

SANDIA NATIONAL LABORATORIES

SNL ADTM

FY18Q4 report for ATDM AD projects to ECP

September 14, 2018

Prepared by: Aaron Pennington

Prepared for:

ECP Confluence updates

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology and Engineering Solutions of Sandia, LLC.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.



Performance to Plan:

- Successfully created the foundational High Level Architecture for CHEETAH.
- The DevOps system for integrating EMPIRE and Trilinos continues to mature.
- The group from the Agile Components project and EMPIRE project work as a unified team. This was critical to the L2 Milestone, but mainly behind the scenes.
- MiniXyce:
 - Another rewrite of the parser and device package to create an infrastructure that is more similar to Xyce's design. The original miniXyce was a small linear circuit simulator with a design nothing like Xyce. In the last two years substantial restructuring of miniXyce have occurred, resulting in a code that is less a complete simulator and more focused on emulating the device loading portion of Xyce that I believe Kokkos can impact.

Milestone 6358: Assess Status of Next Generation Components and Physics Models in EMPIRE (Q4)

Status: [Blue] Complete

Reviews scheduled:

- Initial [9/28/18] | Mid-year [03/23/2018] | Final [8/30/2018]

Brief status:

- EMPIRE underwent a L2 milestone which was designed to assess the performance, accuracy and "next generation readiness" of the EMPIRE code. Correctness was based on a large verification suite that tests over 85% of the EMPIRE code. Next generation readiness was based on incorporating portable performant abstractions such as kokkos (MPI+X), high performance I/O (FAODEL), and time integration libraries which allow for embedded sensitivity analysis (Tempus).
- L2 Milestone Panel concluded that the EMPIRE team met all requirements of the milestone.

Technical results of the EMPIRE milestone:

- The performance was tested on roughly ½ of each Trinity partition (KNL and HSW). The PIC algorithm was shown to have nearly perfect weak and strong scaling, on up to 256k cores on Trinity and problems with up to 1.3B elements and 66B particles.

Milestone 6359: Demonstrate ATDM Reentry Physics Capability (Q4)

Status: [Blue] Complete

Reviews scheduled:

- Initial [Dec 2017] | Mid-year [March 2018] | Final [August 2018]

Brief status:

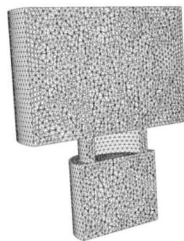
- A comprehensive V&V study of hypersonic flow in SPARC validated against several experiments was produced. This work was successfully completed as an official ASC L2 milestone with an external review of the team's work. Our work has provided a basis for utilizing SPARC as credible analysis tool for hypersonic re-entry flows. The V&V process has been exercised in full breadth including applicable frameworks, professional standards, code and solution verification, calibration, sensitivity analysis and parametric uncertainty.

The full breadth of results has been applied to provide a validation rollup of the uncertainties from the entire modeling process. In addition, this entire process has been integrated with an active code development team. This produced ancillary benefits including enhanced capability development, bug detection and fixes, greater code use, a comparison with other, more established codes and more complete integration with the modeling and simulation software stack. Our work has provided both confidence in the code and models, but also raised important questions for follow-on work. One of our most significant challenges during the year was the archival nature of the experimental results. We felt that the experimental results suffered from several potential deficiencies that required our attention to fully benefit from the detailed comparison of experiment with simulations. We pursued several paths to determine the impact of the issues we identified. Ultimately our attention to these details has deepened our knowledge of hypersonic flows and allowed for a meaningful validation exercise. This milestone effort serves as an exemplar for V&V and code credibility work more broadly at Sandia and externally. The milestone has been documented in a 200+ page report. The External Review Committee found the validation of SPARC to be of very high quality and has recommended using a similar approach for other code validation projects.

News notes/accomplishments:

EMPIRE:

- **Successful completion of ASC-L2 Milestone.** EMPIRE passed a L2 milestone that was designed to assess the performance, accuracy and “next-generation readiness” of the EMPIRE code.

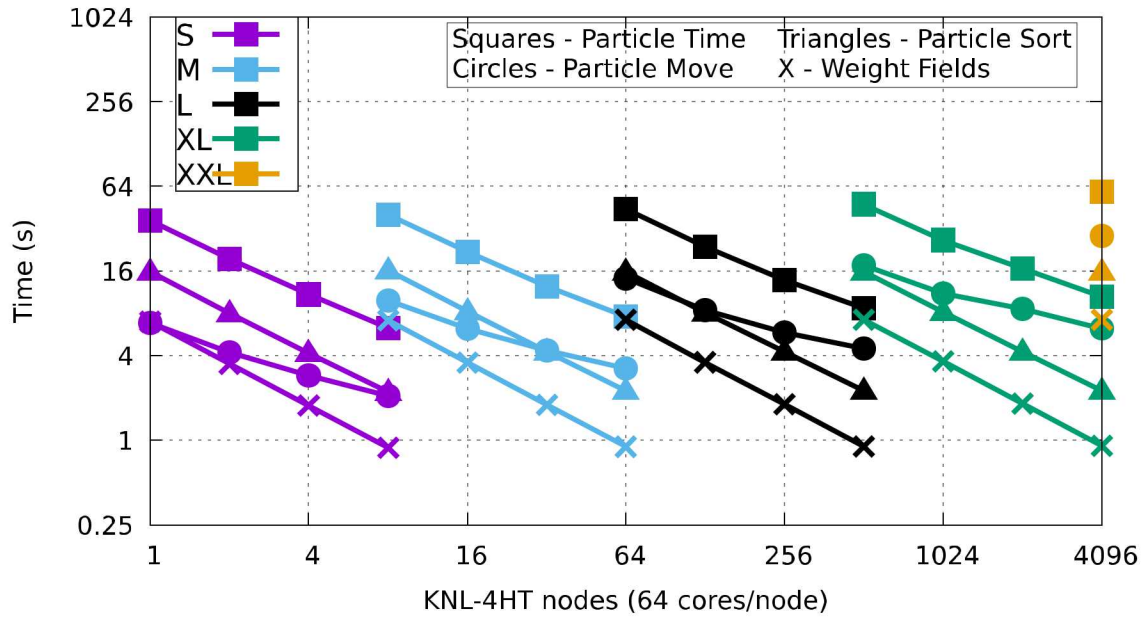


Test Mesh

Correctness was based on the development of a large verification suite that tests over 85% of the EMPIRE code. Next-generation readiness was based on the incorporation of portable performance abstractions such as Kokkos (MPI+X), high performance I/O (FAODEL), and time integration libraries that allow for embedded sensitivity analysis (Tempus). Performance was tested on roughly ½ of each Trinity partition (KNL and HSW). The core Particle-In-Cell (PIC) algorithm was shown to have nearly perfect weak and strong scaling, on up to 256k cores on Trinity and problems with up to 1.3B

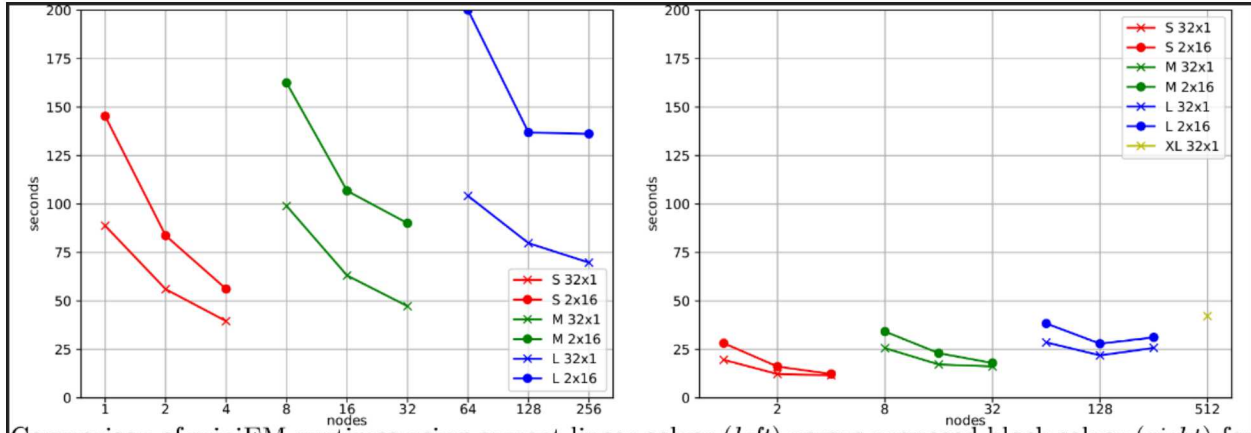
elements and 66B particles. The figure below shows a sample of the scaling results from the KNL portion of Trinity across five levels of refinement of the test problem (mesh shown to the left). (POC: Matthew Bettencourt mbetten@sandia.gov)

(Summary: Successful completion of a L2 milestone demonstrating accuracy, next-generation readiness and performant PIC kernels in EMPIRE.)



Pulsed Power:

Improved electromagnetics linear solver formulation for PIC: Researchers at Sandia National Labs have developed an improved electromagnetics linear solver formulation for time-dependent PIC simulations in the ATDM code EMPIRE. The new formulation relies on an exact block LU factorization of a block two-by-two system. The diagonal matrices are inverted using diagonally-scaled conjugate gradients (CG) and CG preconditioned by a Maxwell-specific algebraic multigrid method from the Trilinos library MueLu. The reformulation has been demonstrated to be approximately five times faster than the solver currently employed by EMPIRE on Cori/Haswell in the proxy application miniEM for a representative weak-scaling 3D unstructured mesh problem. Future work includes testing on larger meshes, optimization of solver settings, and integration with EMPIRE. (POCS: Christian Glusa and Jonathan Hu, caglusa,jhu@sandia.gov).



Comparison of miniEM runtimes using current linear solver (*left*) versus proposed block solver (*right*) for a sequence (S, M, L, XL) of refined unstructured meshes on Cori/Haswell. “32x1” denotes 32 MPI ranks per node, and “2x16” denotes 2 MPI ranks per node, each with 16 threads. The small mesh “S” contains 340k elements; the XL mesh contains 166M elements.

