SAND2018-6553R

SANDIA NATIONAL LABORATORIES

SNL ADTM

FY18Q3 report for ATDM AD projects to ECP

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Prepared for:

ECP Confluence updates

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Performance to Plan:

- **SPARC**: Q4 Deliverable: *L2 Milestone: Demonstrate Application Physics Capability of SPARC Hypersonic Reentry Code*. The milestone effort is progressing very well so far this FY, with several teams coordinating/collaborating on physics model implementations, verification and validation and uncertainty quantification. The team has selected three experimental datasets to validate the code against. The first case is essentially complete, work on the second case began at mid-Q2 and the third case will begin at the start of Q3. Status: On Schedule
- **EMPIRE**: Q3FY18 Verification test suite for particle-in-cell representation: This effort consists building a verification suite which builds a series of tests with analytic solutions to verify different components of the solver. We currently have over 80% code coverage in our automated testing with analytic convergence analysis and code promotion. Status: Complete
- A second **SPARTA** full Trinity run was performed in May, and a third full run is planned for June.
- **Components**: Development of the new SGM geometric modeling capability is progressing well and is on target for completion of phase 1 by the end of Q4. Structured mesh refinement has been demonstrated using SGM on simple test problems running in SPARC.
- Transition the SPARC reacting gas kernels to Kokkos. Completed. All reacting gas flow kernels are now running on GPU and are protected in SPARC testing. Now finished.

Exceeds:

- **SPARC:** An 11-species air model was completed, which is above and beyond what's required for this year's L2 Milestone work, to support the ASC/LSCI project.

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

Status: [Green]

Reviews scheduled:

- Initial [TBD] | Mid-year [03/23/2018] | Final [TBD]

Brief status:

All work proceeding on scheduled.

- Progress continuing on verification test suite; The regression test suite, combined with unit tests, now exercises 81% of the EMPIRE PIC code that has been written thus far (up from 75% in Q2).
- EMPIRE PIC runs on Serrano and Mutrino demonstrating good scalability and performance
- ASD Components
- Solver performance profiling and improvements continuing for KNL (main focus) and GPU.
- Initial checkpoint/restart capability working for PIC and Fluid sides of EMPIRE. Capability has been merged into EMPIRE mainline development branch.
- Tempus integration branch merged into EMPIRE main development branch

The blocked versions of the panzer assembly tools were converted to use kokkos. This resulted in a speedup of ~30x on HSW/KNL systems for RHS Assembly phase in EMPIRE. This brings the RHS assembly times down to ~10% of overall runtime.

Milestone 6359: Demonstrate ATDM Reentry Physics Capability **(Q4)**
Status: [Green]
Reviews scheduled:

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

Brief status:

- Three experimental cases have been identified; calibration, solution verification, UQ and experimental-simulation comparisons have been conducted and continue to be refined.
- The codes for the V&V and UQ are being exercised in the conduct of validation.
- The PIRT completed will be validations and augmented by a PCMM
- The review committee (G. Tipton - chair, S. Domino, E. Draeger, A. Hungerford, D. Bodony, C. Roy), introductory and mid-year review/updates have held

Issues:

- Experimental data shortcomings have been clearly identified and addressed.
- Time and resources will limit the extent of 3D tests will be pursued

News notes/accomplishments:

SPARC:
The SPARC development team has productionized the code for GPU-based systems. This effort involved readying all of the code's perfect and reacting gas models and turbulence model combinations for efficient GPU execution. A noteworthy achievement is that SPARC's key assembly kernel is between 4x and 6x faster on Volta GPUs than on Haswell/Broadwell and Knights Landing processors. The team also worked with the Kokkos Kernels team to integrate the latest GPU-enabled block Jacobi and block tri-diagonal solvers; these solvers give 8x to 10x improvement in execution time compared to the previous generation GPU solvers. These two accomplishments bring the code up to a point of competitive end-to-end execution on ATS-2 early-access systems as well as Sandia's prototype CTS GPU system. The software stack for MPI communication on GPU systems remains a bottleneck; the SPARC team is actively communicating this information with relevant Sandia teams and then up to LLNL and IBM. (POC: Micah Howard, mhoward@sandia.gov)

(Summary: Researchers at Sandia have productionized SPARC for efficient performance on GPU-based systems like ATS-2.)

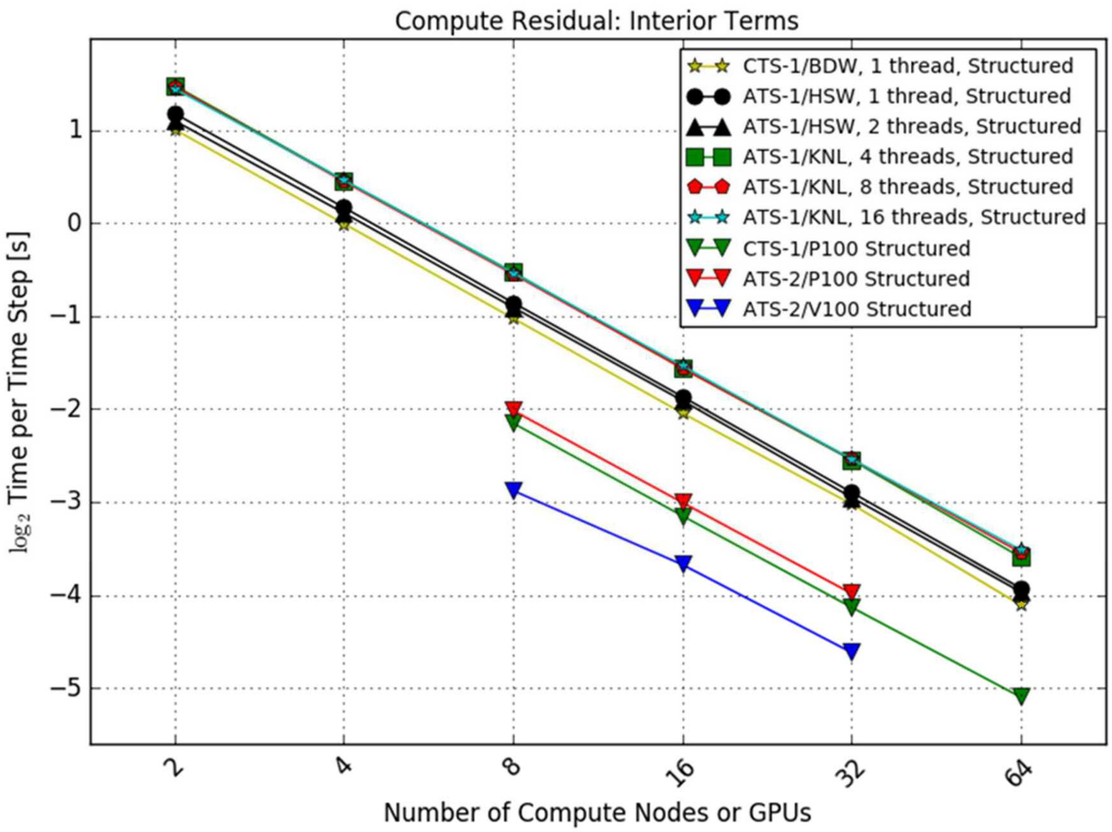

Figure: SPARC's key assembly kernel on a variety of platforms/architectures (CTS-1, ATS-1, ATS-2, Broadwell, Haswell, KNL, P100, V100). Lower is better. Unit of measure: dual socket Broadwell/Haswell node vs. single socket KNL node vs. one GPU.

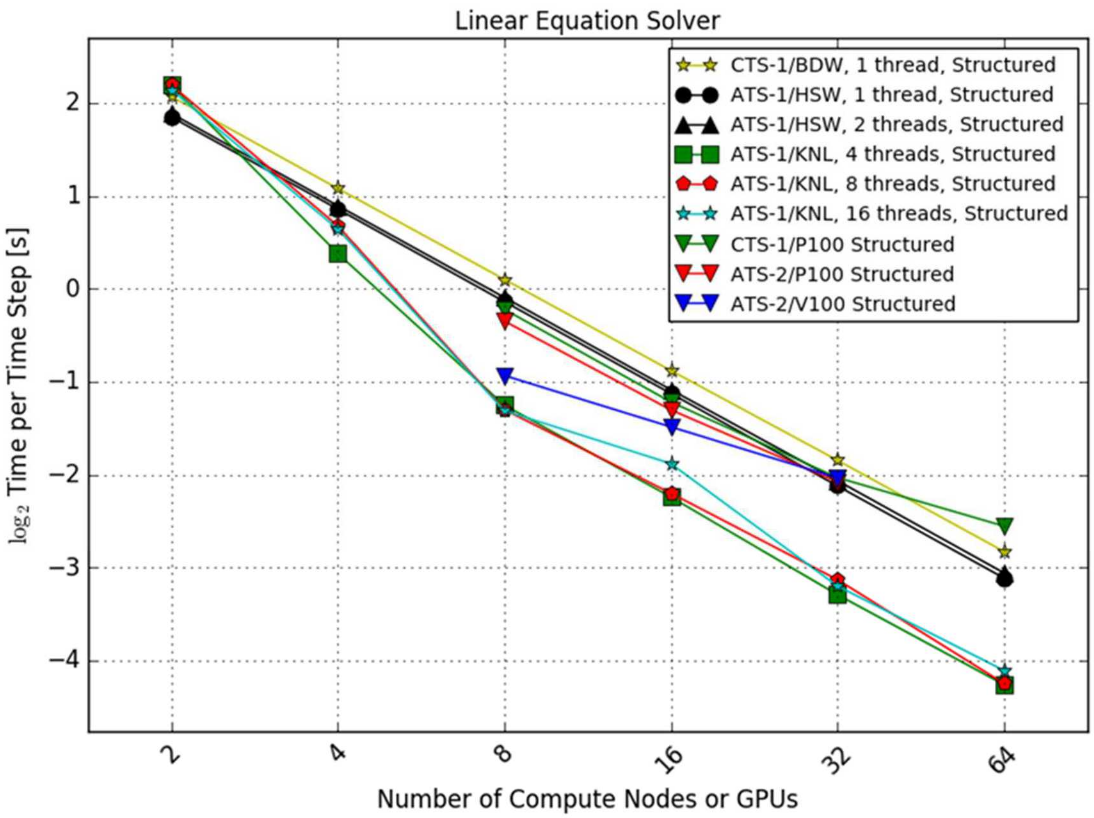

Figure: Kokkos Kernels block tri-diagonal solver on a variety of platforms/architectures. Lower is better. GPU-based solvers are significantly better than prior generation solvers. Further gains to GPU solvers are underway.

EMPIRE:

Automated acceptance, regression and convergence testing. EMPIRE has implemented an automatic testing hierarchy which asserts the code remains stable for analysts while allowing for an agile development processes. This process insolates the EMPIRE developers and users from instabilities in Trilinos in a transparent way. Using a hierarchy of tests (from unit, regression, and automated convergence testing of both EMPIRE and Trilinos), the code is tested on a variety of platforms, an upon success a new EMPIRE version is certified as stable. A key component of this is the automated convergence testing, when a test is created, and an analytic solution can be provided. Through the Sandia SciDev tools, convergence rates are calculated for this test ensuring that we are converging to the correct solution at the expected rates. This process is critical to ensure accurate code performance. (POC: Scot Swan mswan@sandia.gov)

(Summary: Testing hierarchy implemented with automatic convergence and version promotion in ATDM EMPIRE.)

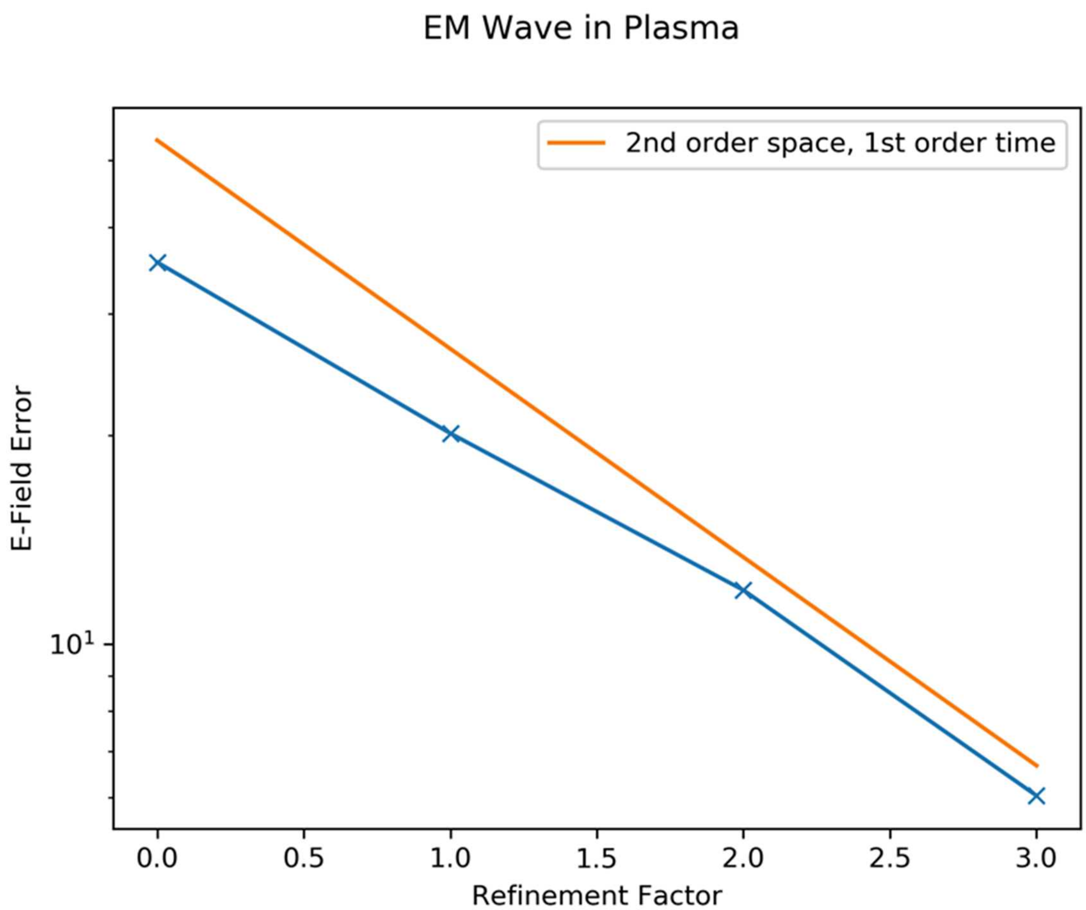

Figure: Automatically generated convergence plot for the EMPIRE code.

Application Algorithms:

Improved Multi-Domain Shock Capturing. Researchers at Sandia National Laboratories have developed a new high-order approach for simulating shocks in structured multi-domain mesh configurations that improves robustness and reduces previously observed simulation anomalies. This work is important for being able to perform direct numerical simulations (DNS) of hypersonic flows in requiring more complex geometric configurations. The new method is a cell-centered, entropy stable Weighted Essentially Non-Oscillatory (WENO) scheme. The cell-centered scheme allows for the nonlinearly adapting divergence operator across the multi-domain interface while maintaining a provable stability estimate, regardless of the interface configuration. Previous usage of an entropy stable node-centered WENO scheme resulted in uncontrolled oscillations when a shock would cross the multi-domain interface, resulting in a larger solution error. The new scheme will be implemented in the ATDM Reentry solver, SPARC, and used in high-order DNS of a hypersonic boundary layer over a sphere-cone geometry. (POC: Jungyeoul (Brad) Maeng, jmaeng@sandia.gov)

(Summary: Researchers at Sandia have developed a new high-order entropy-stable WENO method for simulating shocks on multi-domain structured meshes.)

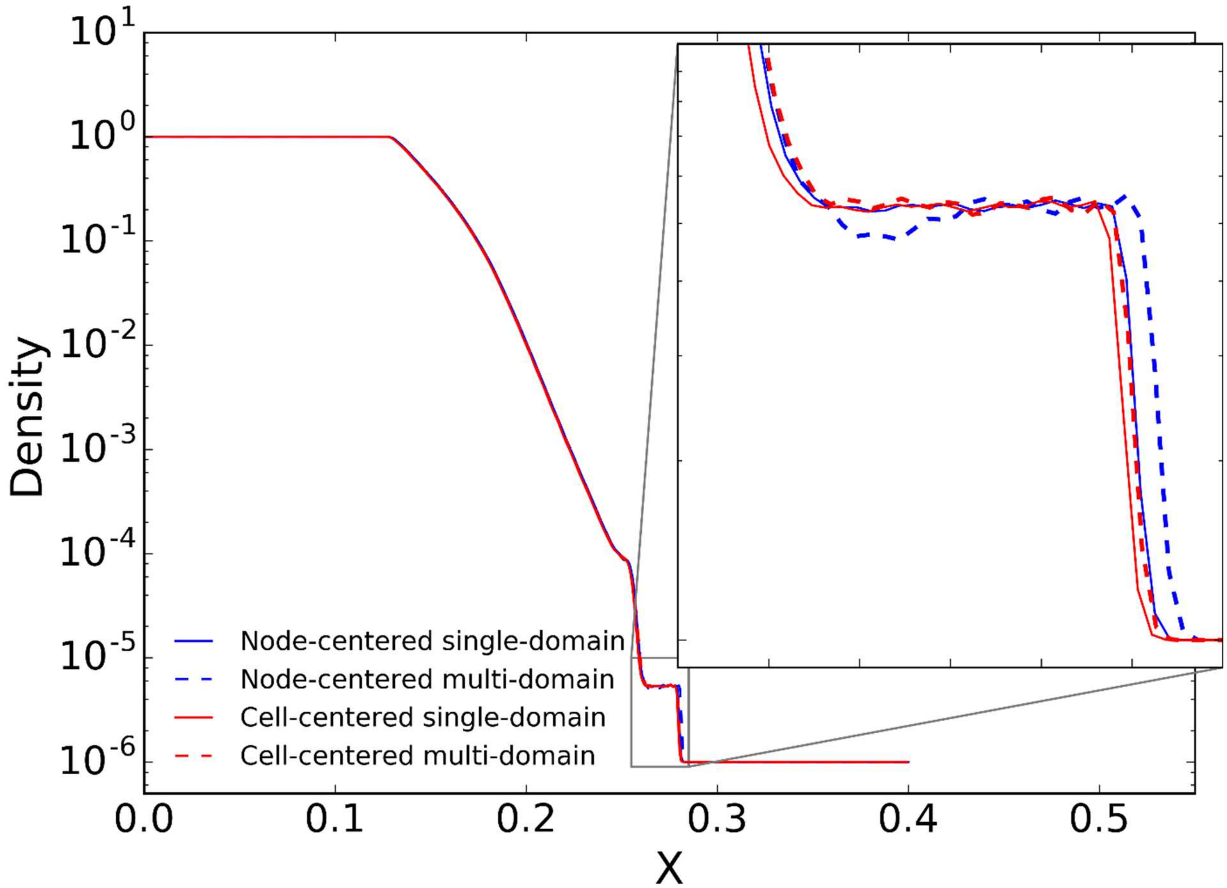

Figure: Shock tube simulation with N = 512 cells, density ratio of 1e6, and final time T = 0.02, showing the elimination of an anomalous undershoot in a multi-domain simulation when cell-centered WENO is used instead of a node-centered scheme.

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