Sierra Thermal/Fluid Update: New Capabilities in Aria and Fuego

SAND2016-12026C

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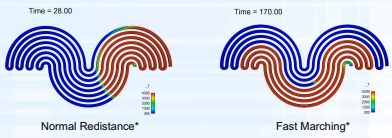
Aria – Energetic Materials & Chemistry

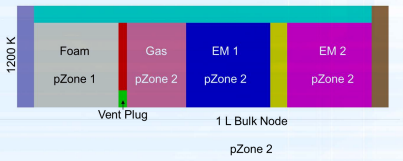
- **Proportional-integral-derivative (PID) controller**
  - PID controlled flux or source
  - Setpoint from a user function
  - Feedback from a data probe global variable
  - Low pass filter on derivative term
- **Total energy accounted for if chemistry is deactivated**
  - User specifies total energy release and release time
  - Also handles gas release for pressurization
  - Available in both ChemEq and General Chemistry
- **Can now enter block-style reactions in ChemEq**
  - Hobbs PBX9501 model (Combustion and Flame, V 173, pp 132, 2016) shown to run about 2X faster with ChemEq
- **ChemEq can detect runaway reactions and limit rate based on complete reactant consumption in a small fraction of the overall time step**

Aria – Burn Front Modeling

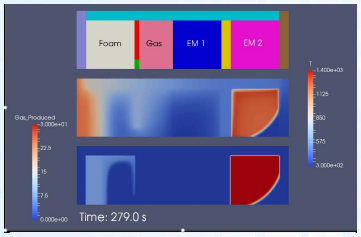
- **Level-set burn model can follow tortuous path**
- **Existing level-set burn model source now time-step independent**
  - A burn front is initiated when any nodes exceed the ignition temperature, and the front is created from all those nodes
  - Each block ignites separately
  - Propagation between blocks is purely thermal
  - Level set distance function can be a global distance, or path-wise distance



Aria- Combination of Capabilities

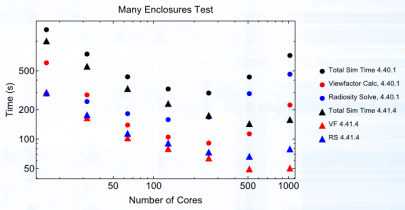


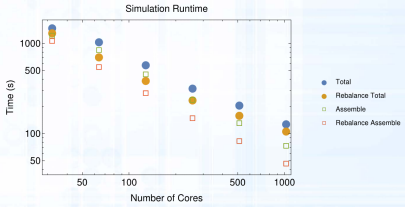
- **One ChemEq Energetic Material + Level Set Burn**
- **One General Chemistry Energetic Material + Level Set Burn**
- **One ChemEq Foam**
- **Two pressurization zones linked by a vent plug that melts at 400 K**
- **One meshed gas region**
- **One bulk node gas region**



Aria- Performance of Enclosure Radiation & Multiphysics Problems

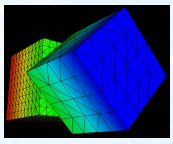
- **Improved communication patterns in Chaparral**
- **Enable Chaparral to simultaneously solve multiple enclosures using different subsets of Aria MPI ranks.**
- **Rebalance multi-criteria weighting improved performance for multi-physics problems with variable cost of element assembly (and dynamic meshes)**





Aria- Thermal Contact

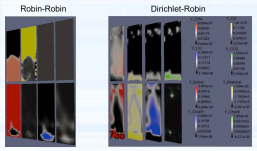
- **Alternative implementation of nonconformal contact**
- **Current support**
  - Discontiguous mesh (Block Skinning)
  - Coverage (Flux mask)
  - Adaptivity
  - Visualization
  - Thermal-Mechanical
- **Coming soon**
  - Automatic tolerancing Shells
  - Shell-to-Shell



Fuego- Aria Coupling Robustness

- **Converted Robin-Robin coupling to Dirichlet-Robin coupling: convergence improved for composite fire**

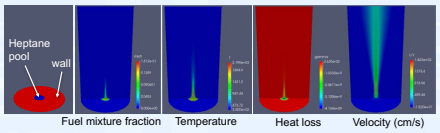
1) epoxy -> char + fuel
2) epoxy + O_2 -> char_trans + fuel
3) char + O_2 -> residue + CO
4) char_trans + O_2 -> residue + CO
5) fiber + O_2 -> residue + CO_2



- **Allowing for the solver to continue after all equations within a submechanics group converged led to significant speedup for the coupled Fuego-Aria composite burn simulations.**

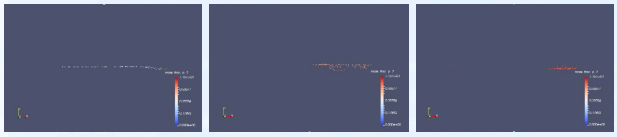
Fuego- Coupling Mixture Fraction Approach and Liquid Pool Boundary

- **Flamelet: reaction is modeled using a set of representative scalars**
  - Mixture fraction, variance, dissipation rate, progress variable, heat loss, etc.
- **Evaporating liquid pool BC is coupled with flamelet**
  - Source of fuel vapor: added to fuel mixture fraction
  - Heat flux through the liquid phase: a sink for heat loss parameter
  - Therefore, non-adiabatic flamelet model is needed
  - Example: evaporating heptane pool surrounded by adiabatic wall



Fuego- Improved Reactive Particle Modeling

- **General chemistry for Fuego particles**
- **Allows for arbitrary reaction mechanism to be specified**
- **Borrows from heated particle dynamics**
- **Allow two-way fluid/particle coupling with enthalpy and chemical source terms**
- **Kinetically-limited versus mass/heat transport limited reactive mechanisms**
- **Test case: cold, liquid particle spay injected into hot fluid, and O2 absorbed onto particle surfaces to form a new liquid compound**



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