SAND2015-3614C

Exceptional service in the national interest

Sandia National Laboratories

Core Capabilities

Delivery

Safety and Security

Sierra Thermal/Fluids Release 4.36

AWE Briefing May 6, 2015

U.S. DEPARTMENT OF ENERGY | National Nuclear Security Administration

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Outline

- Aria – Thermal/Multiphysics
- Aero – High Mach Flows
- Fuego – Low Mach Flows

Aero – Re-entry

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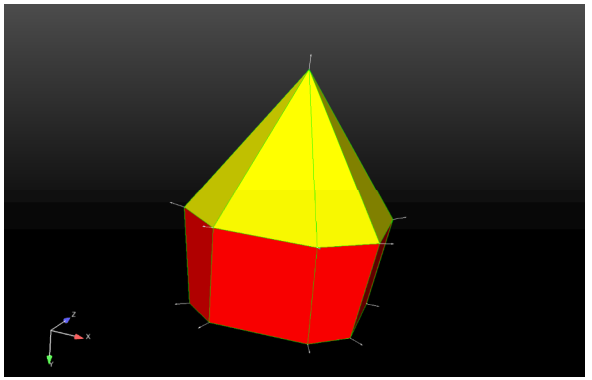
- Goal: Incorporate more advanced physics into simulations of reentry
- Beyond the normal reentry environment
  - High temperatures
  - Unsteady reacting simulations
  - Interacting shocks
- Developed a path forward for running these difficult simulations
- Fixed a bug in reaction temperature clipping when temperature exceeds curve equilibrium constant curve fit
- Developed a verification test for reacting gases (verifies chemical equilibrium state)

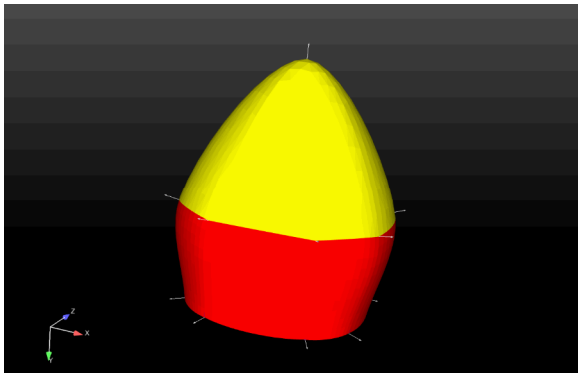
Aero – Mesh Adaptivity and Usability

Sierra/Aero focus is on usability for aero

- Adapt curved geometries
- Ensure useful adaptivity indicators are available
- Support both offline and in-situ run-adapt-run simulations

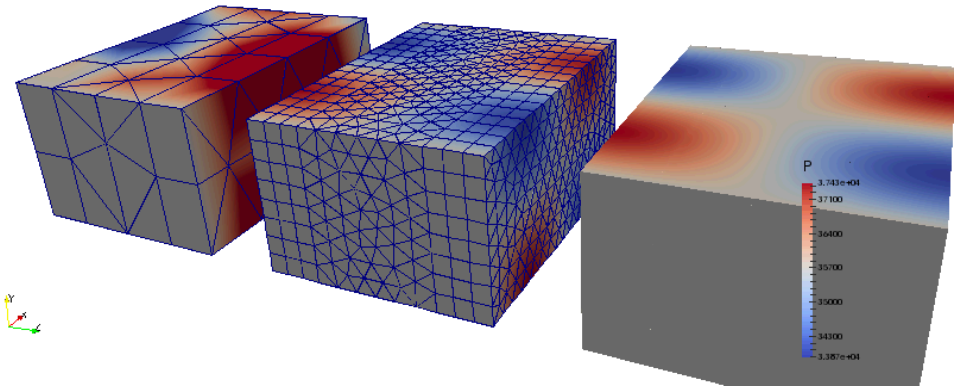
- Curvature Fitting (WIP)
  - Useful when CAD is unavailable or requires significant clean-up
  - Develops skeleton workflow for adapting to curved geometries
  - Needed for high-order curved meshes





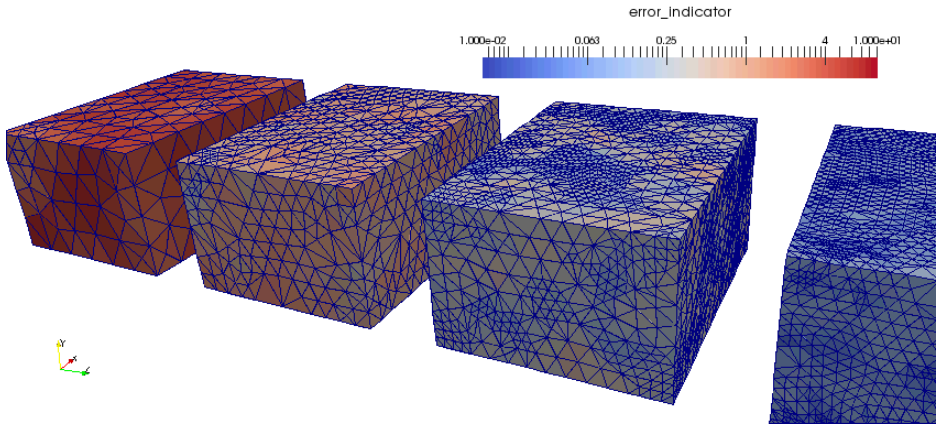
Aero Verification

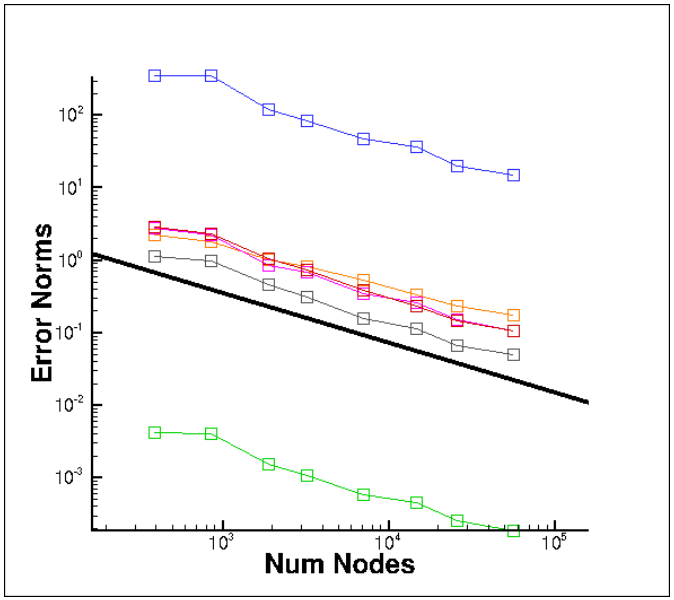
Hybrid mesh verification using Euler MMS test, using transfer for ICs



Offline adaptivity for tet meshes also using Euler MMS;

We see optimal convergence w.r.t. number of nodes

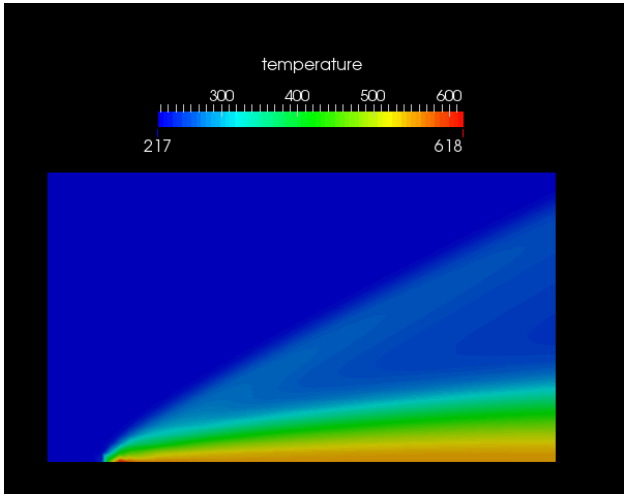


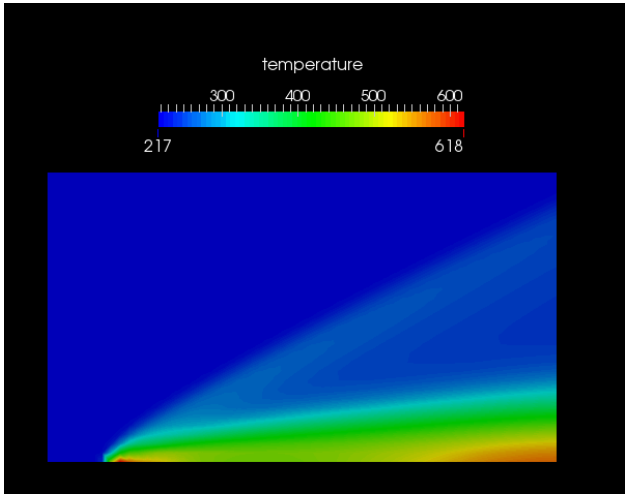


Aero – Other improvements

- Specify Wall Heat Flux and Wall Temperature Profile

Using weak walls ensures consistent imposition of specified temperature and specified heat flux boundary conditions





- Enabled Modified Steger Warming Flux for turbulent flows
- Added append iteration option for DES/unsteady simulations
- Fixed bug in K-epsilon turbulence model

Aero – Strategic Efforts

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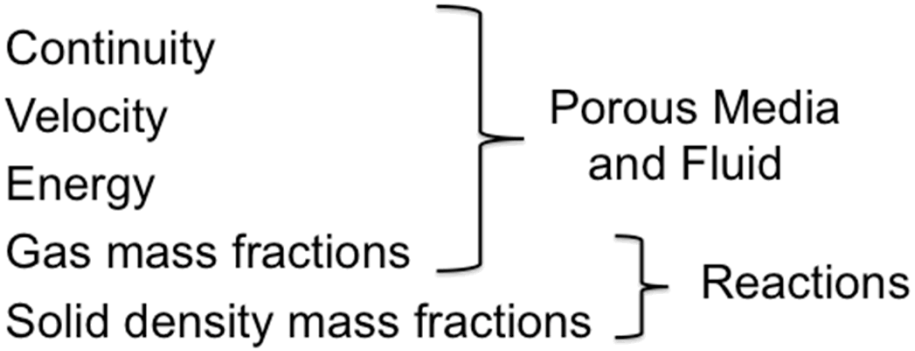
- Features to allow FSI captive carry simulations
  - unstructured higher-order algorithm development
- Performance improvements
- Next milestone: improved robustness of two-way fluid-structure interaction capability (coupling of Aero and SD)
- Increased verification and testing

Aria – Thermal/Mechanical Coupling

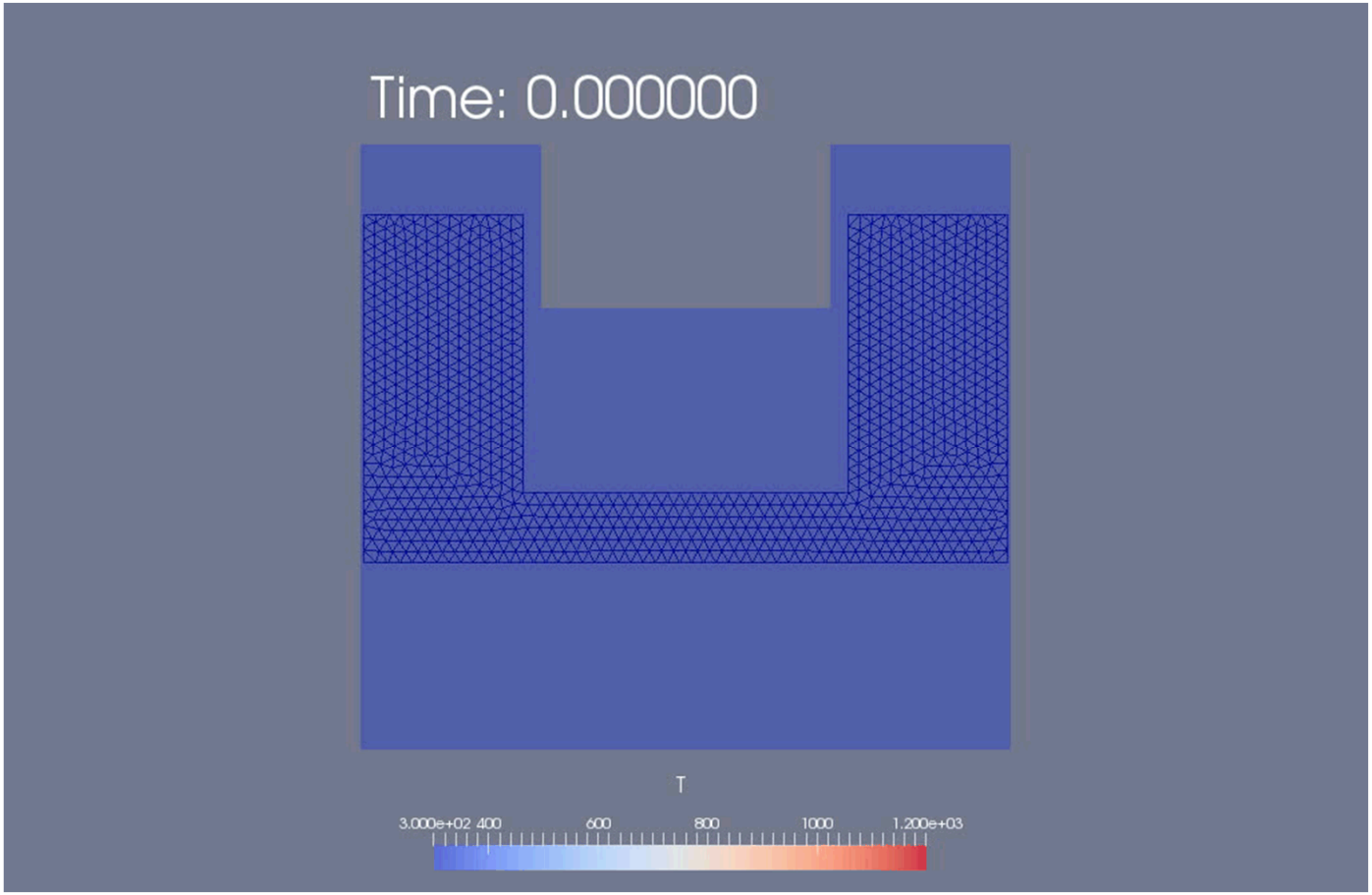
Thermal/mechanical milestone to produce a robust and efficient simulation capability for thermal-mechanical pressurization (from organic material decomposition) to breach

- Improvement of pressure predictions: governing equations



- Major robustness improvements
- Fixed parallel inconsistency bugs
- Improved scalability with robust segregated solution strategy: Enables starting to test 3D

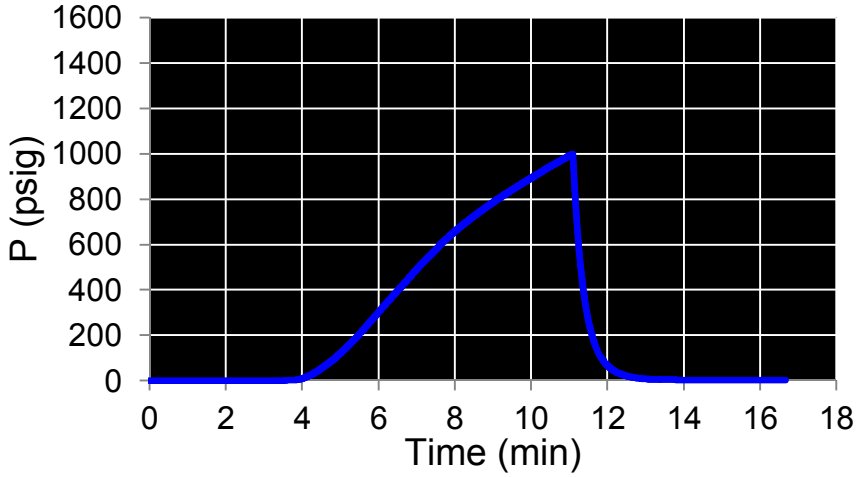
Successful 2D Simulation

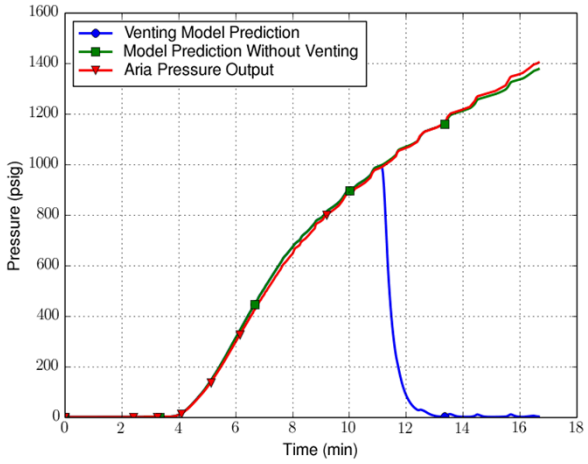


Temperature and Flow

Aria – New ODE Solver

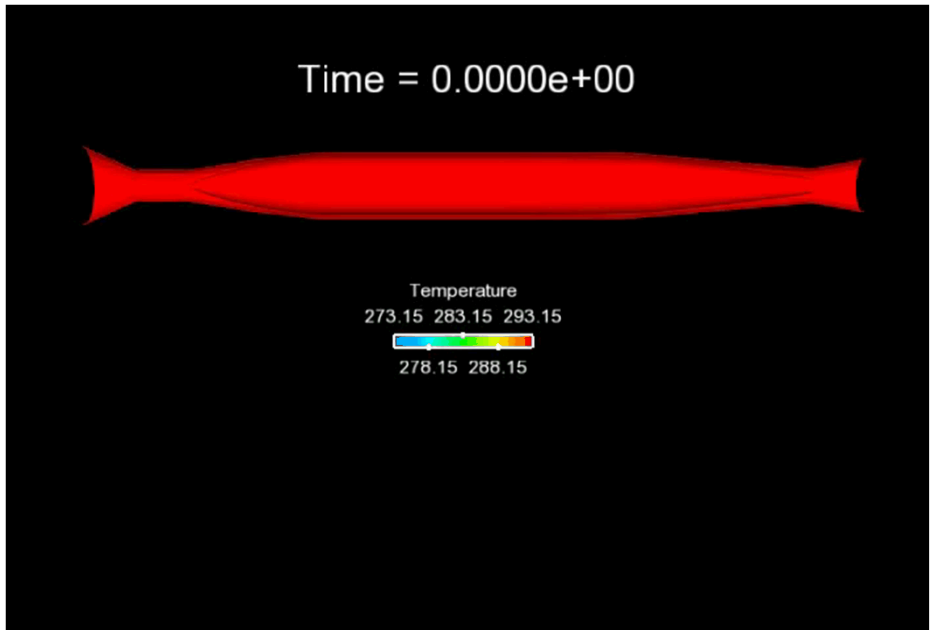
- Users wanted a built-in ODE integrator available for user plugins (pressure venting)
- Added two new capabilities: ODE and ODESolver
- Added example to regression test suite
- ODESolver will be used for upcoming segregated chemistry solver capabilities in the general chemistry module, ChemEq, and electrochemical simulations (allowing faster solves)





Aria – Advective Bar

- Correlations based upon Modified Gnielinski Model
- Restart support
- IC File support
- Axisymmetry
- Heat Transfer Coefficient Visualization



Aria – Harden and Improve

- Simplified Spherical Harmonics (SPN) Radiation Transport: Moment method for solution of the Boltzmann RTE within a radiatively participating medium – computationally efficient
- Elem death flag DEATH_STATUS (1= dead) allows element death use in Arpeggio (coupled Aria/Adagio)
- Post processing changes
- Warning on max nonlinear iterations
- Uniform refinement (to aid in STK transition: node set support currently limited but expected to improve after the STK transition)

Aria – Added Verification Tests

- Anisotropic thermal conductivity from user functions
- Local coordinate system: cylindrical
- Fully 2D enclosure radiation test
- ChemEq pressure-dependent kinetics (time accuracy)

Aria – Strategic Efforts

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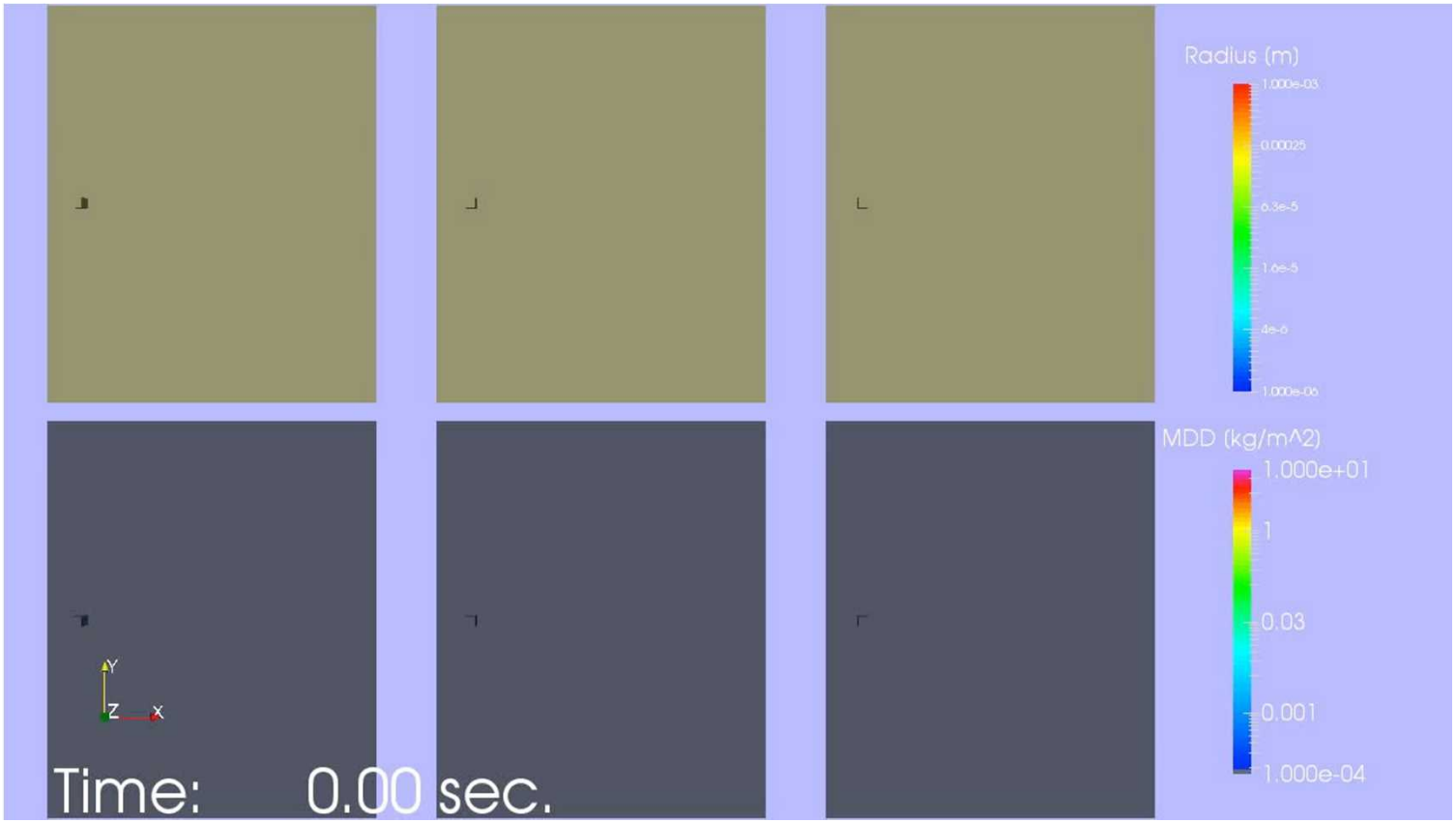
- Continued improvement of physics models
  - Foam and composite encapsulation
  - Thermal batteries
  - Laser welding
  - Energetic materials
  - Organic Material Decomposition
  - Reduced order model additions
- SAW integration
  - Reduce number of extraneous options presented to users
  - Enable better input deck validation by SAW
- Continued improvement on robustness, performance, verification, coupling
- Increased verification and testing

Fuego – Particle Impact and Shatter BC

- Implemented based on Alex Brown's implementation in Vulcan



Fuego – Strategic Efforts

- Improve solid-fuel fire modeling capabilities
- Improve particle capabilities
- Increased verification and testing
- Improve robustness, performance