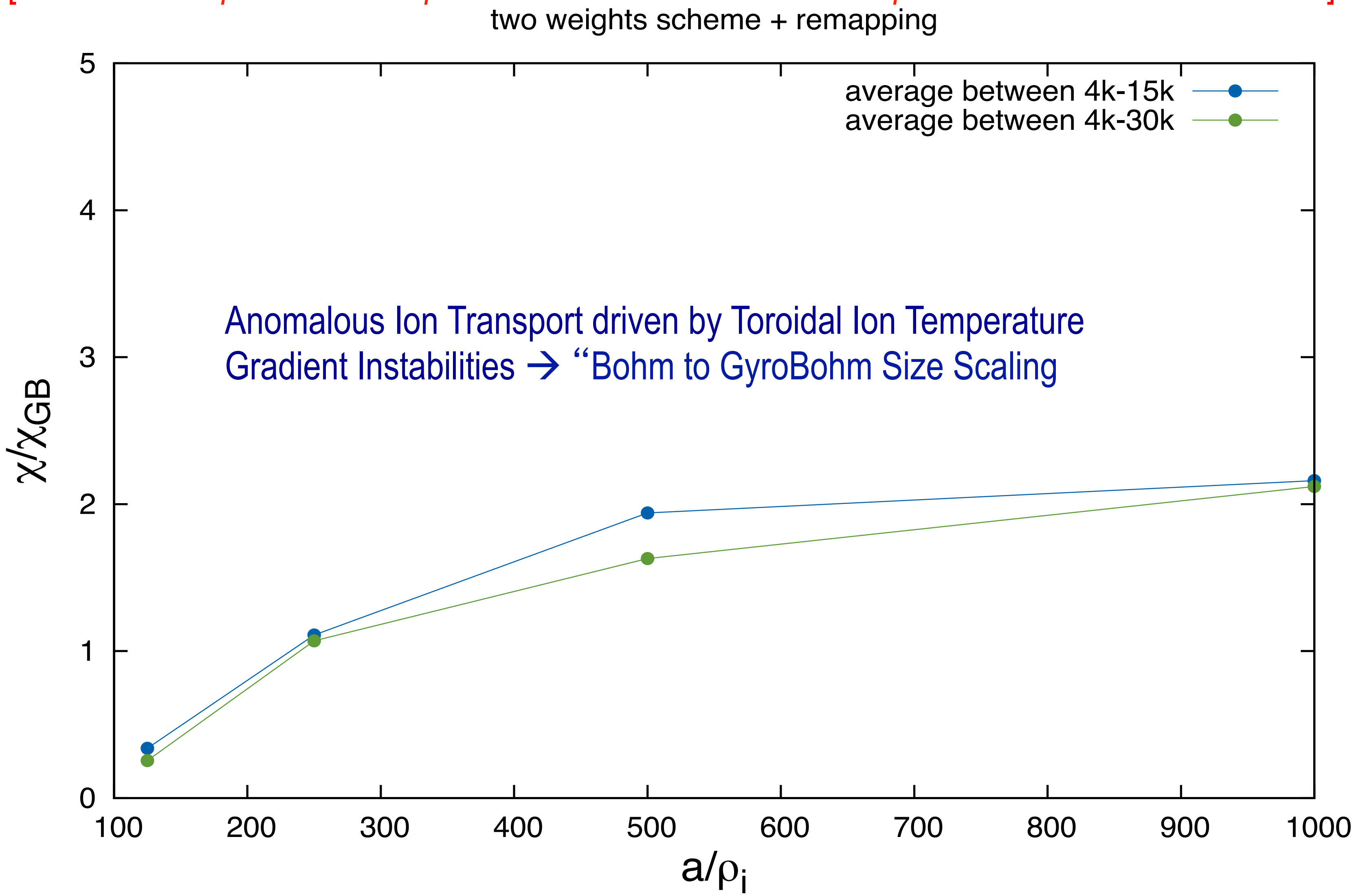
[Results from C-version GTC-Princeton Code for ITER (D-size) Case on IBM BG-Q]

Time History of Thermal Diffusivity from ITG Instability @ Different Resolutions



High Resolution Ion Transport Scaling Results enabled by "Mira" at ALCF

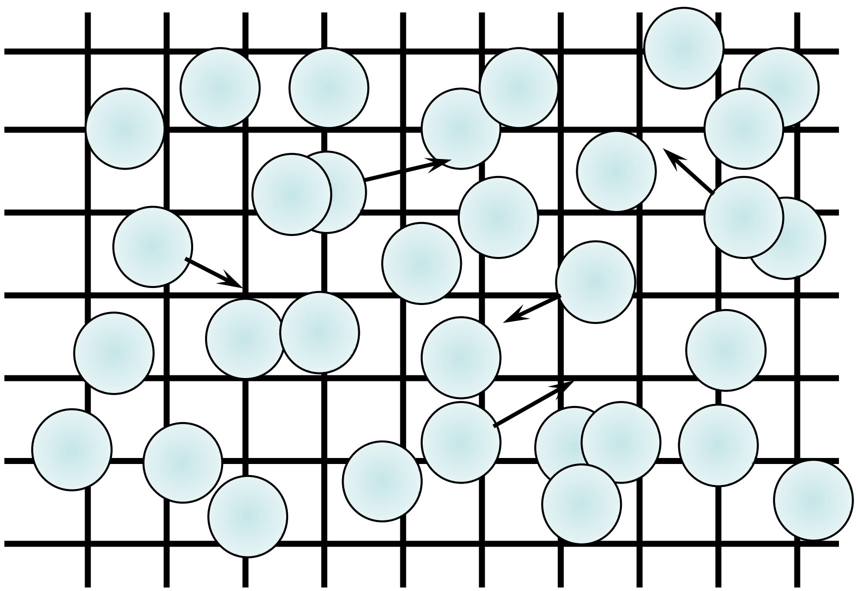
[*vertical axis represents transport level and horizontal axis the plasma size with ITER at 1000*]



<u>New Trends:</u> "rollover" significantly more gradual than established earlier in much lower resolution, shorter duration studies with magnitude of transport now reduced by ~ 2

Picture of Particle-in-Cell Method

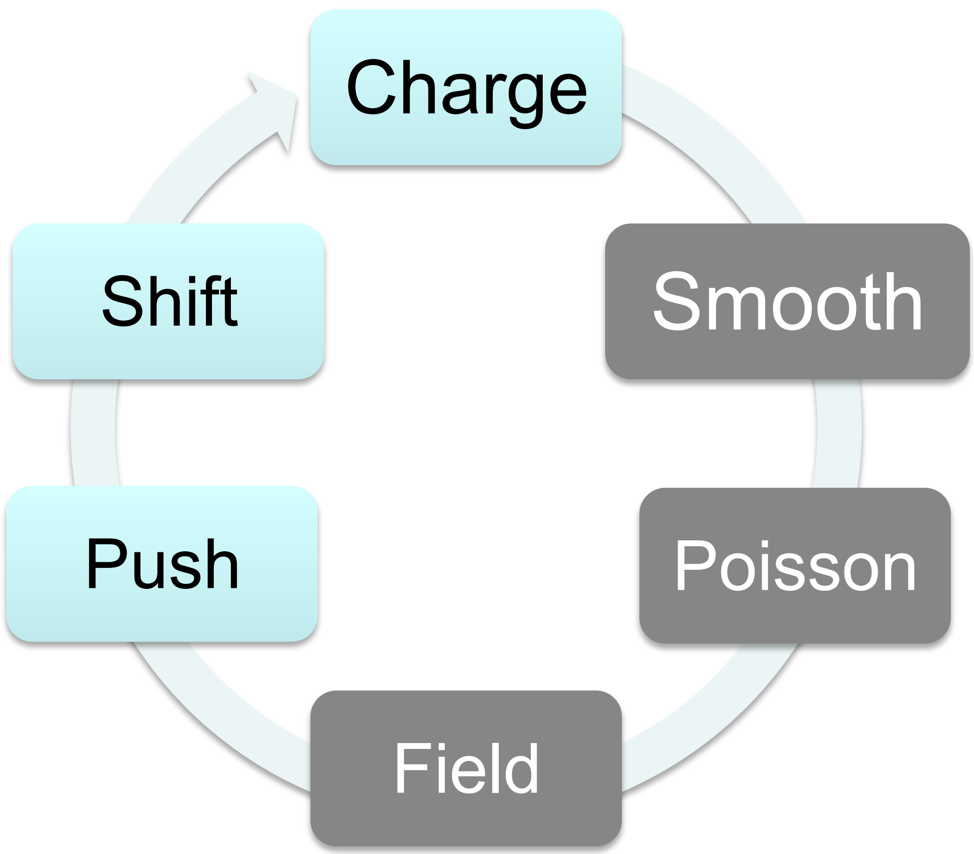
- Charged particles sample distribution function
- Interactions occur on a grid with the forces determined by gradient of electrostatic potential (calculated from deposited charges)
- *Grid resolution dictated by Debye length ("finite-sized" particles) up to gyro-radius scale*



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…*

GTC-P: six major subroutines



- **Charge**: particle to grid interpolation (SCATTER)
- **Smooth/Poisson/Field**: grid work (local stencil)
- **Push**:
  - grid to particle interpolation (GATHER)
  - update position and velocity
- **Shift**: in distributed memory environment, exchange particles among processors

KEY ROLE OF OPEN-MP in ADDRESSING MODERN HPC CHALLENGES

Open-MP-enabled scalable scientific software for extreme scale applications: FES as illustrative application domain

- **Extreme concurrency:** → *Adopting OpenMP is one of most efficient algorithmic approaches to facilitate efficient multi-threading methods*
- **Portability:** → *except for GPU hardware, OpenMP works with **all** multicore processors*
- **Ease of Deployment**: → *OpenMP is now a mature implementation relatively easy to use*

  -- easiest approach to deploy OpenMP is at *loop level;*

  -- OpenMP worked best at loop level beginning in late 1990s/early 2000s and has *remained best approach since then*;

  -- Example: deployed this way *in all prominent Global FES PIC codes* – GTC-P, GTC, GTS, and XGC;

KEY ROLE OF OPEN-MP (continued)

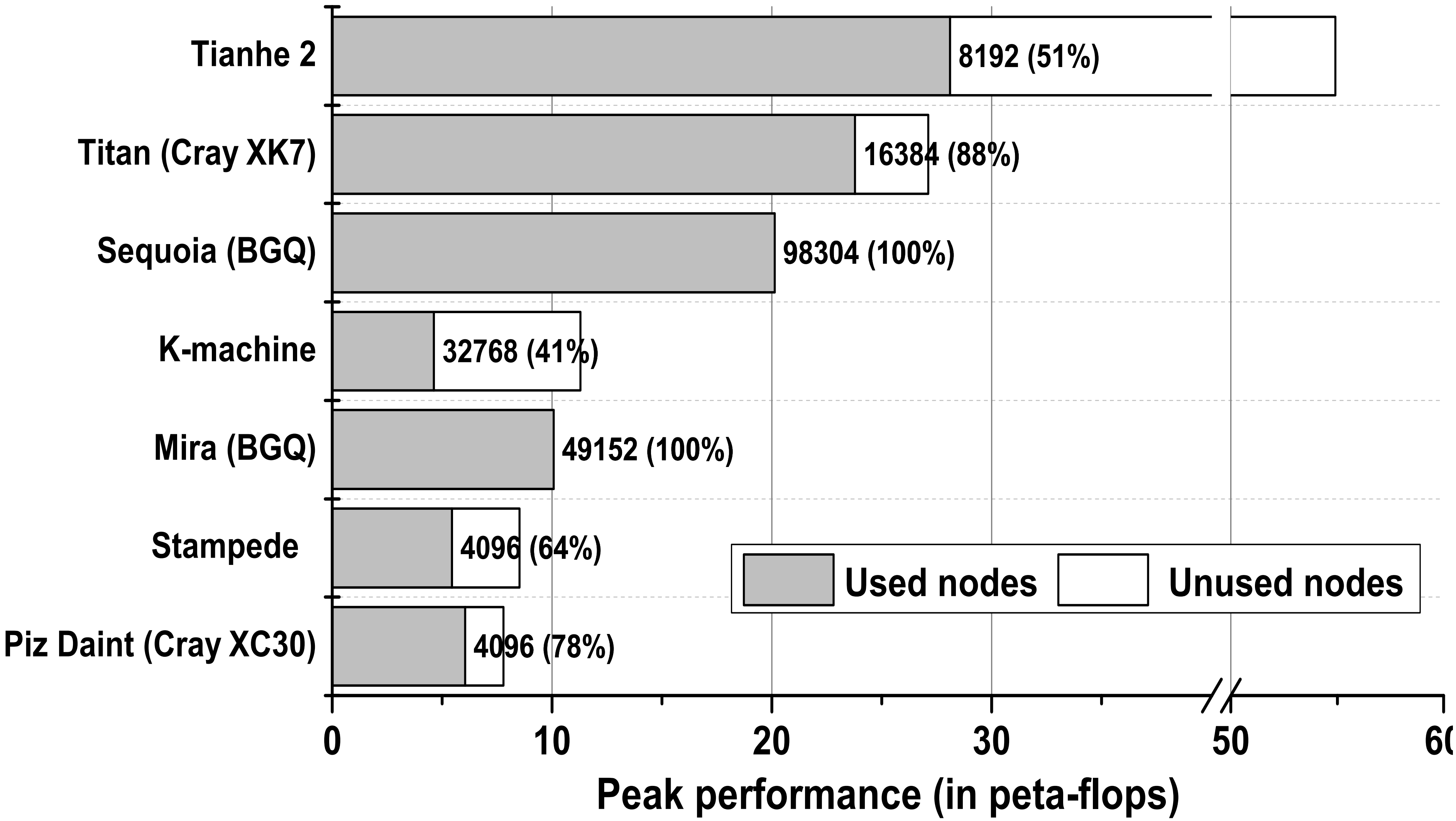
- ***NEED FOR OPEN-MP CAPABILITY IN MULTI-GRID SOLVERS SUCH AS LLNL'S "HYPRE"***

-- **Significant challenge/goal**: *Incorporation of multi-grid Poisson solvers with OpenMP to efficiently deal with extreme concurrency, multi-threading issues characteristic of near-future systems (e.g., 100 PF systems such as Summit and Aurora)*

-- **FES Application**: GTC (UC Irvine) & GTC-P Project in Fusion Energy Science were selected for current portfolio of OLCF CAAR Early Science Program for Summit → *will require multi-grid electromagnetic field-solver with OpenMP such as HYPRE*

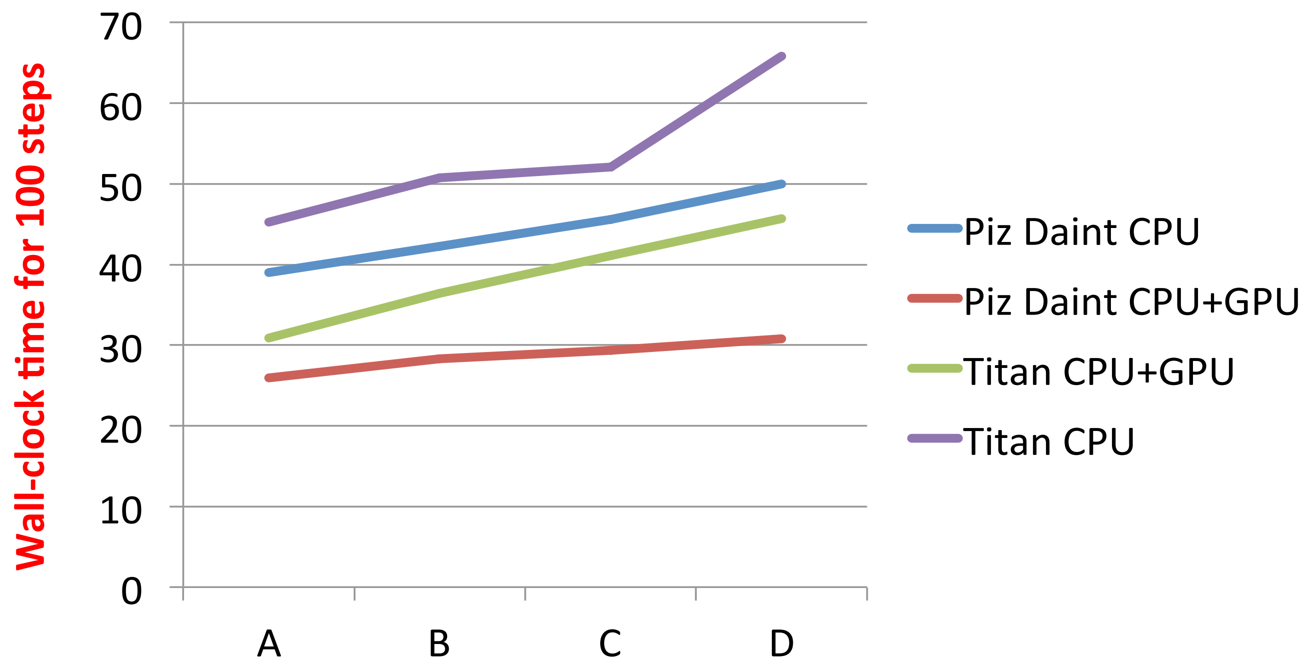
→ ***Choosing a portable and threaded solver (e.g., HYPRE) is critically important for GTC and GTC-P***

ILLUSTRATION OF GTC-P CODE PORTABILITY



- Broad range of leading multi-PF supercomputers worldwide
- Percentage indicates fraction of overall nodes currently utilized for GTC-P experiments
- NOTE: Results in this figure are only for CPU nodes on Stampede and TH-2

Weak Scaling of GTC-P (GPU-version) on Heterogenous (GPU/CPU) "Titan" and "Piz Daint"

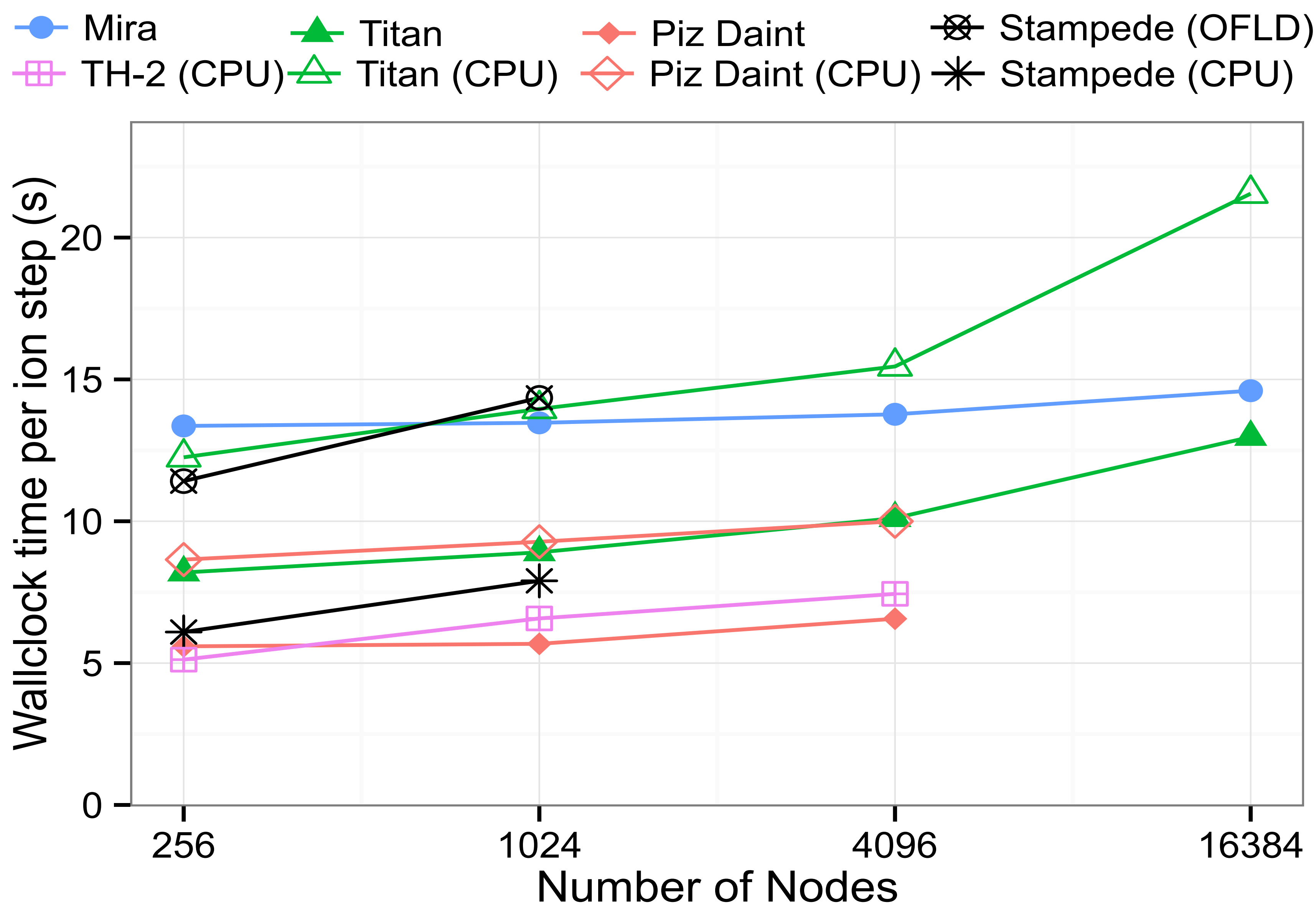


# of nodes: 64 256 1024 4096

- **The number of particles per cell is 100**
- **GTC-P GPU obtains 1.7x speed up**

***Same code** for all cases → Performance difference solely due to hardware/system software*

**Aries Network on Piz Daint*



GTC-P (kinetic electron) weak scaling performance using a fixed problem size per node across all systems allows comparisons of node performance.

"ENERGY TO SOLUTION" ESTIMATES
(for Mira, Titan, and Piz Daint)

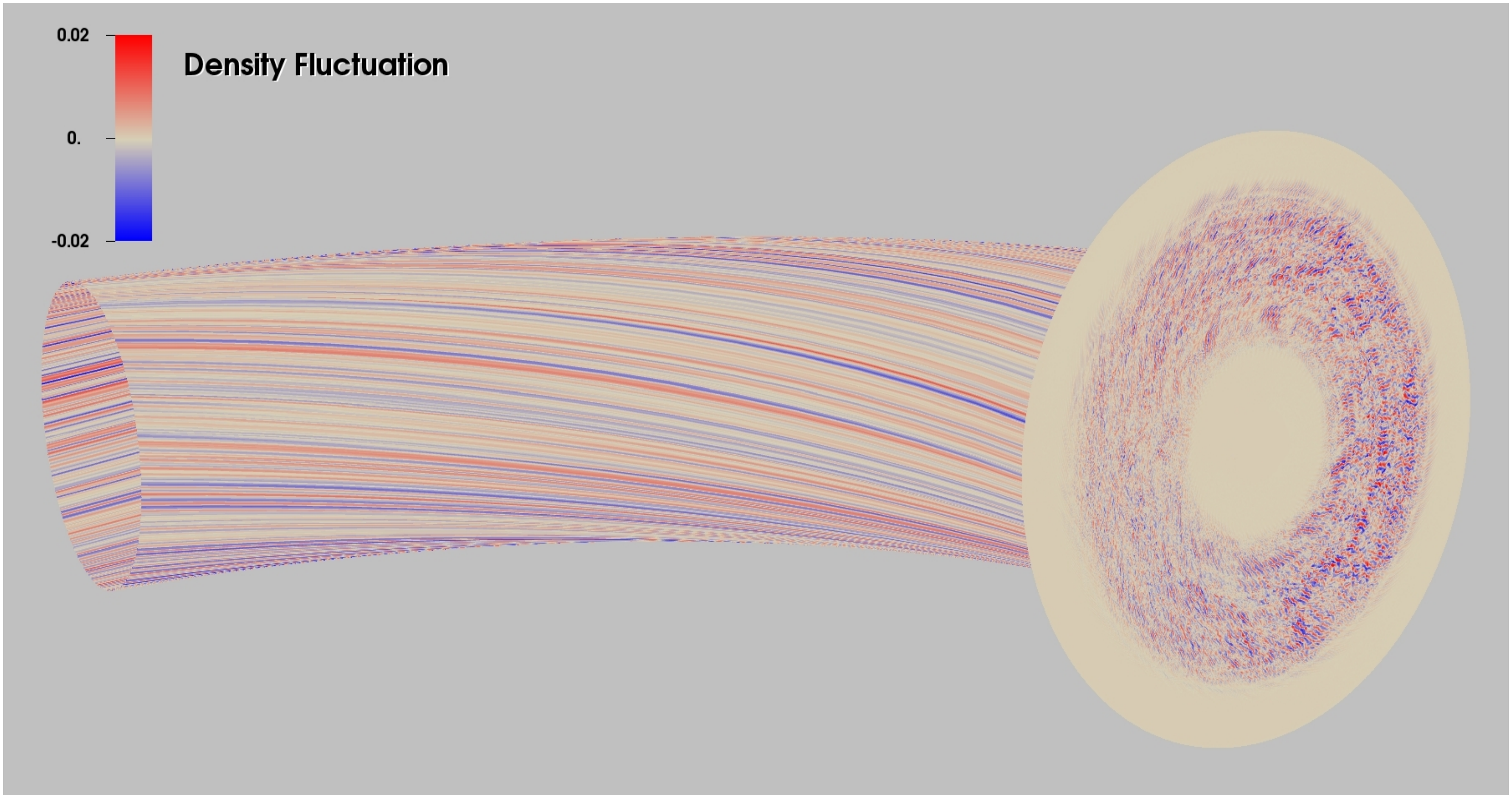
	CPU-Only			CPU+GPU	
	Mira	Titan	Piz Daint	Titan	Piz Daint
Nodes	4096	4096	4096	4096	4096
Power/node (W)	69.7	254.1	204.9	269.4	246.5
Time/step (s)	13.77	15.46	10.00	10.11	6.56
Energy (KWh)	1.09	4.47	2.33	3.10	1.84

- **Energy per ion time step (KWh) by each system/platform for the weak-scaling, kinetic electron studies using 4K nodes.**

(Watts/node) * (#nodes) * (seconds per step) * (1KW/1000W) * (1hr/3600s)

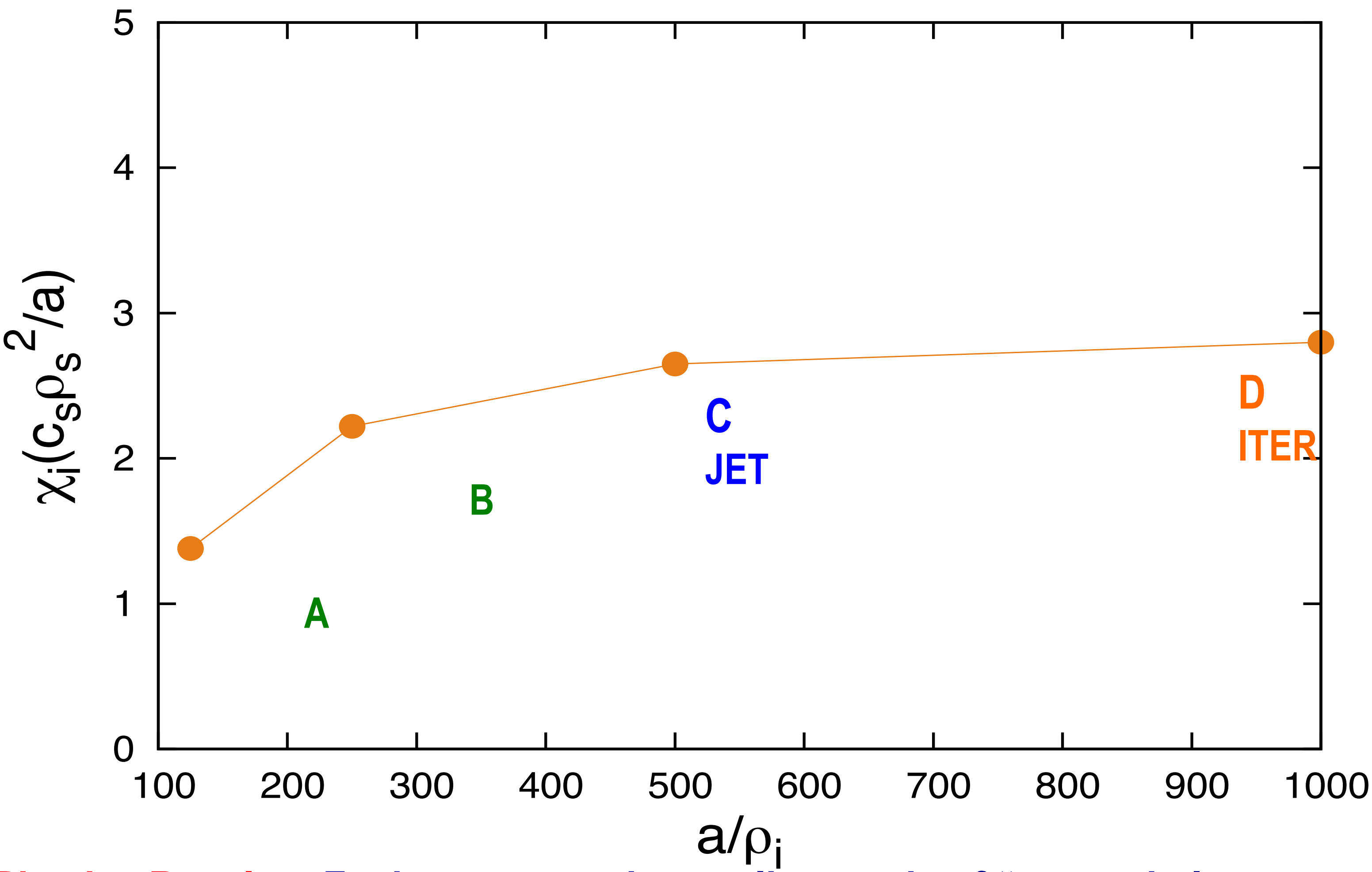
- **Power/Energy estimates obtained from system instrumentation including compute nodes, network, blades, AC to DC conversion, etc.**

GTC-P SIMULATION OF MICROTURBULENCE IN ITER-SIZE PLASMA



Density fluctuations during the non-linear phase of an ITER-size GTC-P simulation of plasma microturbulence

ILLUSTRATION OF GTC-P CODE CAPABILITY FOR INCREASING PROBLEM SIZE

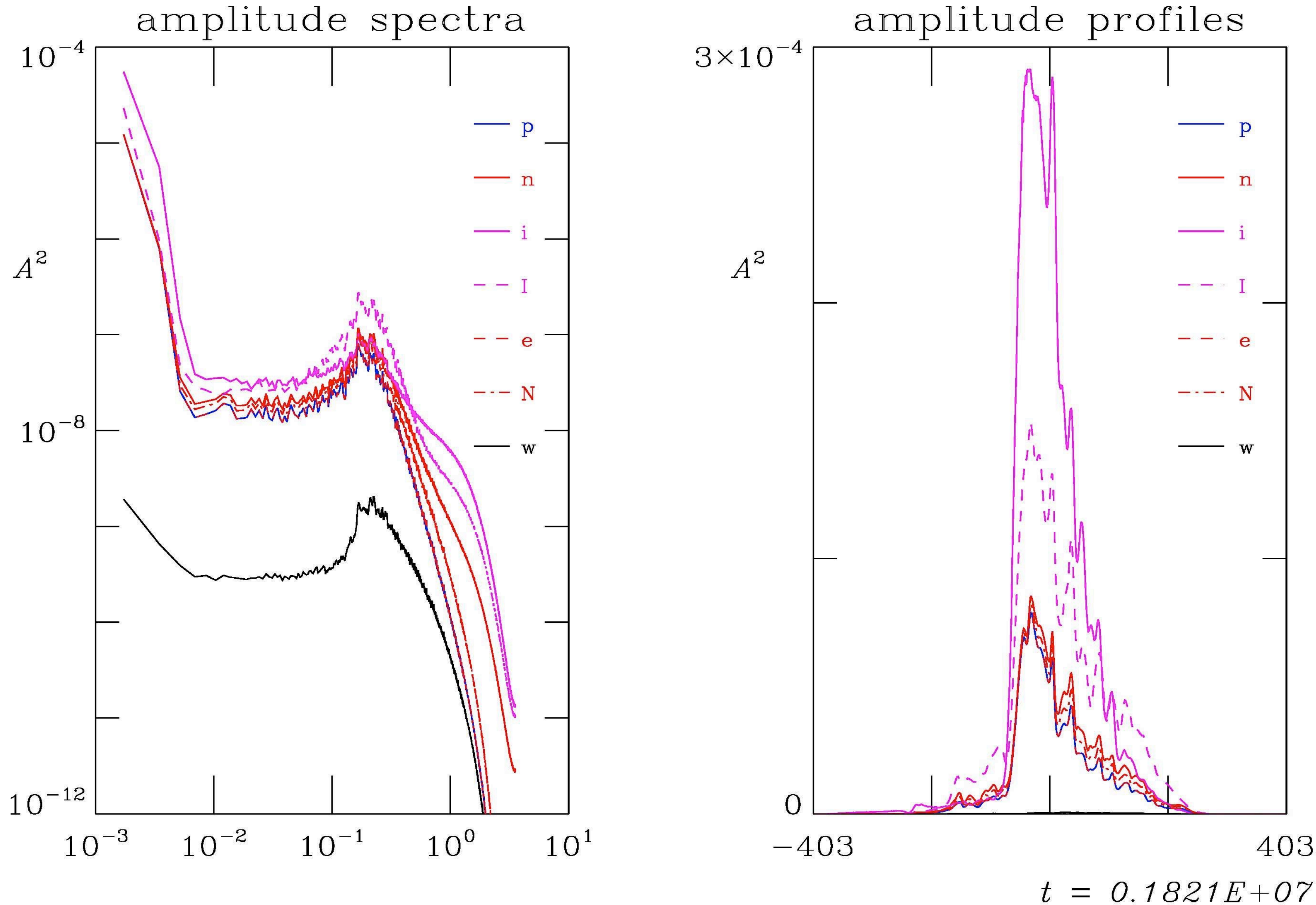


New Physics Results: Fusion system size-scaling study of "trapped-electron-mode" turbulence showing the "plateauing" of the radial electron heat flux as size of tokamak increases.

• **Verification** – *via (1) GTC Simulation Results (up to C) – Y. Xiao, Z. Lin (PRL – 2009); and (2) Analytic Foundations –* ***Liu Chen*** *& Z. Lin hybrid kinetic model for electrons*

Kolmogorov-like Rollover Spectral Results from GTC-P on multi-PF BG-Q "Mira"

(collaboration with B. Scott, IPP-Garching)



Associated Findings

• Advanced phase space remapping and Krook-type collision models deployed for long temporal duration global PIC simulations with GTC-P (*Bei Wang and Bruce Scott*)
→ Current findings of realistic Kolmogorov-type spectral roll-over indicate:

(i) numerical dissipation in some form needed to ensure proper “steady state” behavior for “collisionless” systems;

(ii) while further improvements are needed, present results from remapping and Krook-type collision models effectively reduce noise levels for long-duration simulations where the amplitudes are small; and

(iii) Inherent turbulence-driven dissipation sustainable in meaningful way – without invoking “ad-hoc” artificial dissipation models

APPLIED MATH LOCALITY CHALLENGE: *GEOMETRIC HAMILTONIAN APPROACH TO SOLVING GENERALIZED VLASOV-MAXWELL EQUATIONS*

Hamiltonian → Lagrangian → Action → Variational Optimization → Discretized Symplectic Orbits for Particle Motion

I. "Ultrahigh Performance 3-Dimensional Electromagnetic Relativistic Kinetic Plasma Simulation

Kevin J. Bowers, et al., *Phys. Plasmas 15, 055703 (2008)*

- ➔ Basic foundation for symplectic integration of particle orbits in electromagnetic fields *without frequency ordering constraints*
- ➔ Foundational approach for present-day simulations of laser-plasma interactions on modern supercomputing systems
- ➔ ***Limited applicabiity with respect to size of simulation region and geometric complexity***

II. "Geometric Gyrokinetic Theory for Edge Plasmas"

Hong Qin, et al., *Phys. Plasmas 14, 056110 (2007)*

- ➔ Basic foundation for symplectic integration of particle orbits in *electromagnetic low-frequency plasma following GK ordering*
- ➔ Still **outstanding challenge**: Address reformulation of ***non-local Poisson Equations structure*** for electromagnetic field solve

Concluding Comments

• Modern FES HPC domain application code capable of scientific discovery while providing good performance scaling and portability on top supercomputing systems worldwide – together with illustrating the key metrics of "time to solution" and associated "energy to solution"

Reference: "Scientific Discovery in Fusion Plasma Turbulence Simulations @ Extreme Scale;" W. Tang, B. Wang, S. Ethier, Computing in Science and Engineering (CiSE), vol. 16. Issue 5, pp.44-52, 2014

• Current physics and computational progress enabled by *deployment of innovative algorithms within a modern application code (GTC-P) that delivers new scientific insights on world-class systems → currently: Mira; Sequoia; K-Computer; Titan; Piz Daint; Blue Waters; Stampede;TH-2*

with future targets: Summit (via CAAR), Cori, Aurora, Stampede-II, Tsubame 3.0, -----

• Future progress will require *algorithmic & solver advances enabled by Applied Mathematics – in an interdisciplinary "Co-Design" type environment together with Computer Science (e.g., OpenMP4.5, OpenACC, etc.) & Extreme-Scale HPC Domain Applications*