SciDAC GSEP & CSEP: Gyrokinetic Simulation of Energetic Particle

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NERSC FES Requirements for 2017
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1. Project Description: GSEP

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• Summarize your project(s) and its scientific objectives through 2017

extend the capability of highly scalable gyrokinetic (GK) turbulence codes based on the complementary particle-in-cell GTC and continuum GYRO to study the energetic particle (EP) driven Alfvén modes and their interaction with background thermal plasmas
1. Project Description

• Our present focus is ...
2008-2011: extend GK from microturbulence (micro-scale) to EP Alfven modes (meso-scale); V&V.
2011-2016: study EP turbulence & transport; extend GK to MHD (macro-scale).
First-principles, integrated, peta-scale GK simulation of kinetic MHD: microturbulence, EP, MHD, neoclassical...
• By 2017 we expect to ...
2016-?: study EP interaction with background thermal plasmas (microturbulence & MHD); extend global code from kinetic MHD to include heating/current drive.
Exa-scale simulation of multi-physics processes.
Linear Simulations of TAE, RSAE, BAE Verified

- DIII-D shot # 142111, GTC, GYRO, and TAEFL frequency up-sweeping, mode structures, and transition of RSAE to TAE in good agreement with experiments.
- BAE [H. Zhang et al, PoP2010]
- RSAE [W. Deng et al, PoP2010]

GTC simulation of RSAE to TAE transition with real geometry & kinetic electrons [W. Deng et al, NF2012]

RSAE in DIII-D shot # 142111 at 725ms [D. Spong et al, PoP2012]
GTC Nonlinear Simulations of BAE Find Fast Chirping

- Fast, repetitive, mostly downward chirping, sub-millisecond period
- $90^\circ$ phase shift between intensity oscillation and frequency chirping
- Simulation features observed in recent NSTX TAE, ASDEX BAE
  - EP transport enhanced by chirping
- No sources and sinks. Chirping mechanism? Universal dynamics?

[M. Podesta et al, NF2011; PPPL-4719]
2. Computational Strategies

• We approach this problem computationally at a high level by …
  GK particle-in-cell GTC and continuum GYRO

• The codes we use are …
  GTC, GYRO, TAEFL, HMGC

• These codes are characterized by these algorithms: …
  PIC, continuum, gyrofluid, MHD-PIC hybrid

• Our biggest computational challenges are …
  Improve efficiency while maintaining scalability

• Our parallel scaling is limited by …
  linear solvers, I/O

• We expect our computational approach and/or codes to change (or not) by 2017 in this way …
Gyrokinetic Toroidal Code (GTC)

- Confinement and stability properties of fusion plasmas depend on nonlinear interaction of multiple physical processes
  - Microturbulence, energetic particle (EP), magnetohydrodynamic (MHD) modes, heating/current drive using radio-frequency (RF), ….

- **GTC Physics Integration**: first-principles simulations of microturbulence + EP + MHD + RF
  - General geometry & experimental profiles
  - Kinetic electrons & electromagnetic fluctuations
  - Gyrokinetic or fully kinetic ions
  - Equilibrium current; δf or full-f
  - Scalable to $10^5$ cores; GPU acceleration

[Z. Lin et al, Science1998]
[I. Holod et al, PoP2009]

[http://phoenix.ps.uci.edu/GTC]
3. Current HPC Usage (see slide notes)

- Machines currently using
  Hopper, Jagarpf, Tianhe-1A, Titan, Edison
- Hours used in 2012 (list different facilities)
  Hopper: 20M; Jaguarpf: 5M/24M (ALCC); Tianhe-1A: 5M (ITER-CN)
- Typical parallel concurrency and run time, number of runs per year
  \(10^3\)-\(10^5\) cores, 1-20 hours, hundreds of runs per year
- Data read/written per run
  restart files: 0.01 to 0.1 of total node memory
- Memory used per (node | core | globally)
  0.1 to 1 of node memory
- Necessary software, services or infrastructure
  linear solvers, I/O
- Data resources used (HPSS, NERSC Global File System, etc.) and amount of data stored: HPSS: 7unit
4. HPC Requirements for 2017
(Key point is to directly link NERSC requirements to science goals)

• Compute hours needed (in units of Hopper hours)
  1 billions hours
• Changes to parallel concurrency, run time, number of runs per year
  parallel concurrency increases with core #, run time/number of runs stay unchanged
• Changes to data read/written
  size increases with core #
• Changes to memory needed per ( core | node | globally )
  Memory stays unchanged per core, increases with code # per node/globally
• Changes to necessary software, services or infrastructure
  linear solvers (e.g., petsc by ANL), I/O by ORNL
5. Strategies for New Architectures

• Our strategy for running on new many-core architectures (GPUs or MIC) is ... 
  Collaboration with CS.

• To date we have prepared for many core by ... 
  Multi-level parallelism: MPI/OpenMP
  Production version: GTC-GPU via CUDA Fortran & OpenACC (NSCC-TJ & Nvidia)

• We are already planning to do ... 
  MIC optimization (NSCC-TJ).

• To be successful on many-core systems we will need help with 
  Linear solver (ANL), I/O (ORNL)
5. Summary

• What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  
  First-principles, integrated simulation of cross-scale interaction between multiple physics processes.

• Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science heterogeneous, multi-level concurrency.

• NERSC generally refreshes systems to provide on average a 2X performance increase every year. What significant scientific progress could you achieve over the next 5 years with access to 32X your current NERSC allocation?
  
  Coupling between microturbulence, EP, MHD, neoclassical, e.g., Neoclassical tearing mode, resistive wall mode, sawtooth etc.

• What "expanded HPC resources" are important for your project?
  
  Linear solvers with multi-level parallelization

• General discussion