LA-UR-17-28580
Approved for public release; distribution is unlimited.

Title:	FY17Q4 Ristra project: Release Version 1.0 of a production toolkit
Author(s):	Hungerford, Aimee L. Daniel, David John
Intended for:	Report
Issued:	2017-09-21

LA-UR-17-XXXXX

Date: September 18, 2017

To: Doug Kothe, Erik Draeger

cc: Mike Lang

From: Aimee Hungerford and David Daniel, 1.2.2.01/LANL ATDM Ristra

Milestone Deliverable — FY17Q4 Ristra project: Release Version 1.0 of a production toolkit

Milestone Due Date: 09/30/2017

Milestone Completion Date: 09/30/2017

Description of Milestone:
The Next Generation Code project will release Version 1.0 of a production toolkit for multi-physics application development on advanced architectures. Features of this toolkit will include remap and link utilities, control and state manager, setup, visualization and I/O, as well as support for a variety of mesh and particle data representations. Numerical physics packages that operate atop this foundational toolkit will be employed in a multi-physics demonstration problem and released to the community along with results from the demonstration.

Completion Proof of the Milestone:
This milestone delivery includes integration of Portage, FleCSI and initial visualization capabilities (delivered in previous quarters of FY17) with numerical physics application codes. Demonstration of the integrated capability is showcased through a set of verification test problems. These test problems showcase that Ristra's integrated framework can support complex multiphysics applications, and can facilitate swapping of physics and runtime components in a fashion that allows separation of computational physics and computer science concerns. In addition, a milestone review presentation to senior members of the ECP management was conducted on September 12, 2017.

Tasks to Complete the Milestone:
The Ristra project at LANL exists under the Advance Technology Development and Mitigation (ATDM) heading of the Exascale Computing Project (ECP). Ristra is aimed at developing new multi-physics simulation tools that address emerging HPC challenges of massive, heterogeneous parallelism using novel programming models and data management. Modern codes will be developed through co-design of applications by laboratory scientists and engineers. The end product of this work is a next-generation set of simulation tools for LANL's diverse mission space.
In FY17, the annual Ristra ECP milestone targeted delivery of an integrated multiphysics application code built upon a toolkit with utilities for simulation control and state management, as well as

remap and link capabilities. Quarterly milestones throughout FY17 demonstrated progress in the individual toolkit components. The infrastructure to support simulation control and state management is encapsulated in a package called FleCSI (Flexible Computational Science Infrastructure). From FleCSI's inception, it targeted the goal of achieving a separation of concerns between the computational science and computer science aspects of the software, so as to isolate architecture uncertainty and diversity as much as possible from physics code implementation. Connecting this abstraction layer with both a computational physics application code, as well as a parallel runtime, were the major tasks in a proof-of-principle demonstration.

Co-design work between FleCSI code developers and Ristra computational scientists resulted in the FleCSALE/FUEL and Puno codes. FleCSALE/FUEL is a low-energy density multi-physics application code that employs cell-centered Lagrange hydrodynamics and includes a treatment for material strength. Puno is a low-order P1 radiation transport application code. The co-design of the FleCSI interface to these application codes has resulted in some key advances for enabling flexibility. Figure 1 shows a Marshak wave test problem run in Puno using both 2D (bottom) and 3D (top) unstructured mesh topologies. Puno's development was carried out using the 2D unstructured mesh topology specialization through FleCSI, and then extended to 3D by swapping out the 2D mesh specialization for a 3D unstructured FleCSI mesh specialization. This swap of mesh topology was accomplished without any change to the physics code package. In both the 2D and 3D cases, the mesh specialization code was completed by an independent team from the Puno code development team.

An additional demonstration of FleCSI's successful separation of computational physics and computer science concerns is shown in Figure 2. It shows results from a 2D shock box test problem (essentially 2 Sod shocktube problems at 90 degrees to eachother). These results are using FleCSALE in 2D with a Godunov method (64X64 quadrilateral cells with reflective boundary conditions). The left panel shows the result employing a MPI parallel runtime through FleCSI, and the right panel is for the Legion parallel runtime. Again in this case, swapping out the parallel runtime was accomplished with no change to the physics code package.

While these proof of principle test problems demonstrate good promise for our goal of "separation of concerns", it is equally important to show that FleCSI is also capable of supporting the complexity of multi-material, multi-physics simulations. The broad research portfolio at LANL requires this. Figure 3 shows results from a 3D Lagrange FUEL simulation for a cylindrical test problem with 5 materials (including both gases and metals). The physics being represented in this problem are varying by material, with strength calculated for the metals, but not the gases. This test scenario represents a level of simulation complexity that was the team's goal for our low-energy density physics focus in FY17.

The results above were delivered with a set of codes that have been released under a Ristra Toolkit version 1.0 for our open source codes (FleCSI, Portage and FleCSALE). Internal codes like FUEL and Puno are being made available to the internal LANL ASC community. Ristra development will continue in FY18 with a shift in focus to high-energy density applications, such as ICF, but with a continued focus on achieving this within our FleCSI abstraction paradigm. More details for this milestone can be found in a longer report that will be uploaded through the ECP Jira site once a document release number is assigned.

Person(s) Responsible for Completing the Milestone:

Results in support of this milestone were presented by LANL staff Aimee Hungerford, David

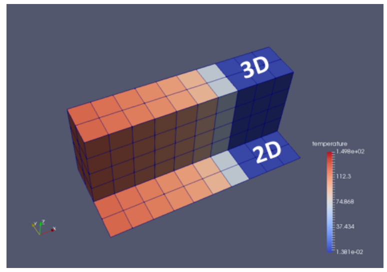

Figure 1: Temperature field of the Marshak problem from a simulation with Puno built on both a 2D (lower) and 3D (upper) unstructured FleCSI mesh specialization.

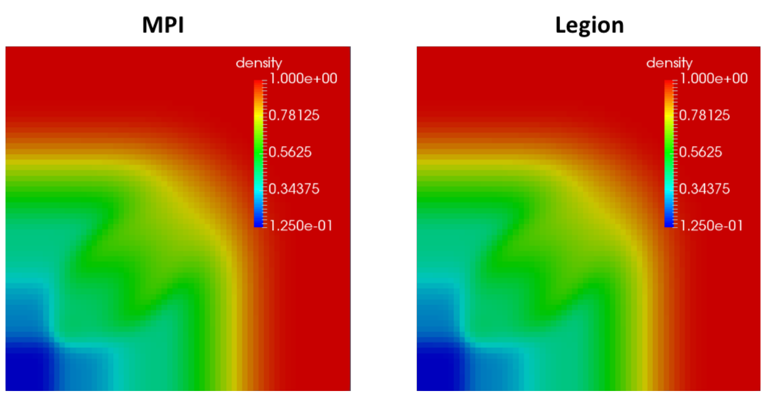

Figure 2: Shock box test problem (essentially 2 Sod shocktube problems at 90 degrees to eachother). These results are using FleCSALE in 2D with a Godunov method (64X64 quadrilateral cells with reflective boundary conditions). The left panel shows the result employing a MPI parallel runtime through FleCSI, and the right panel is for the Legion parallel runtime.

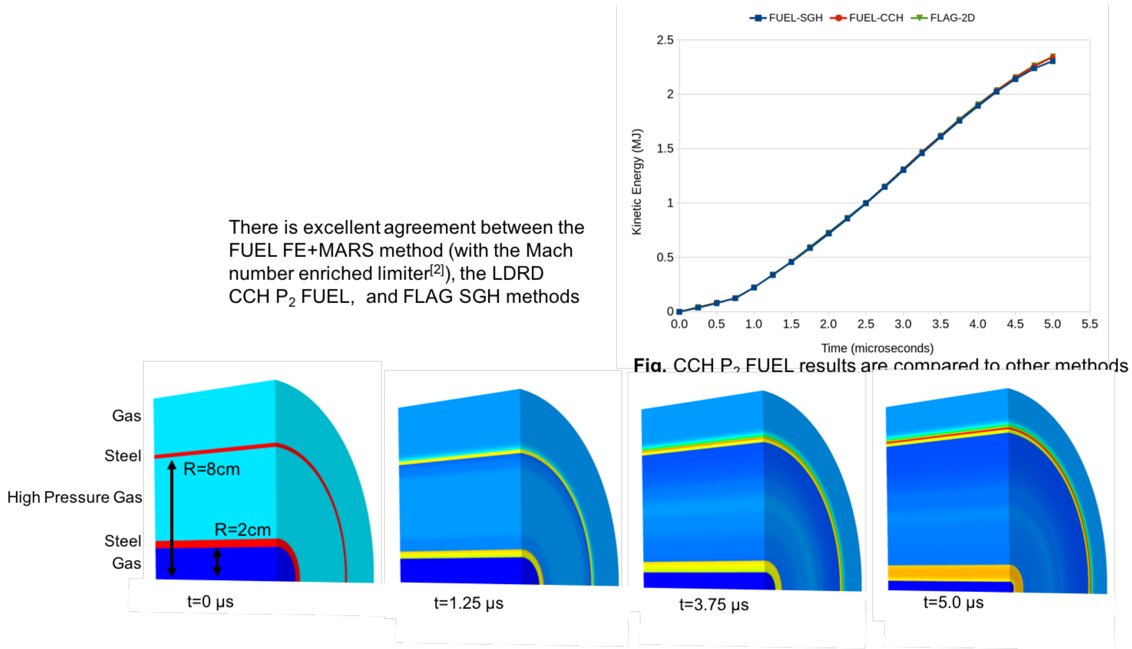

Figure 3: This 5-material test problem has contact discontinuities, shocks, release waves, and disparate material models represented. The results shown here were run with FE SGH and CCH FUEL, as well as the FLAG code, all using Lagrange hydro with multi-material, Gruneisen EOS and PTW strength model.

Daniel, Angela Herring, Ben Bergen, and Nathaniel Morgan, as representatives for work completed by the entire Ristra team.

Regards,
Aimee Hungerford and David Daniel