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SNL ADTM

FY20Q3 report for ATDM AD projects to ECP

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Performance to Plan:

- SPARC:
 - The SPARC team has completed much of the workflow development needed for the coupled and uncoupled analyses needed to support our flight test validation work.
 - The SPARC team has continued to make progress on development activities to support unsteady, full reentry vehicle aero analysis, which have focused on turbulence modeling, uniform mesh refinement, in-situ visualization (with the Paraview/Catalyst team), and performance analysis.
 - The SPARC team is making solid progress towards our Q4 goal of demonstrating an improved Wall Modeled Large Eddy Simulation (WMLES) capability for standard geometries using high-order finite difference, discontinuous Galerkin, and low-dissipation finite volume methods.
 - The SPARC team has met the minimum completion criteria for parts of the L1, including documenting performance and scaling of SPARC on Trinity, Sierra and Astra, and performing runs for the flight test validation case.
- EMPIRE:
 - The milestone remains on target. The team is maximizing its use of the additional time to improve performance for EMPIRE-PIC and enhance capability for EMPIRE-Hybrid.
 - EMPIRE development in Q3 focused on performance improvements and memory use reduction: for the milestone SGC problem, kernel optimizations in the particle push halved runtime for that part of the simulation, and, through careful segregation of the Trilinos components (Panzer), runtime memory use has been reduced by 60%.
 - Dynamic particle load balancing is maturing with performance improvements targeted for Vortex/Sierra. The same infrastructure, based on the Checkpoint library co-developed with VT, is being used as the basis for a checkpoint-restart capability for EMPIRE-PIC. This was fast tracked as a risk mitigation strategy based on issues with MPI AllReduce reported on Sierra.
- Applications:
 - EMPIRE hybrid capabilities have been demonstrated on a beam-in-box prototype test problem that serves as a prequel to simulation of the HERMES courtyard experiment. Hybrid compares favorably with PIC and shows good performance.
 - Progress continues on the SPARC and EMPIRE V&V efforts. Notable Q3 accomplishments include an initial warm diode analytic solution for EMPIRE verification, and execution of Generic Re-entry Vehicle (GRV) simulations using SPARC.
- Components
 - SGM History capability is complete. Solid model generation capability is greatly enhanced by ability to back up step by step, and go forward again, quickly and reproducibly.

- Higher-order implicit methods in SPARC now running with Kokkos on GPUs. Various nonlinear solver approaches implemented and tested.
- Fine-grained memory management in Panzer has led to 2x-3x decrease in memory usage for EMPIRE-PIC.

EXCEEDS

- EM Survivability: A substantial reduction in turnaround time to build EMPIRE and run the test suite has transformed team productivity and code stability. Improved infrastructural stability and utilization of the ASC Build&Test farm brought the build and test completion time from 8 hours to two, meaning three runs can now be completed per day. This allows developers to catch and address problems much faster.
- Applications & Algorithms: The SPARC trajectory modeling workflow has been extended to handle multiple turbulence and reacting gas models, trajectory resolution, and atmospheric variability.

Lessons Learned:

- Applications:
 - Recent collaboration between the SPARTA and SEMS teams has been beneficial, producing improvements to the SPARTA build and test systems.
 - The development of automated diagnostics for the SPARC trajectory workflow has proven valuable for FY20 activities and is expected to be beneficial to future analyst work as well.



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