Nonlinear Collision becomes Practical from Multi-Threading
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ASCR− SciDAC Highlight: Three-way collaboration among SUPER, FASTMath, and Fusion-EPSI

Objectives

- **Develop nonlinear Fokker-Planck-Landau collision operation on the highly non-Maxwellian edge plasma for the first time.**

Impact

- **Higher fidelity prediction for ITER's fusion performance by accounting for non-equilibrium edge plasma**

Accomplishment highlight

	Main loop time	Collision routine time
Multi threaded collision	200 s	32 s
Single threaded collision	340 s	171 s

Challenges

- **New nonlinear Fokker-Planck collision solver has been developed in EPSI for fusion kinetic codes but initial implementation in XGC1 proved impractical: *New collision solver nearly doubled total compute time of XGC1***
- **Insufficient work in a single grid cell to fully exploit OpenMP multi-threading capability of XGC1**
- **Effective OpenMP across grid cells needs to include Picard iteration, which solves many small sparse linear systems (currently using PETSc, not thread-safe)**

Solution

- **Thread-safe version of PETSc created by FASTMath (B. Smith)**
- **Multi-threaded nested OpenMP parallelization across grid cells achieved in collaboration with SUPER (E. D'Azevedo, P. Worley)**
- **Collision solver accelerated by over 5X, and XGC1 by 1.7X**

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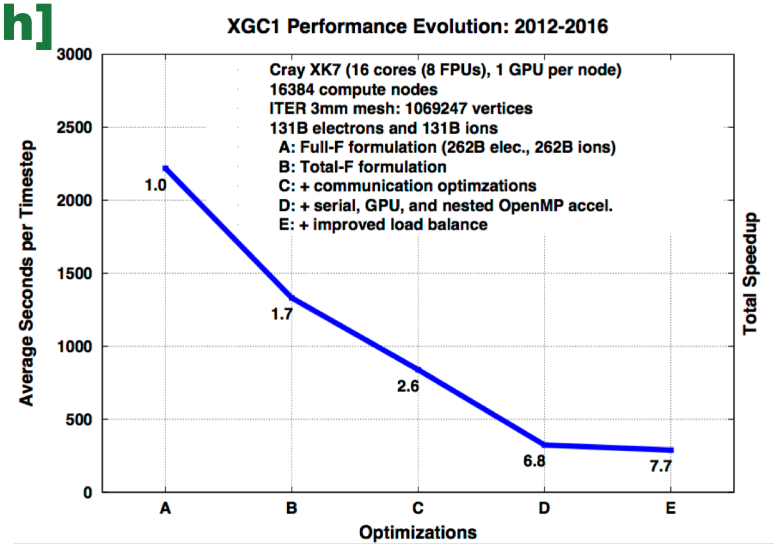
Performance Evaluation and Analysis Consortium End Station: [XGC, SUPER & FASTMath]

Science Objectives

- **Enable ITER simulation on Titan by XGC kinetic code**
- Develop new programming models and runtime systems
- Update and extend performance evaluation of Leadership Class (LC) systems
- Port, further develop, and make available performance tools and middleware on LC systems
- Develop and validate performance prediction technologies
- **Analyze and help optimize LC applications codes**



Performance of XGC1 ITER simulation on Titan as a function of algorithmic improvements.

OLCF Contribution

Have OLCF resources such as hardware resources, liaisons, user support, data resources, training, website, etc. contributed thus far to the success of the project?

- Science experiments using XGC1 are feasible only on the full Titan system.
- OLCF system staff have been vital in identifying hardware and software issues that cause failures in XGC1 runs, and in proposing workarounds and improving fault tolerance.

Science Accomplishment and Impact

- In a collaboration between the EPSi SciDAC projects and the SUPER & FASTMath SciDAC institute, documented a greater than **7.6 times performance improvement** in the XGC1 particle-in-cell code on Titan over the past 4 years, due to
  - New formulation, requiring half as many particles
  - New parallel algorithm, significantly decreasing interprocess communication overhead
  - Port of primary particle computation kernel to GPU
  - Serial and parallel implementation improvements in nonlinear collision operator
  - New hybrid load balancing scheme
  - I/O enhancement not included