

SANDIA NATIONAL LABORATORIES

SNL ADTM

Monthly report for ECP ATDM ST projects

August 21, 2018

Prepared by: Aaron Pennington

Prepared for:

ECP Monthly reporting

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.



ATDM Tools and DevOPs

In August the team was able to get CUDA-9.2 up and running on white. Ride is not update to be the same as White, to support Trilinos testing. CUDA-9.2 builds are up on both. The team also expanded ATDM testing for SPARC and finished up the KNL build. Worked on ATDM Trilinos configuration to include the packages necessary for SPARC

ATDM Math Libraries

In August The EMPIRE solvers team identified and fixed a bottleneck in the block operator matrix-vector product. This led to a 1.5x speedup in the overall EMPIRE electrostatics simulation time on the R1 mesh (2.7m elements, 256 Haswell cores). The team progressed integrating the Trilinos electromagnetics solver into EMPIRE, performance assessment is underway. The team succeeded in getting NOX working in SPARC as a precursor to Tempus. Completed the milestone on reducing space interface between ROL and Tempus, working toward demonstrating an inversion for SPARC/ROL.

ATDM Data and Visualization

In August, the team made progress on the TuckerMPI compression writer, with substantial testing framework to handle corner cases. The team made improvements on SPARC/Catalyst integration with Tucker/MPI. Progress toward SPARC/Catalyst working on trinity. Progressed on CPR for EMPIRE. Progress on EMPIRE; restart for field data and now, along with particle. Now is ready for review by EMPIRE team for merging into their code base. The team also revisited I/O support for SPARC.

ATDM Software Ecosystem

In August the team identified best ways to use Kokkos when the goal is serial execution and parallelism is minimized. Joined a working group called COMPASS to collaborate on Cray. The Sierra team started a sprint on Contact work with Tech demonstrator and GPU. The team also expanded the use of Kokkos in the tech demonstrator so that all I/O features are enabled