Answers to PSACI-PAC charge from CPES

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A. Three of the most important scientific accomplishments that impact predictive capability

1. Gyrokinetic edge code: Gyrokinetic 2D equilibrium solution from XGC1 across the toroidal magnetic separatrix in the edge
2. Verification of the XGC1 linear ITG mode capability in cyclone geometry
3. Effect of resonance magnetic perturbation (RMP) on edge pedestal

B. To what extent is the code validated

1. Good agreement with R. J. Goldston, "Charge-exchange measurements of the radial profiles of parallel and anti-parallel ion energy distribution on ATC", Nuclear Fusion, 18, 1611, 1978
2. RMP simulation compared reasonably well with DIII-D
3. Anisotropic ion temperature seen in DIII-D as predicted by XGC

C. What deliverables were you not able to obtain, why?

1. Everything was delivered as scheduled except the DEGAS2 integration into XGC0. The job schedule was modified to accommodate another important task within the same laboratory. The job will be accomplished according to the modified schedule.

D. Up to three key contributions from Science Applications and Enabling Techology Centers

1. TOPS: Provided solvers and algorithms
2. SDM: Kepler work flow and dashboard, Data management
3. PERI: Performance enhancement
4. GPSC: Gyrokinetic turbulence techniques
5. CEMM: M3D and NIMROD code coupling to XGC

E. What is the science enabled by maximum number of CPUs used, efficiency?

1. We have used up to 16,384 processors (1.64B particles).
2. Noise convergence with particle numbers in XGC1 nonlinear ITG verification was enabled.
3. Efficiency was about 7% a few months ago (XGC1 is a particle code). PERC team has been continuously improving the efficiency (the same team as for GTC).

Specific questions to CPES

A two fluid E&M code coupling to XGC0 until we get the E&M capability in XGC1?

This will be a good idea if we can find an adequate code. We will try to find one.

If we have to spend too much time to make the fluid code coupling work in the edge, however, it may be better to put the resource on the kinetic code development. The E&M technology from GEM is a candidate for XGC1 E&M.

2. How is your Proto-FSP integration/coupling approach going to fit into the next phase FSP framework?

a) We hope our Kepler framework develop into the next phase FSP framework (very flexible, fast IO, has all the features for FSP, can contain other framework including CCA), however

b) Framework has moving targets. Should not be fixed too early. Different framework developments will become the bases for the future FSP framework

c) There are two aspects of the framework:
   - Software (Kepler, Python, CCA, etc)
   - Integration methods between different physics
     Kinetic-kinetic (same level, but multiscale)
     Kinetic-fluid (different level)
     Dimensionality difference,
     Geometry difference

d) Edge has its own integration properties
   Data-2D-3D-Kinetic-fluid (MHD)-geometry-core coupling

3. Plans for code verification and experimental validation?

Verification: XGC code verification was reported at the 2007 US-EU Transport Task Force Workshop. Manufactured solution method is an excellent one. Comparison with a known analytic result and already verified code results are other good methods we have been using.

Validation: Lehigh University’s specific mission is validation. We have domestic and international validation partners: Zweben (PPPL), Maingi (ORNL), Greenwald (MIT), Groebner, Leonard , Osborn (GA), Kamada (JT60U), Horton (ASDEX-U), Fundamenski (JET).

We identify specific validation data together.

“Computers are incredibly fast, but incredibly stupid. Humans are incredibly slow, but incredibly smart. Together, they perform incredibly smart science at incredibly fast speed through SciDAC Proto-FSPs” (A. Einstein)