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# FY20Q4 report for ATDM AD projects to ECP

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ECP Confluence updates

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## Performance to Plan:

- SPARC:
  - The SPARC team has demonstrated the ability to run two-way coupled SPARC/Aria simulations for a thermal ablation test problem.

  - The SPARC team has demonstrated use of all of its targeted ATDM components (performance portable/scalable solvers, scalable I/O, uniform mesh refinement) except in-situ visualization for full vehicle reentry analysis.

  - SPARC is on track for successful completion and documentation of its part of the L1 milestone. Performance and scaling of SPARC on Trinity, Sierra, and Astra is complete. Qualitative and quantitative comparisons between SPARC and US3D are complete. The flight test validation case is complete. Work on the unsteady full RV analysis case is in progress and will be complete in time for the L1 final review in December 2020.

- EMPIRE:
  - The milestone remains on target. The additional time has been used to improve performance for EMPIRE-PIC, which has paid off in the good scaling results, and enhance capability for EMPIRE-Hybrid.

  - Thanks to the efforts of the UMR and Cubit teams, meshing of the SGC ceased to be a concern for the milestone. An alpha version of Cubit was made available to the EMPIRE team to address the bug that was preventing a r=2 mesh from being generated, with the result that mesh quality is now more consistent across refinement levels.

  - The checkpoint/restart capability started in Q3 has made great progress. We can now restart electromagnetics problems in EMPIRE, and we are on track for restarting EMPIRE-PIC by the end of September. This effort was facilitated by close collaboration with the VT team who provided much of the core framework.

  - Dynamic load-balancing has been demonstrated on a L1 milestone problem following resolution of a memory leak and many performance issues. For the long-running gas-filled SGC physics run, we were able to reduce the out of balance ratio (max-min)/(avg) from 1.2 to 0.07, thus attaining essentially perfect balance.

- Applications:
  - EMPIRE-Hybrid has been demonstrated for simulation of the HERMES courtyard experiment in support of the L1 Milestone, confirming hybrid as a

viable solution method relative to pure PIC. This work is a culmination of many efforts among EMPIRE-Fluid, EMPIRE, and additional ATDM teams. Preliminary results indicate significant performance improvements over PIC. Additional comparisons with PIC results are underway for early simulation time.

  - An EMPIRE-Fluid nonlinear warm diode problem has been completed for verification of the coupling between EM and pressure forces, and the coupling of EM/fluid inflow-outflow boundary conditions. The warm diode test includes formal verification (error norms, rates of mesh convergence) for EM and fluid QoI against a quasi-analytic solution. Findings are documented in a manuscript currently in preparation (Hamlin, Beckwith, Smith, Roberds).

  - For the SPARC V&V effort, a framework has been completed for the propagation of uncertainty through a full sequence of re-entry calculations: 1) creation of a set of trajectories, 2) a subsequent series of SPARC aero simulations to determine heat BC for each trajectory, and 3) a set of thermal-ablation simulations for each BC. The net result is an ensemble calculation giving a measure of uncertainty in QoIs (temperatures at thermocouples) as a function of variability in trajectory.

- Components
  - SGM: Multi-threading of volume-volume intersection calculations has provided a 7X speedup in SGM tests. Runtime for the intersection tests was reduced from 23 minutes to 3 minutes on a typical development machine.

  - UMR: MR generated a mesh of 1.9 billion tetrahedral elements refined from a coarse mesh to enable EMPIRE to demonstrate performance scalability on Trinity, Sierra, and Astra HPC platforms.

  - UMR: Mesh quality of the refined mesh was improved by UMR choosing the best refinement pattern for each tetrahedral element based on a quality metric

  - SPARC: Constructed and presented documentation about the basics of performance on GPUs in SPARC using Kokkos.

  - SPARC: Reduced SPARC build time of files which utilize Trilinos components including Belos, Tpetra and Kokkos.

  - EMPIRE Components Support: Refactored the deploy pipelines to consistently deploy Trilinos and EMPIRE to half a dozen platforms. Stood up automated testing of merge requests, including simultaneous merge requests across repositories.

- Panzer: Added overwrite/restart capability to Panzer's STK_Interface.

## EXCEEDS

- EM Survivability: An EMPIRE-PIC reference implementation paper has been completed and is under review by external collaborators. It will be submitted to Computer Physics Communications.

- Applications & Algorithms: The SPARC trajectory modeling workflow has been extended to handle multiple turbulence and reacting gas models, trajectory resolution, and atmospheric variability.

- Components: The successful refactoring of the DevOps pipeline for integrating Components in EMPIRE has led to much improved stability of the EMPIRE code base across targeted platforms.

## Lessons Learned:

- SPARC:
  - The SPARC team has prepared a presentation about its ongoing work to improve code developer productivity. This elaboration was requested by the L1 milestone panel and will be included as part of the L1 final review.

  - The EMPIRE team was able to partially mitigate issues with Astra scheduling and utilization by teaming with SPARC on job submission and fair use. This will need to continue through October and completion of the milestone requirements with cooperation and patience on all sides.

- Applications:
  - Collaboration between the SPARTA and SEMS teams has been beneficial, producing improvements to the SPARTA build and test systems including cdash/ctest support and automation of Github pull-request testing.

  - The VVTest toolset has proven to be valuable for integrating V&V, capability development, and analysis activities. VVTest increases efficiency in multiple phases of research, development, and application, providing long-term confidence via a formal testing methodology.

- Components:
  - Investigation into poor mesh quality after multiple refinement steps in tet meshes shows that significant decreases in quality can result from "overconstrained" tet

elements that continue to flatten as finer and finer mesh is snapped to the geometry. In the future we should consider mesh topology changes (such as edge or face swaps) to eliminate these overconstrained tets to maintain higher quality meshes.