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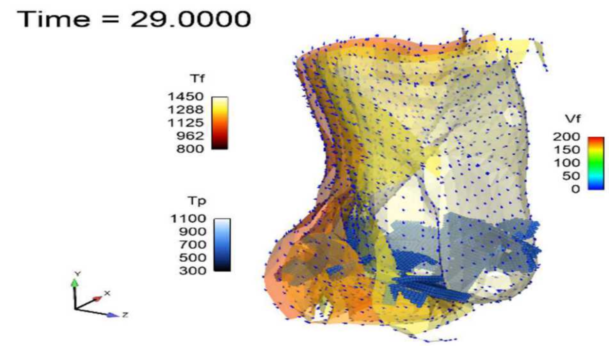

Composite Material Combustion Modeling Using Thermally Interacting, Chemically Reactive Lagrangian Particles

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Sandia National Laboratories

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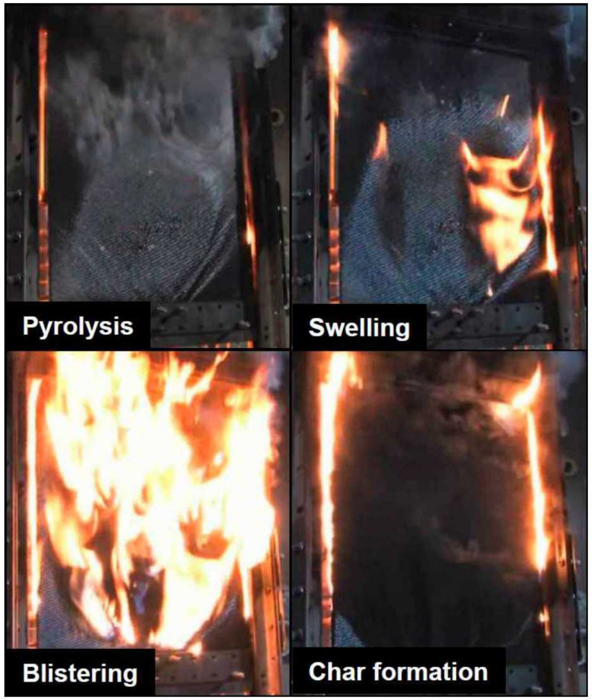
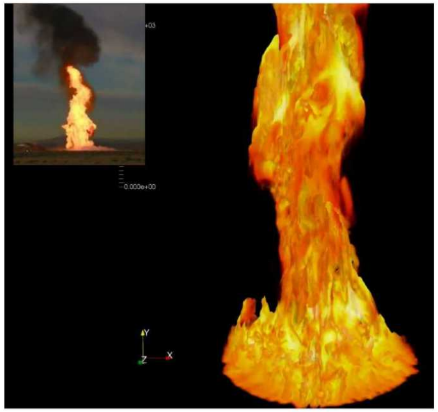
Carbon Fiber - Reinforced Epoxy Composites

LM F-22 Raptor



- Accidents involving aircraft composed of carbon fiber–reinforced epoxy composites can involve mixed fuel fires
  - Liquid fuel
  - Composite rubble
- Complicated combustion processes
  - Chemical Reactions
    - Solid Phase
    - Gas Phase
  - Thermal transport
    - Convection, conduction, radiation
  - Interaction between solids/liquid/gas



Modeling Approach - Fluid

- Fluid (CFD) Description
  - Sierra low Mach Fuego
  - CVFEM
  - Variety of turbulence models
  - Gas phase combustion model
    - EDC – Eddy Dissipation Concept
- Particle/Fluid Coupling
  - Momentum (drag)
  - Energy (heat, enthalpy)
  - Mass
  - Species

SIERRA/Fuego/Syrinx
Low Mach Fluids/Radiation Transport Code

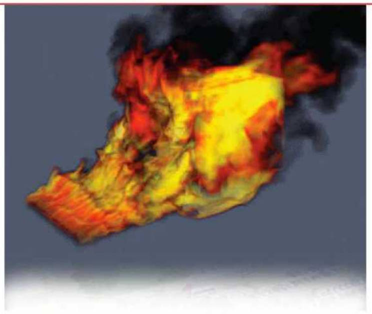
Thermal/Fluids Computational Engineering Sciences Department 1541 at Sandia National Laboratories provides high-fidelity, verified, software-quality assured, massively parallel multi-mechanics coupled analysis codes to the tri-lab community to solve complex problems. SIERRA/Fuego/Syrinx, with coupling to SIERRA/Calore, supports the capability to simulate the abnormal-thermal environment (i.e., transient object heat-up in hydrocarbon pool fire environments that might arise during transportation or storage-accident scenarios).

SIERRA/Fuego/Syrinx

has been developed under the object-oriented SIERRA Frameworks to easily facilitate multi-mechanics coupling to provide a robust simulation capability for highly sooting, buoyancy-driven turbulent-reacting flow mechanics. The core capability in SIERRA/Fuego is simulation of three-dimensional low-Mach-number turbulent-reacting flows on heterogeneous topological meshes (e.g., a mixture of hexahedral, tetrahedral, pyramid, and wedge elements). An approximate projection algorithm is used with Control Volume Finite Element Method (CVFEM) discretization. SIERRA/Syrinx solves the steady radiation transport equation using Streamwise Upwind Petrov-Galerkin discretization. The combined capability, in addition to coupling of the thermal-analysis code SIERRA/Calore, is required in the qualification effort for weapons in abnormal thermal environments.

Applications

SIERRA/Fuego/Syrinx is widely used to simulate applications as diverse as fire environments and laminar natural convection environments. The code primarily simulates buoyancy-driven turbulent-reacting flow in abnormal thermal environments (fluids, participating media radiation [PMR], and heat conduction). However, the core capability of this simulation tool is laminar/turbulent fluid mechanics and a combination of thermal/isothermal and uniform/nonuniform (with reactions) transport.



SIERRA/Fuego/Syrinx/Calore simulation of the proposed Thermal Test Complex Cross Wind Facility. The simulation includes one fluids and [S4] PMR region with two conduction regions (only outside container seen). 400 million dof; 5000 processor Red Storm run; shown is the volume-rendered temperature field.

Features

Unique features of SIERRA/Fuego/Syrinx that enable the code to solve complex problems include the following:

- Scalable, parallel solutions (optimal scaling demonstrated up to available resources, i.e., 40 million node mesh; 4096 processors).
- RANS turbulence models including the v^2-f model of Durbin, standard k-ε with wall functions, low Reynolds number models, and Large Eddy Simulation (LES) models including k-sgs, dynamic Smagorinsky and TFNS.
- Heterogeneous topology support (e.g., hexahedron, tetrahedral, pyramid, and wedge elements).
- Conjugate heat transfer coupling capability either with simple SIERRA/Fuego conduction region(s) or complex SIERRA/Calore conduction region(s).
- Seamless, state-of-the-art solver/preconditioners (e.g, multi-level methods, through input file declarations of solver libraries such as Trilinos, PetSci, Hypre, Prometheus, etc.).
- Advanced user subroutines

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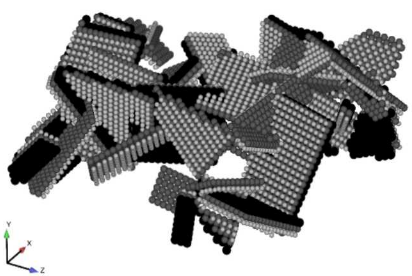
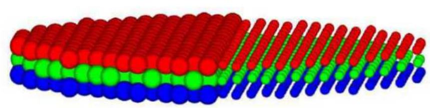
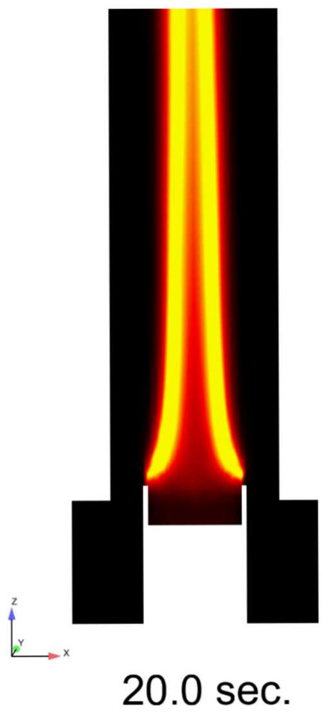
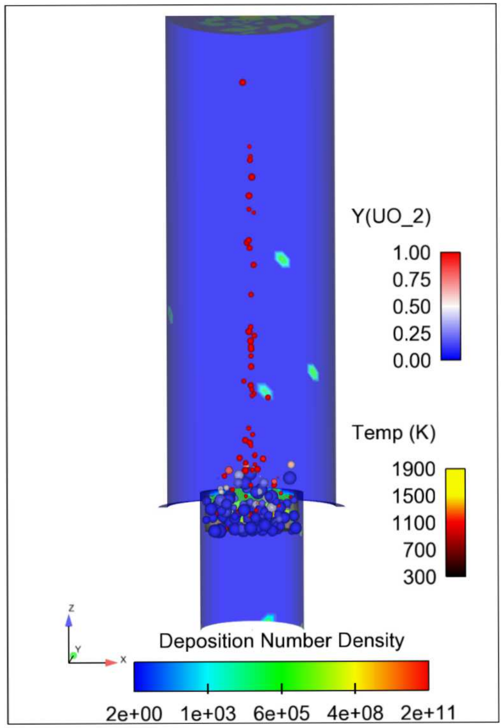
Modeling Approach - Particles

- Composite Materials Description
  - Bars/Layers of Lagrangian particles
- Particle/Particle thermal Interactions
- Particle Chemical Reactions
  - Fuego General Chemistry model

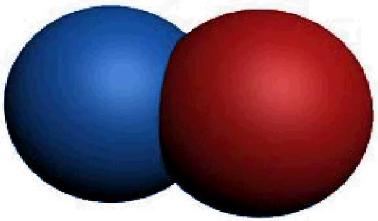


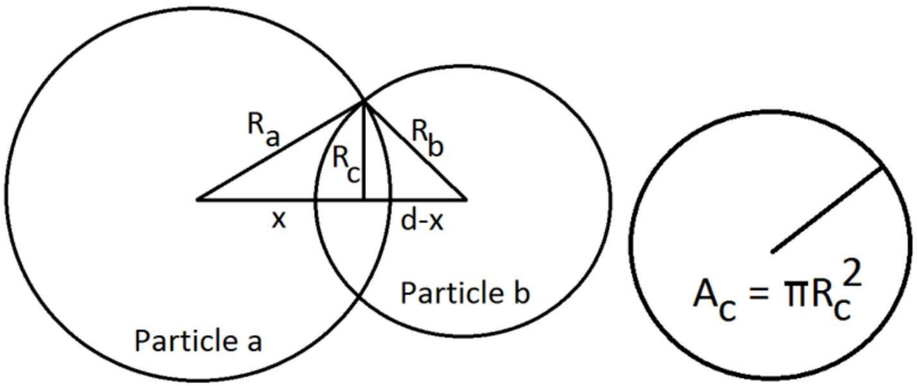






Particle/Particle Thermal Interactions





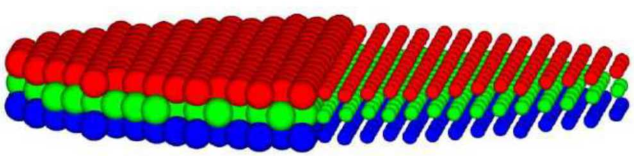
$$x = \frac{d^2 + R_a{}^2 - R_b{}^2}{2d}$$

$$R_c{}^2 = R_a{}^2 - x^2\,,\; A_c = \pi R_c{}^2$$

$$P_{a,b} = \frac{A_c(T_a - T_b)}{\frac{d-x}{k_b} + \frac{x}{k_a}}$$

Thermal exchange - pairwise conduction

- Circular contact area
- Particle size/conductivities can differ
- Particles exist in composite **Bars** made of **Layers**
  - Same layer/bar - full conduction
  - Same bar/neighboring layers – reduced conduction
  - Different bar|non-neighboring layers – no conduction



Particle Reactions – General Chemistry Mechanism

$$A \rightarrow 0.5B + 0.5CH_4 \qquad \omega = f \exp\left(-\frac{E_a}{RT}\right)$$

- Decomposition reaction
  - Arrhenius form
    - ω(T)
    - T changes due to thermal coupling to background fluid/neighboring particles
  - Solid + gas phase products
    - ex: B/CH_4
  - CH_4 (gas) combustion – post production
  - More complex forms available

Fuego input section

```
BEGIN PARTICLE DEFINITION solid_particles
    USE PARTICLE SPECIES = A B C D E
    PARTICLE TYPE IS GENERALIZED_PARTICLE
    USE SPECIES MATERIAL materialA for A
    USE SPECIES MATERIAL materialB for B
    USE SPECIES MATERIAL materialC for C
    USE SPECIES MATERIAL materialD for D
    USE SPECIES MATERIAL materialE for E
    ADD PARTICLE INTERFACE parameterSpec
    particle is stationary
    BEGIN GENERAL CHEMISTRY reactiveMechanism
      Begin Reaction R1
        Reaction is A -> 0.5B + 0.5CH4
        Rate Function = Arrhenius A = 3.33e+15 Ea = 226140000 R = 8314.
        Concentration Function = Standard mu = A 1.0
         Heat of Reaction = 0
         Temperature Phase = LIQUID_PHASE
         Pressure    Phase = LIQUID_PHASE
       End   Reaction R1
```

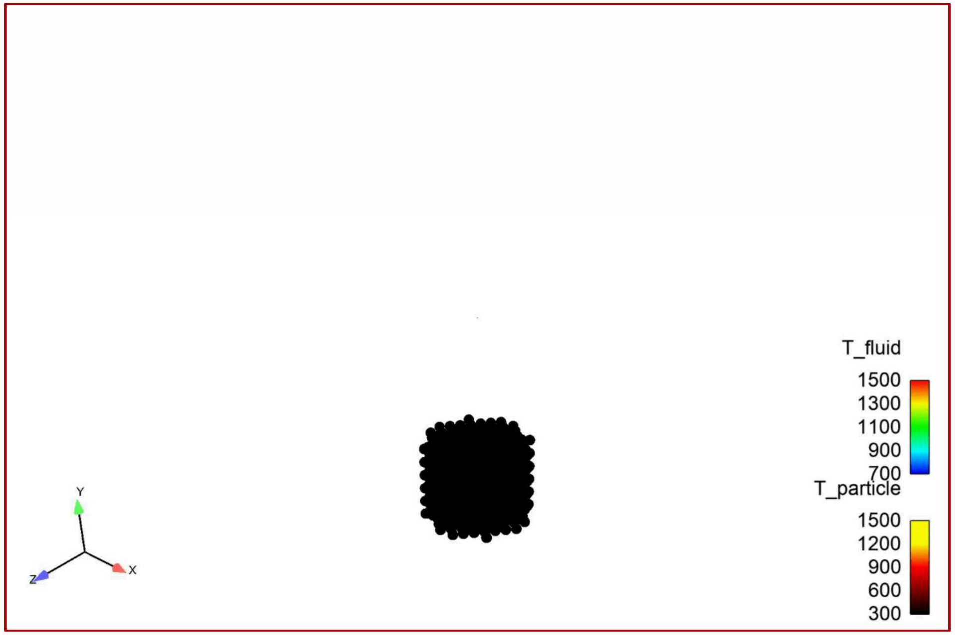
Demonstration Case 1 : Details

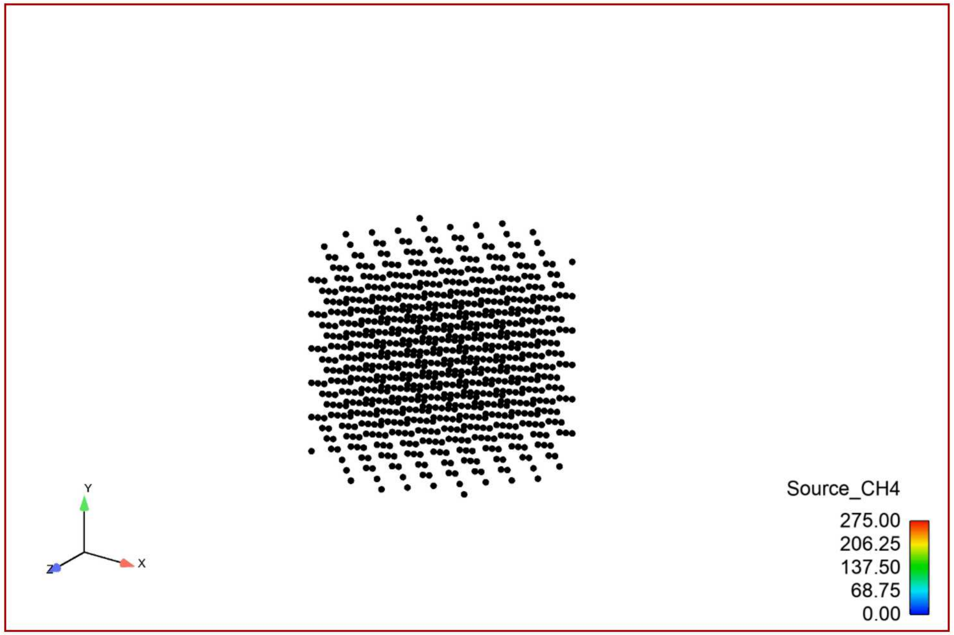
- **Simulation time**: 500s
- **BCs**:
  - 1 m/s upward inflow from inlet base (-Y) at T = 1000K
  - Side walls (and lower boundary around inlet) at T = 800K
  - upper open boundary at T = 800K
- **Particles**:
  - 886 particles of size d = 0.02m in
  - 11 layers, 2 bars
  - T_p (time = 0) = 300K

- **Particle Materials**

```
# Material Properties for species A
   BEGIN PARTICLE MATERIAL materialA
      DENSITY                 = 1779.0 # kg/m^3
      SPECIFIC_HEAT           = 866.0  # J/Kg-K
      ABSORPTIVITY            = 1.0    # no units
      EMISSION_MULTIPLIER     = 1.0    # no units
      VISCOSITY               = 100
      THERMAL_CONDUCTIVITY    = 50.0   # J/m-s-K
      FILM_PRANDTL_NUMBER     = 1.0    # no units
      SURFACE_TENSION         = 1.0e3  # J/m^2
   END   PARTICLE MATERIAL materialA
```

Demonstration Case 1: Temperatures (T_f/T_p) and CH_4 Source





Hot inflow on reacting particles.

- When $T_p \approx 800K$, particles release CH_4
- CH_4 combustion (EDC) → $T_f > 1400K$ (T_f isosurfaces shown)
- After particles release CH_4 they cool to inflow T ~ 1000K

Source of CH_4 : where particles heat up and release CH_4

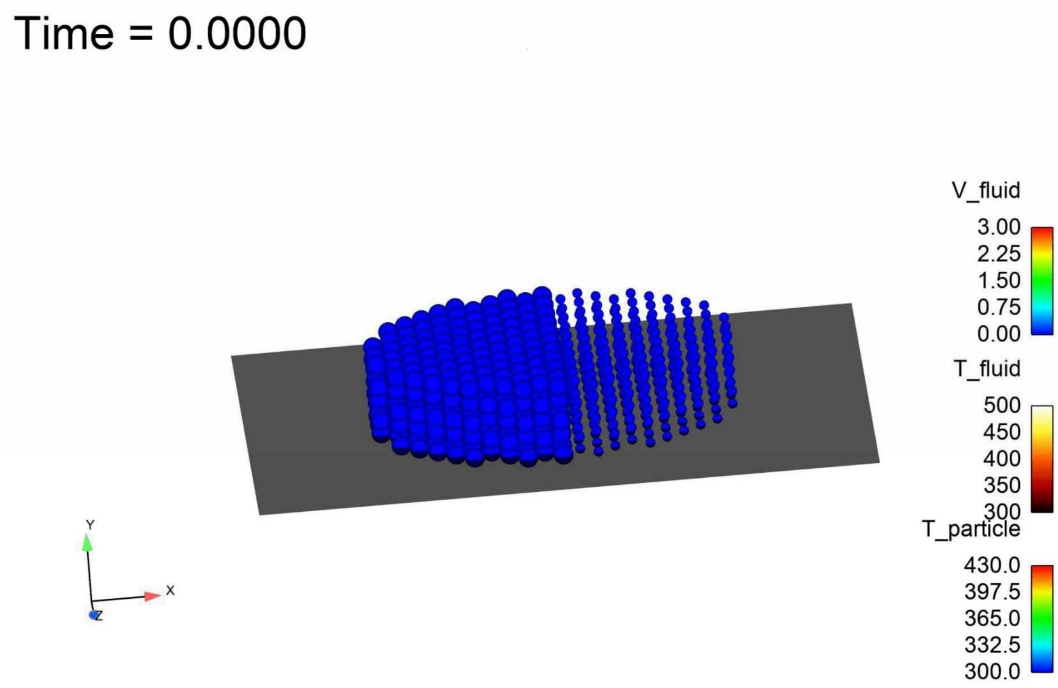
Last particles to burn out - those at center of particle pack

CH_4 source isosurfaces shown

Demonstration Case 2: Neighboring Bars w/ Layers

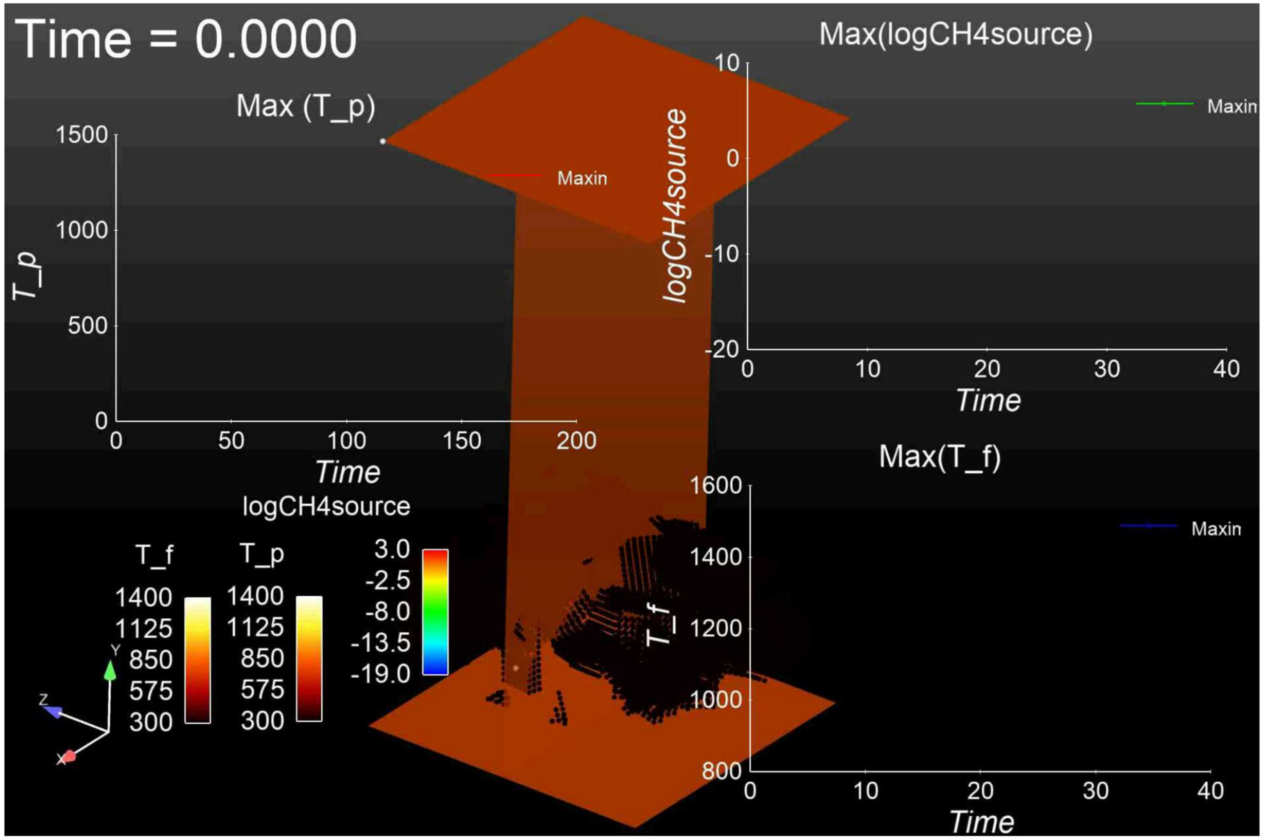
Different Conditions

- BCs:
  - Base:
    - a: V_f = 1.0 m/s (up) - square inlet at @ T = 1000K
    - b: V_f = 0.1 m/s (up) - surrounds inlet @ T = 300K
  - Sides: walls @ T = 300K
  - Top: open boundary at T = 300K
- 875 particles of size d = 0.02m in
  - 5 layers, 2 bars
  - T_p (t = 0) = 300K
- Isosurface T_f = 500K shown
- Particles heated by fluid/conduction
  - Hot particles near hot fluid
- Particles visualized with size scaled by bar#
- T_p not high enough to activate reaction for CH_4 production (as in previous case)
- t_{late} : different bars show obvious thermal non-contact



Demonstration Case 3 – Rubble Pile

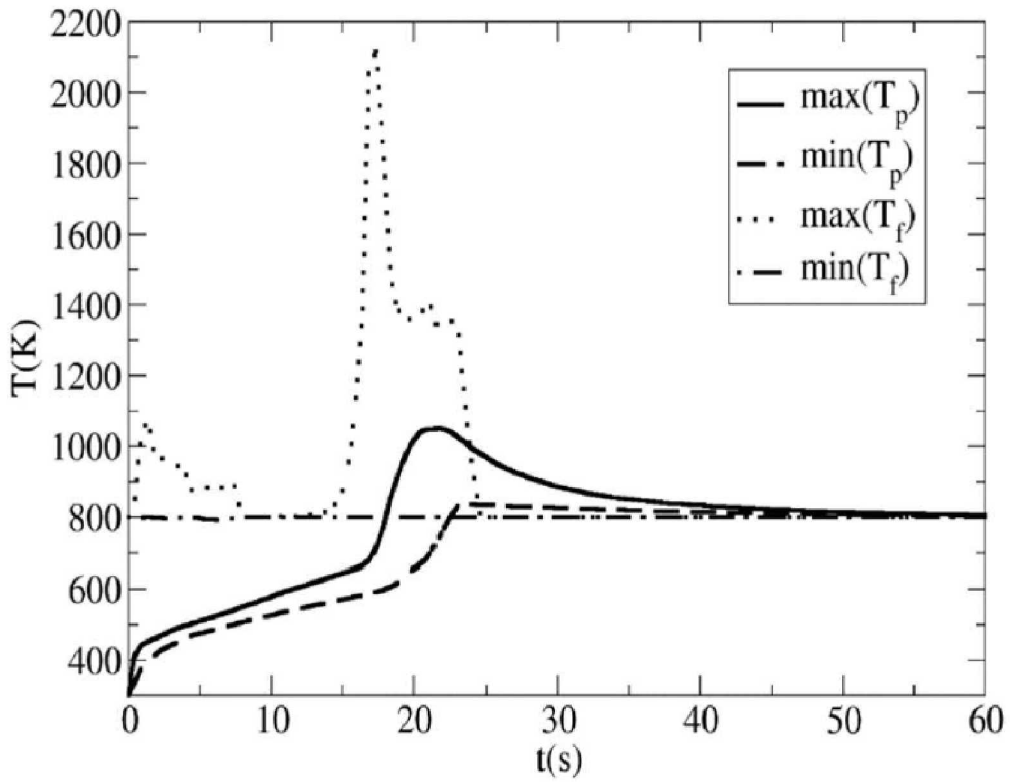
- Rubble pile configuration: Randomly placed/oriented bars - multiple layers



- T_p, T_f, CH_4 source shown vs. time
- 200s time internal

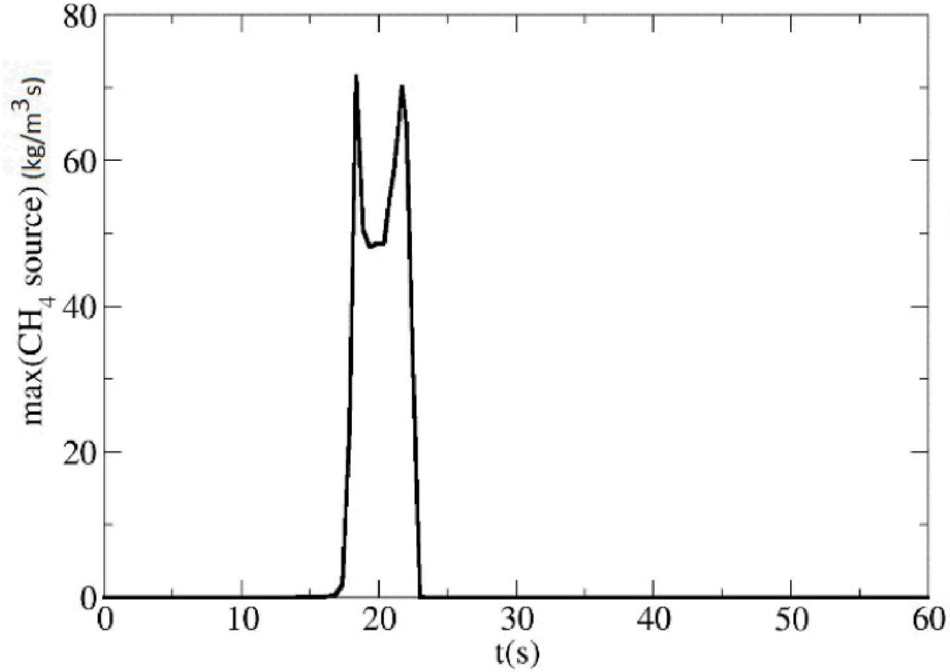
Particle/Fluid Temperature Evolution

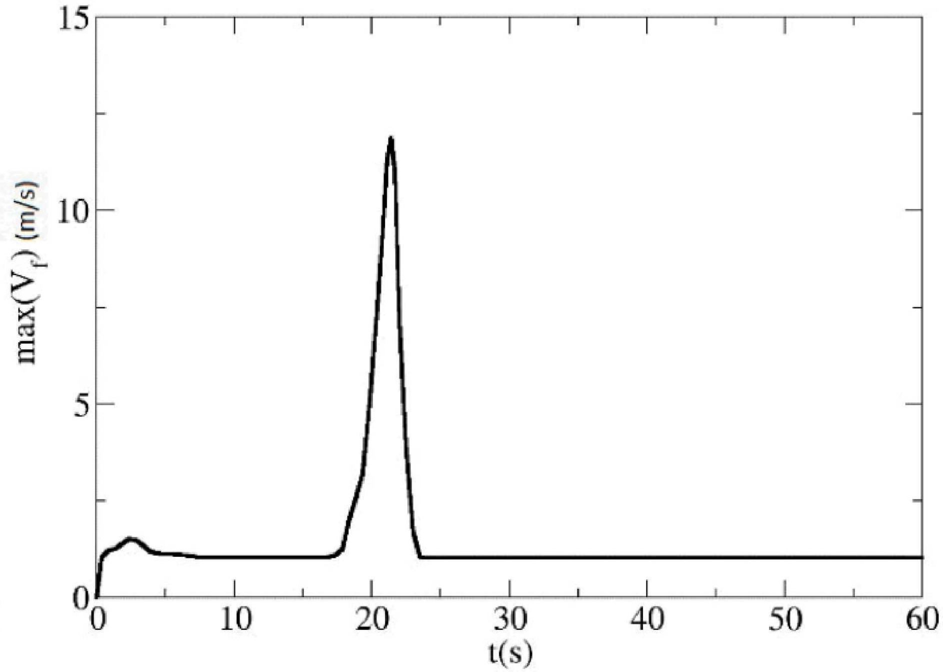
- T_p ↑ from initial (300K) due to hot inflow (800K)
- Highest T_p/T_f when CH_4 combusting
  - Climbing: 15-16s
    - T_p ~ 650K
  - Falling: 22-23s
  - T_p max lags T_f
    - Particle thermal mass
- After particle CH_4 release, particles/fluid cool to ambient
  - T_p again lags T_f – thermal mass difference



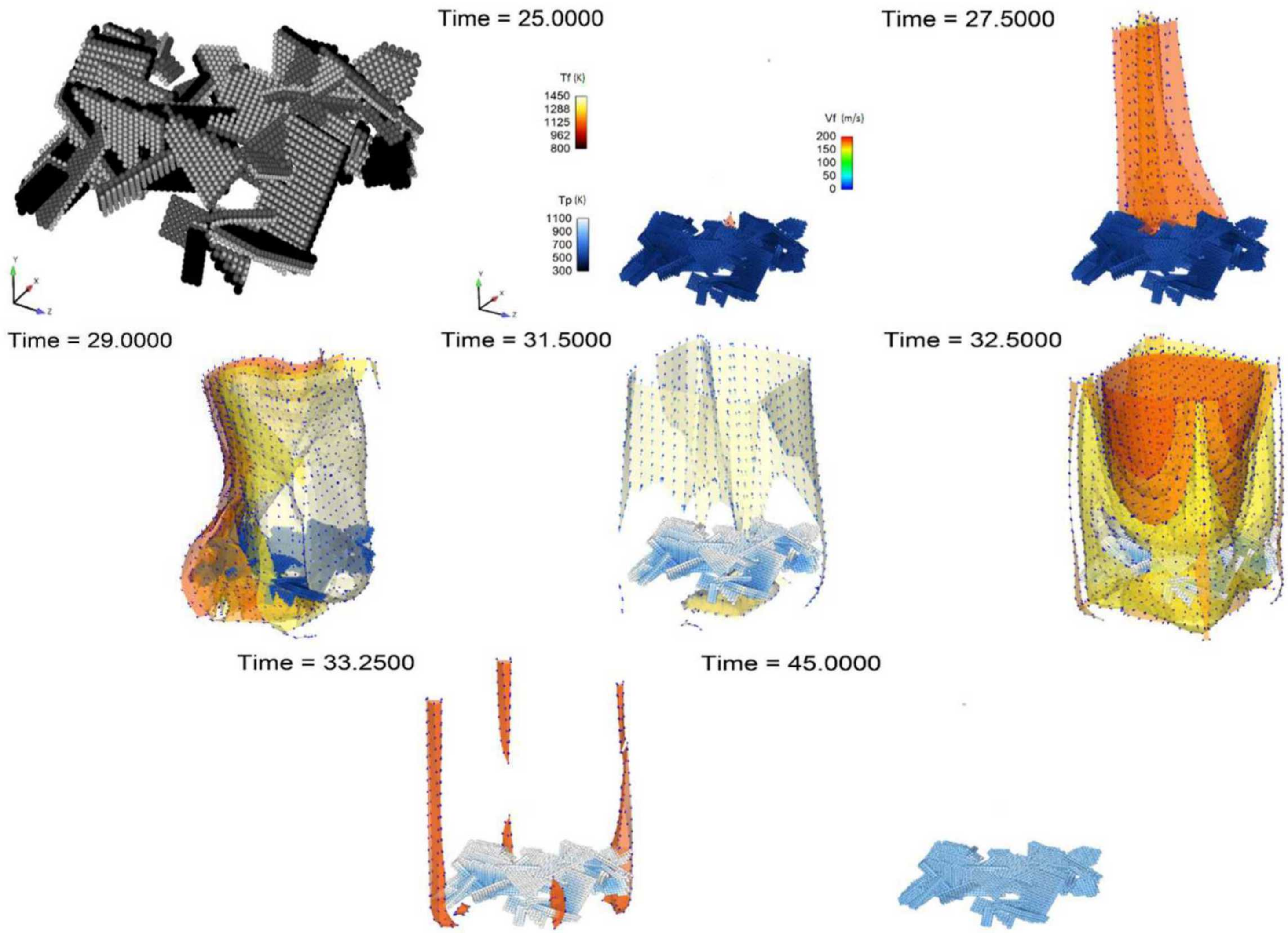
Evolution of CH_4 release rate / Fluid Velocities

- Particle CH_4 release between 16 – 23 s
- Fluid Velocity during this interval





Temporal Evolution of System

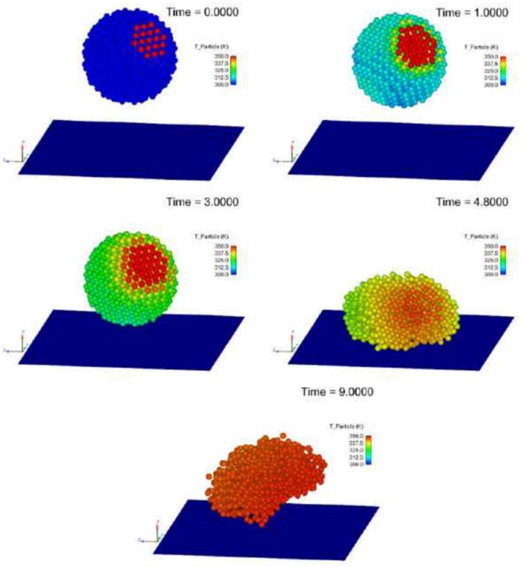


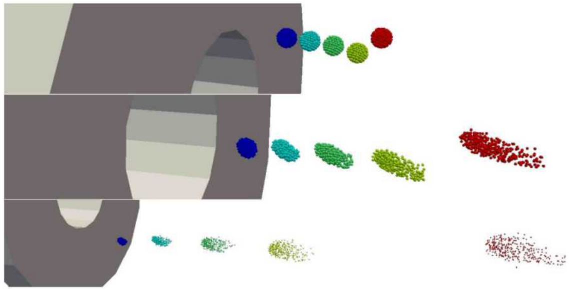
Conclusions

- Reacting/Thermally interacting particles provide effective description of solid phase combustion as seen in carbon fiber – filled expoxy composites
- Useful in context of mixed fuel fires (liquid + solid)
- Evaporating volume of fluid (VOF) capability
  - in progress
  - Can be coupled to bar/layer reacting description to address full mixed phase fuel problem
- Work remains to be done
  - Rubble geometry currently doesn’t change

For the Future

- Better Chemistry Mechanisms
  - More representative of these materials
- Sophisticated fluid/particle coupling
  - Sandia LDRD - proposal stage of Fuego/LAMMPS coupling
  - Would allow for material motion
    - Layer collapse
    - Ember lofting
    - Interaction with fluid
  - Ongoing progress – significant additions to particle/particle, particle/fluid capabilities to Fuego





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