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Computational Methods for Simulating Rocket Motor Cookoff

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

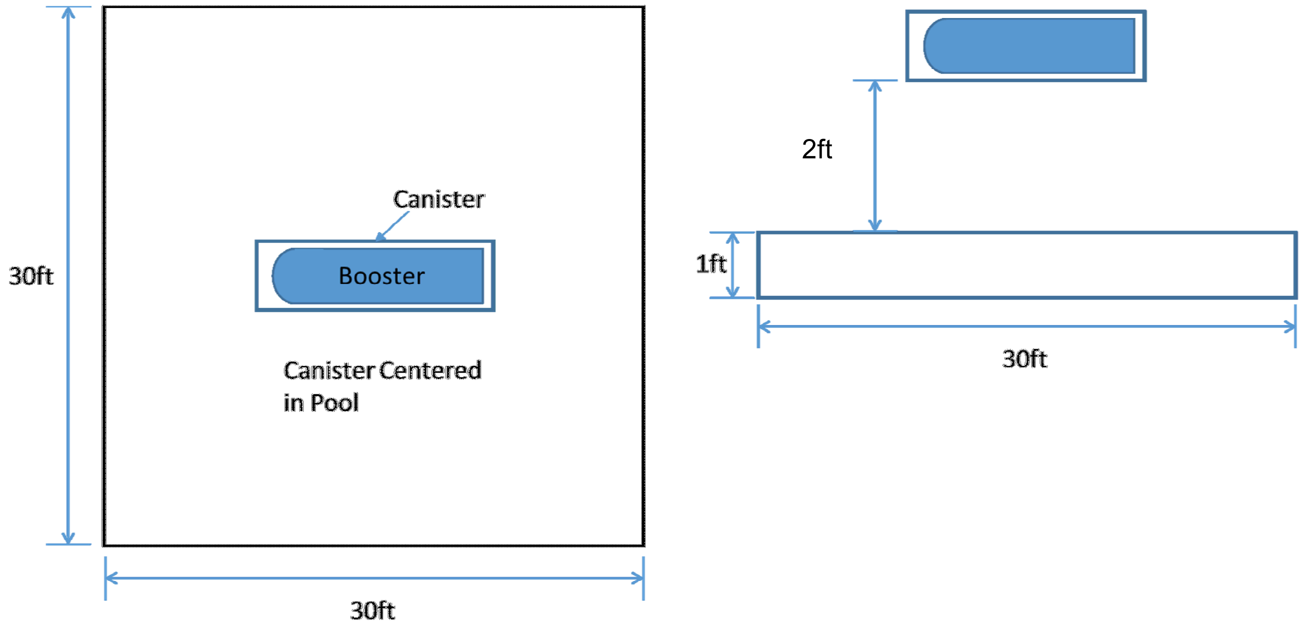
- Introduction
  - Why we are simulating this scenario?
  - Scenario of interest
- Approach
  - SIERRA simulation tools
  - Conjugate modeling capabilities
  - Simulation Matrix
- Results and Discussion
  - Fire simulation results
  - Heat transport simulation

Why this scenario?

- The fast cookoff of a rocket motor contributes to the transportation safety case
  - Is a requirement for transportation approval
- A booster motor was exposed to an engulfing fire
  - This environment is hard to instrument
  - Models can help deduce the reason for test behavior
- The scenario is being modeled by NSWCDD, Sandia to create a physical model of the event
  - Can help interpret the data
  - Useful for assessing other configurations without resorting to expensive experimentation

The Scenario

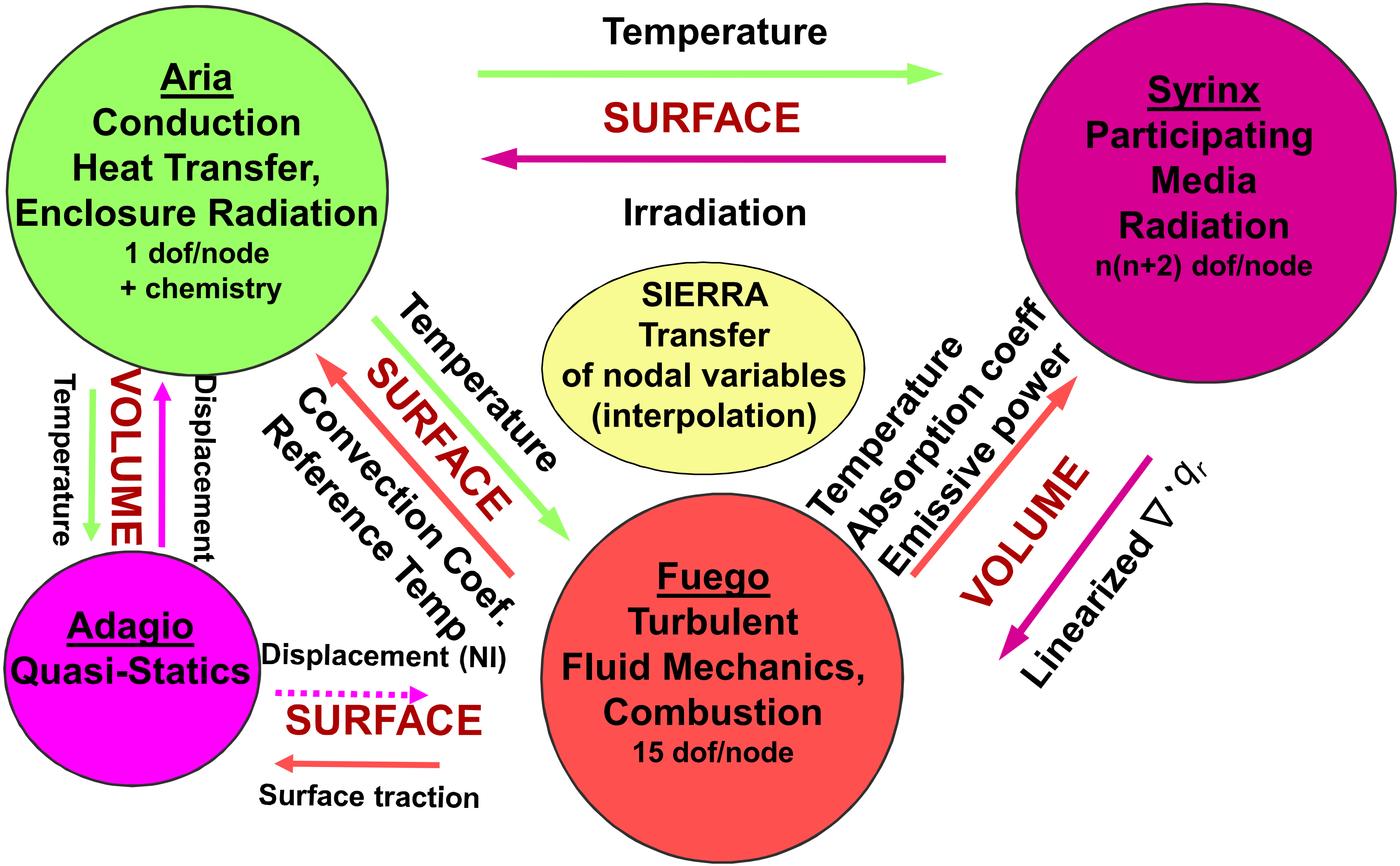
- The booster canister with munition was located 2 feet above a 30’ x 30’ kerosene fuel pool, engulfed for 15 minutes
- Booster propellant is simulated with a kinetic function
  - Failure (run-away) criterion was dT/dt > 30ºC/sec
- Canister is mostly carbon-fiber/epoxy, a complicating factor
  - Thermal conductivity varies by about x40, directionally dependent



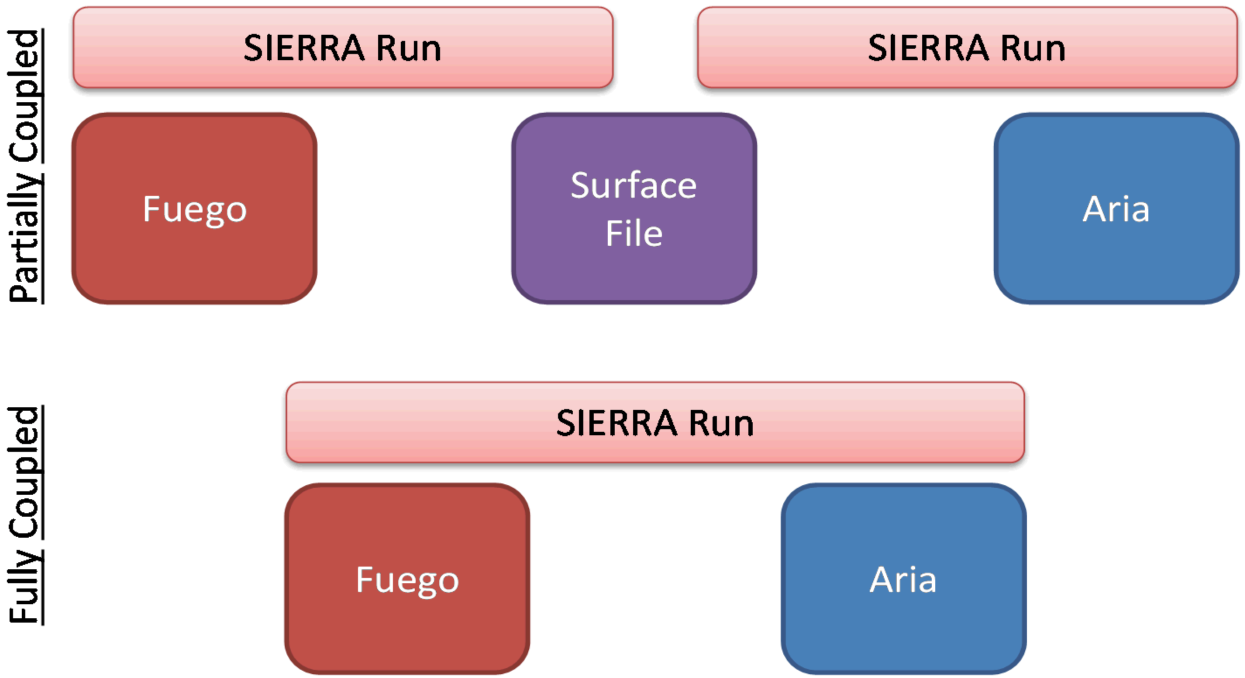
Approach

- SIERRA is an architecture for massively parallel simulations for simulating a variety of engineering problems
  - Many modules couple between each other for complex environment predictions
- SIERRA/Fluid Mechanics modules enable conjugate heat transfer simulations for fire environments
  - SIERRA/Aria primarily simulates conductive heat transport in solids
  - SIERRA/Fuego simulates fire environments
  - Recent code development enables simulating burning composite materials
- Large-scale fire environments are challenging to simulate for 15 minutes
  - Utilize DOE supercomputing resources to produce environment simulations
  - Develop best model for thermal response of the motor and container
- A minor parametric study was also included in the study
  - Mesh refinements to understand solution convergence
  - Various heat transfer model methods for the cavity between the booster and canister

SIERRA Enables Coupling (example)

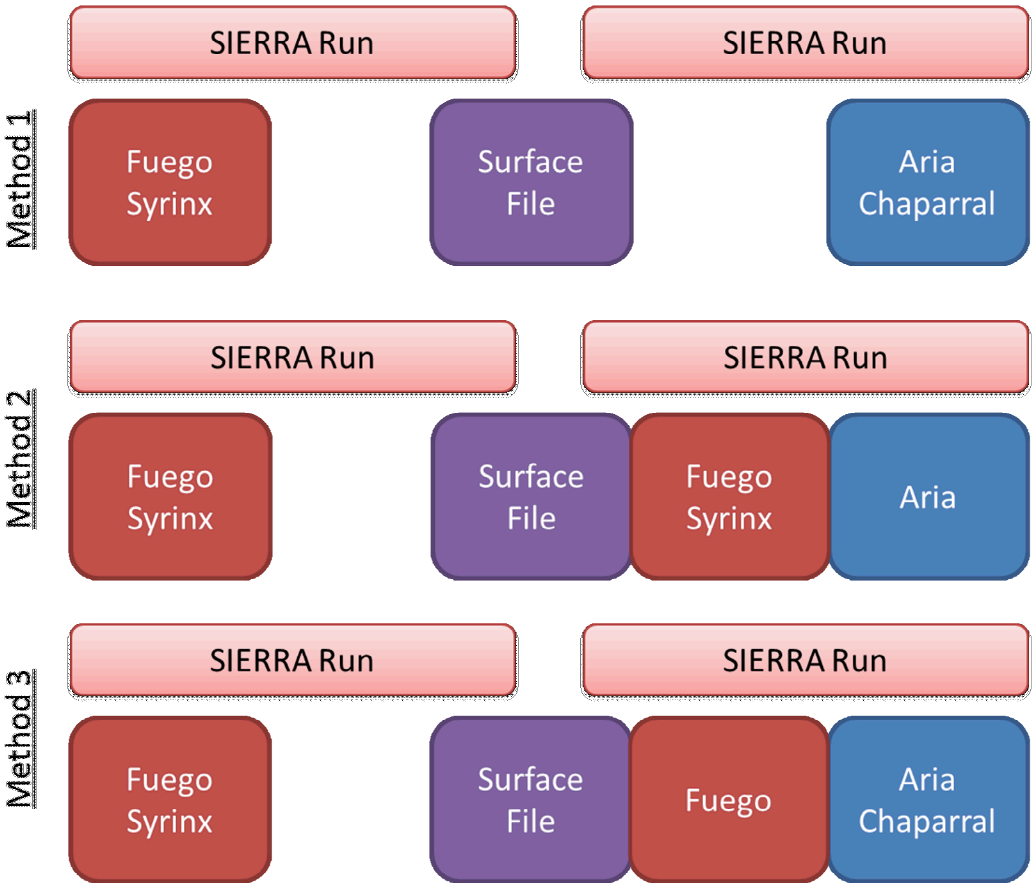


Partial and full coupling



- Full coupling in this case is computationally impractical
  - Simulations take too long
- Partially coupled scenarios leverage the steady-state nature of the fire condition to enable 15 minutes of computation

Partial coupling methods (this study)



- Three methods were used for simulating the event
  - Method 1 uses Aria convection and radiation
  - Method 2 uses Fuego convection and radiation
  - Method 3 uses Aria radiation, Fuego convection
- Comparisons help elucidate model sensitivities to cavity radiation and convection models

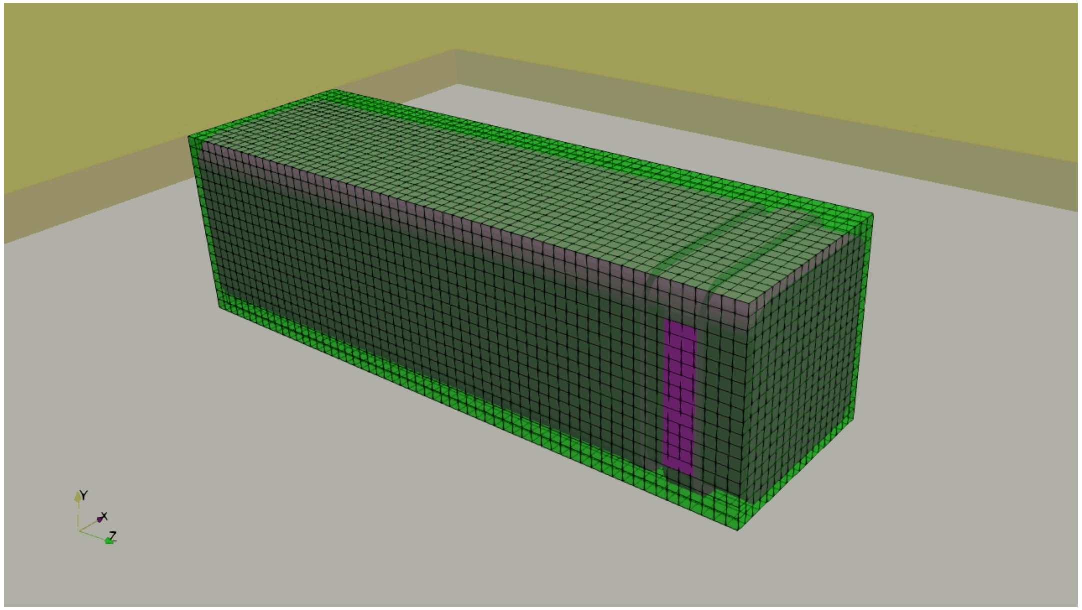
Simulation Matrix

- Seven simulations constitute the simulation matrix for this exercise
  - Fire mesh constituted three simulation variations
  - Radiation and convection methods also varied (method 1-3)
  - Chaparral is the Aria view factor radiation model
  - Syrinx is the Fuego participating media radiation model
  - Enclosure convection in Aria assumes mean cavity temperature for convection; Fuego uses CFD wall models for convection

Fire Mesh	Method	Radiation	Convection
coarse	1	Chaparral	Enclosure
medium	1	Chaparral	Enclosure
fine	1	Chaparral	Enclosure
coarse	3	Chaparral	Fuego
coarse	2	Syrinx	Fuego
medium	2	Syrinx	Fuego
fine	2	Syrinx	Fuego

Meshes

- A 'calorimeter' mesh was used for surface transfers
- Finest fire predictions used 5 cm resolution
- Internal fluid medium mesh results were nearly identical to coarse meshes (results omitted)
- Nominal Aria mesh not varied

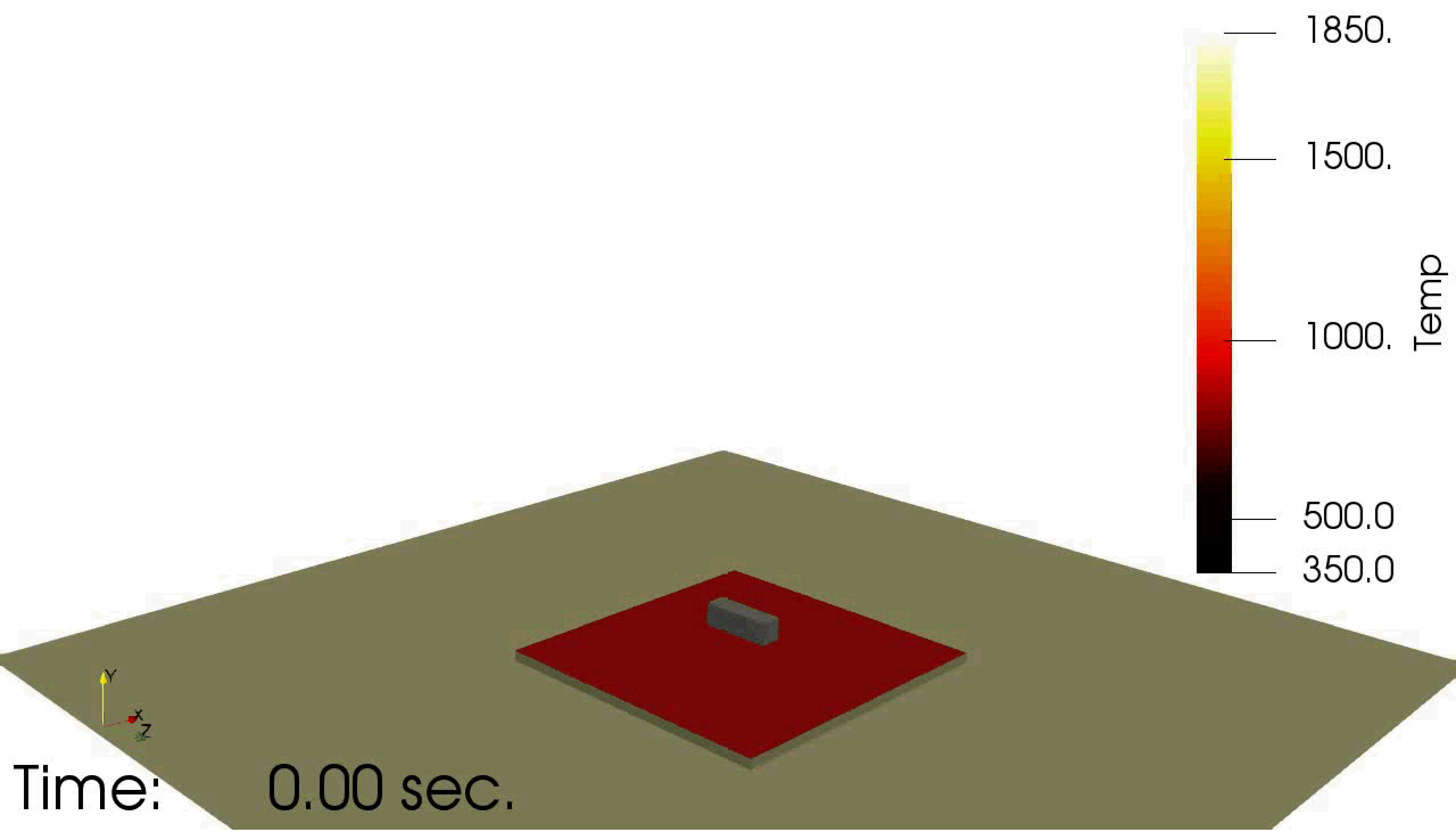


Mesh	Code	Nodes	Nominal Size (m)
fluid fine	Fuego/Syrinx	8,202,852	0.05
fluid med	Fuego/Syrinx	3,151,882	0.075
fluid coarse	Fuego/Syrinx	1,663,116	0.10
calorimeter fine	Fuego-conduction	71,344	0.017
calorimeter med	Fuego-conduction	22,021	0.025
canister and booster	Aria	815,564	-
internal fluid coarse	Fuego/Syrinx	66,604	0.02
internal fluid med	Fuego/Syrinx	493,429	0.01

Selected Model Parameters

- Fire reactions with EDC (Magnussen et al.)
- Turbulence with TFNS (Tieszen et al.)
- Directional conduction with a conductivity tensor through composites
- Composite did not off-gas to the fire or to the cavity
  - Fire was otherwise nearly steady-state
  - Fully transparent cavity
- Fuel pool modeled with a constant fuel velocity
  - We have a 1D pool model that predicts the burn rate in response to thermal feedback from the fire that was not used
- Discrete Ordinates PMR solver, quadrature order 4

Fine Fire Simulation Video



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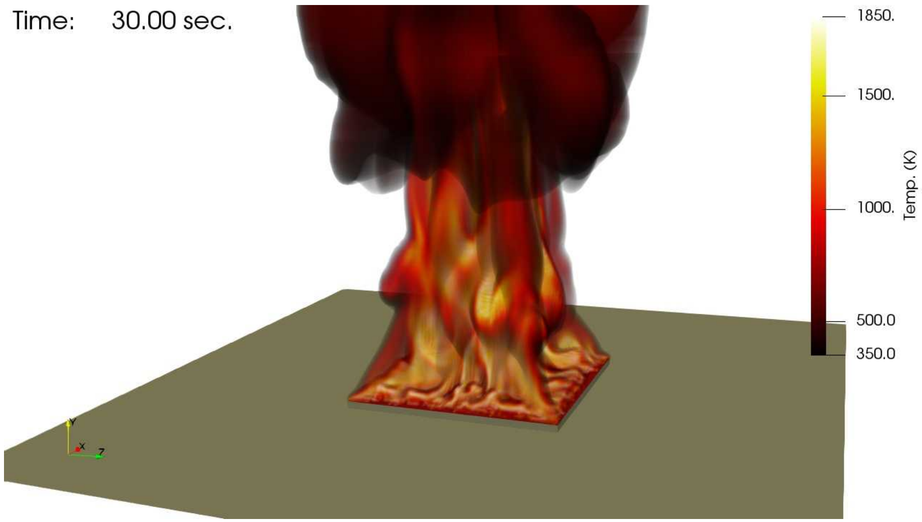
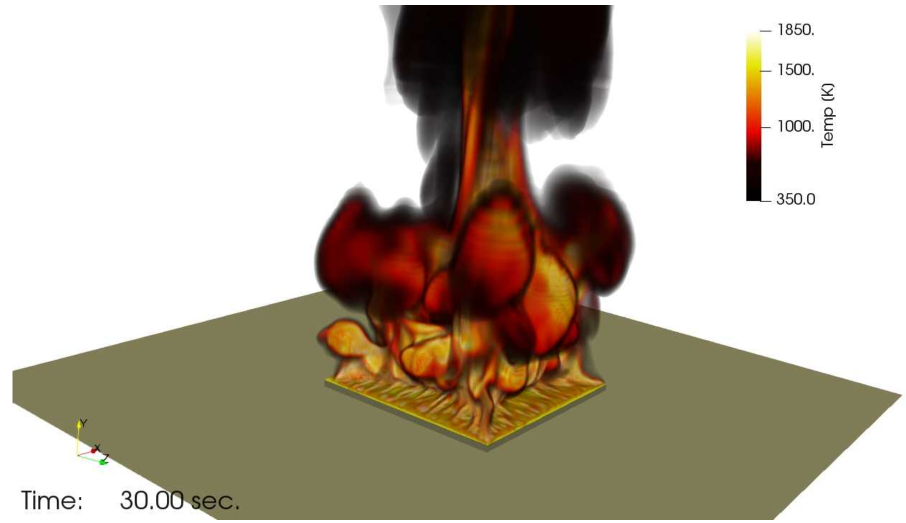
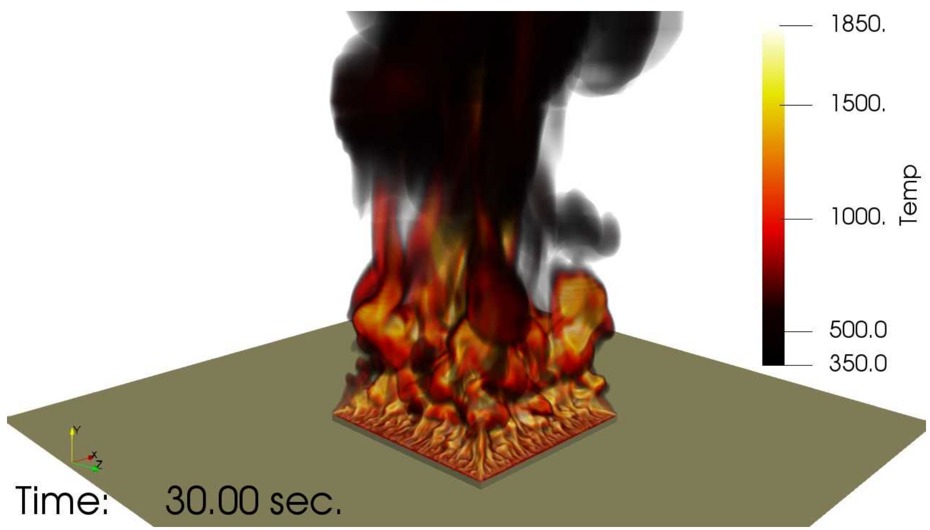
Fire Resolution Comparison



Coarse

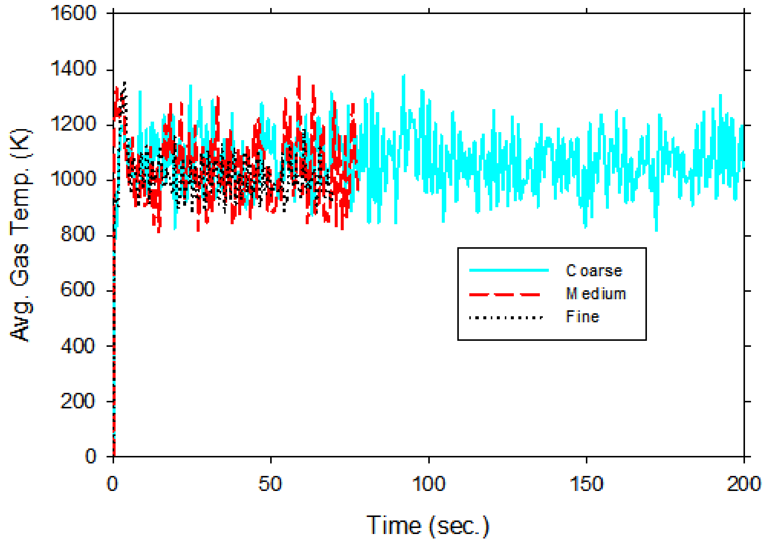


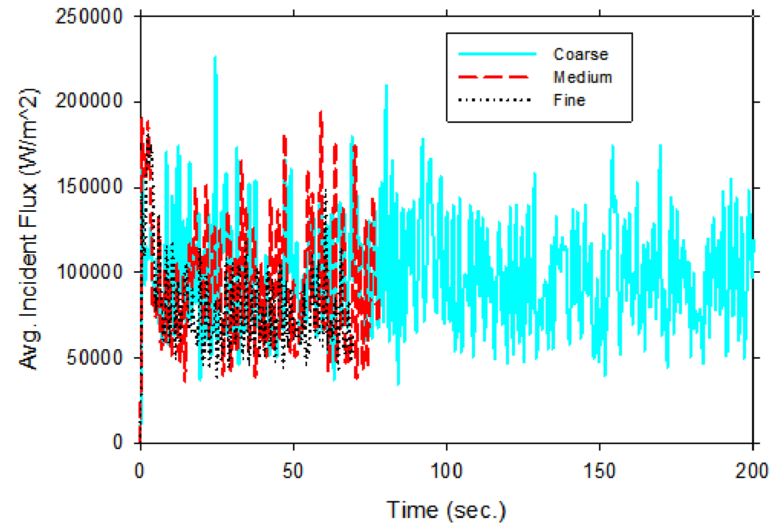
Medium

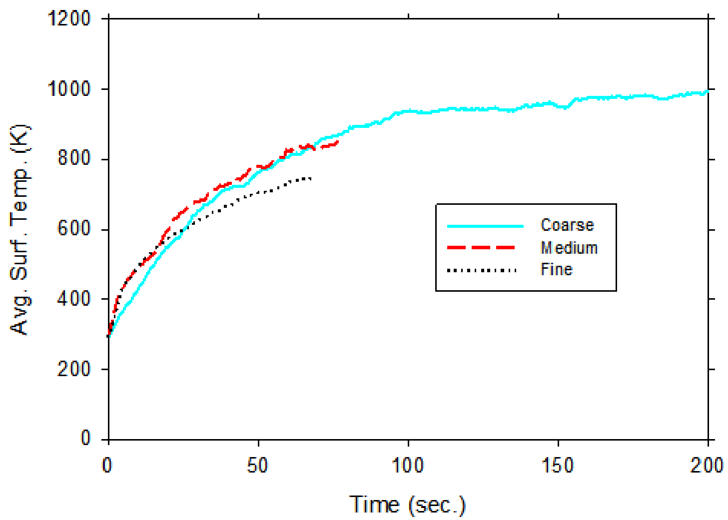


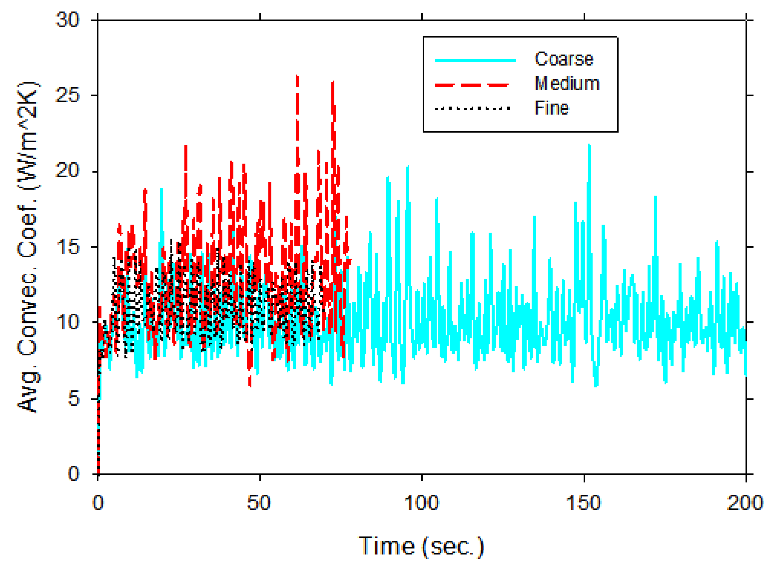
Fine

Fire Environment Convergence







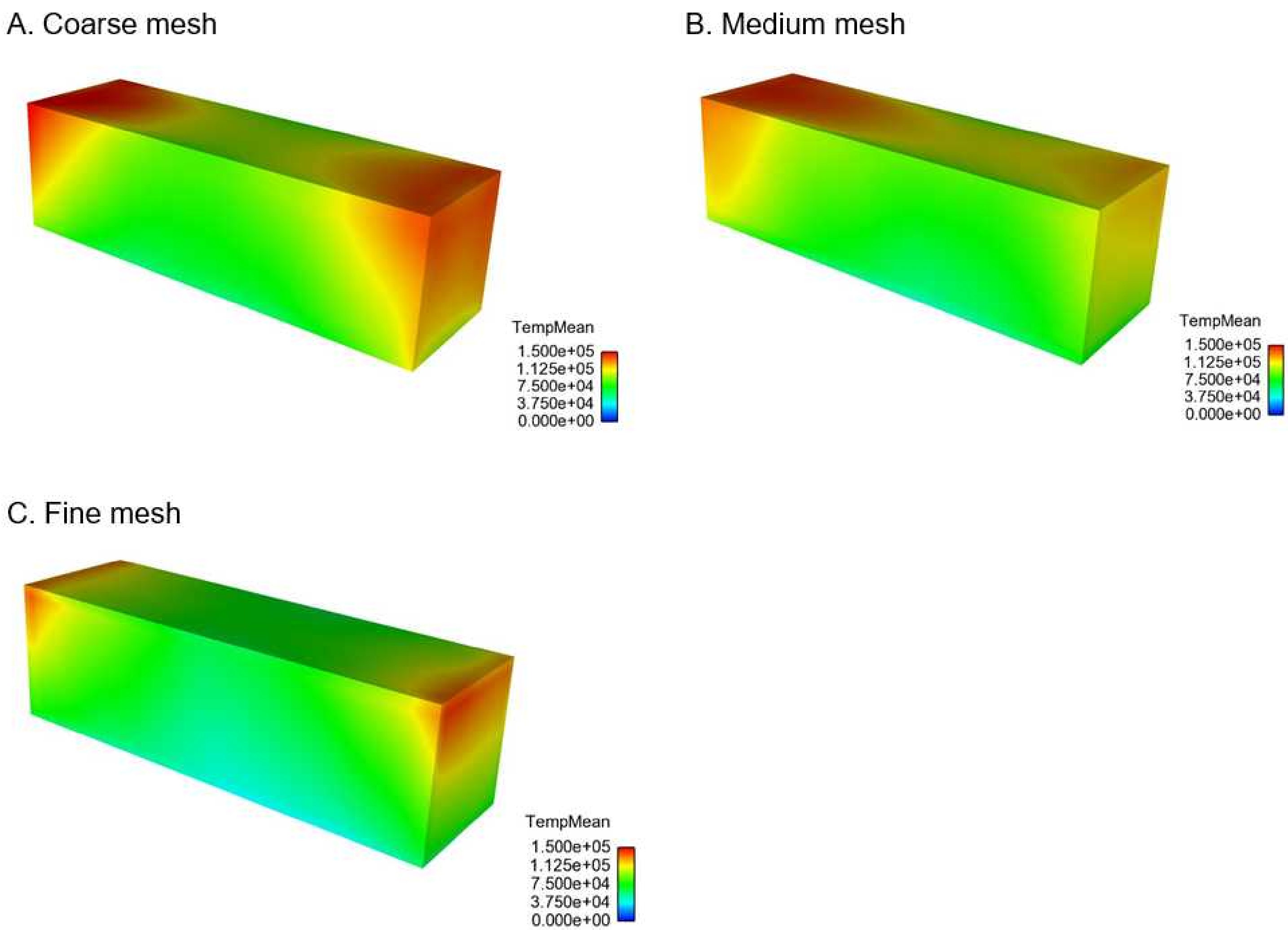


30 sec.+ Means

- Coarse/Medium suggest convergence
- Medium/Fine comparison is curiously less similar
  - Would have done further refinement, but time/resource did not permit
- Mesh resolution expected to be a significant factor in thermal results

Mesh	Convection Coefficient	Incident Flux	Gas Temperature
Unit	*W/(m²K)*	*W/m²*	*K*
coarse	10.05	95,415	1062
medium	13.22	91,349	1036
fine	10.98	73,635	997

Some Asymmetry in Mean Flux

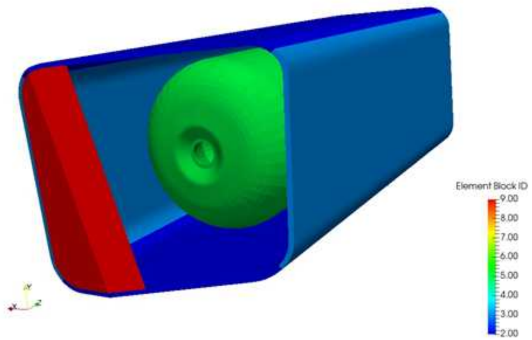


Suggests potential benefit of increased run time for medium/fine cases

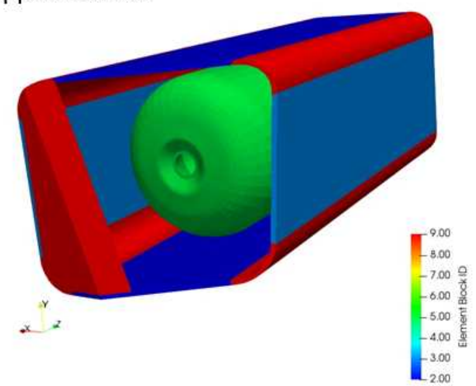
Composite Model

- Targeted mesh preparation was key to an appropriate continuous model of the composite surface

A. Parallel plate approximation



B. Flat plate and cylindrical section approximation



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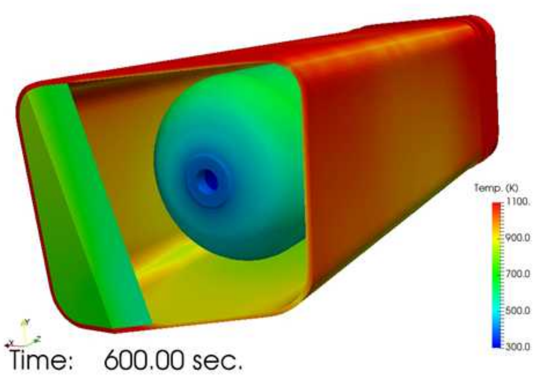
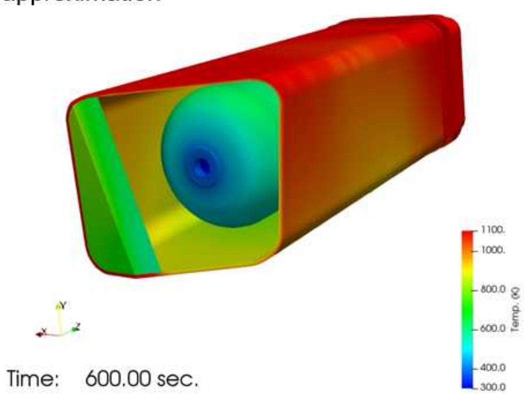


B. Flat plate and cylindrical section approximation



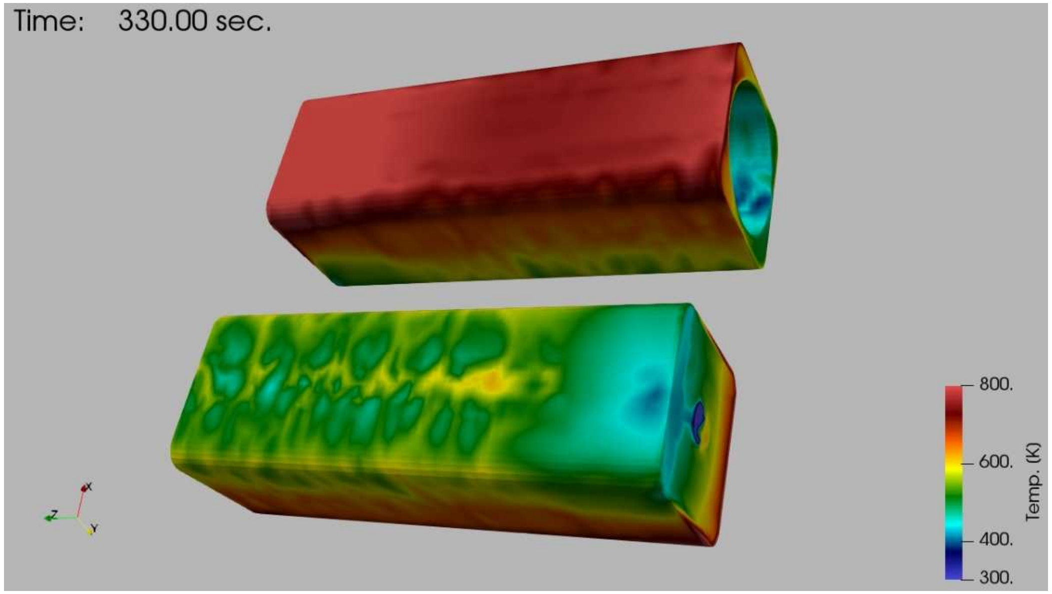
Thermal Race Results

- As suspected, Fine Fire Mesh is significantly slower for run-away than coarse and medium
- Compare coarse method 2 to method 3
  - Substantial effect of radiation model
- Compare coarse method 3 to method 1
  - Relatively large effect of convection approximation

Fire Mesh	Method	Rad.	Conv.	Run-away Time (s)	Avg. Enclosure Temp. (K)
coarse	1	Chap.	Encl.	672	774
medium	1	Chap.	Encl.	696	772
fine	1	Chap.	Encl.	813	739
coarse	3	Chap.	Fuego	814	791
coarse	2	Syr.	Fuego	687	755
medium	2	Syr.	Fuego	730	757
fine	2	Syr.	Fuego	868	726

Mean Convection Temperature

- The mean convection temperature approximation appears to be fairly crude
  - Notice the significant variation in surface temperatures in the below figure
- Fluid region open boundary condition needs to be reconsidered, likely contributing to convection differences



Path Forward

- Look at resolving or better understanding the convergence issue
- The cavity will likely be filled with soot
  - Need to develop modeling methods for this
- Sensitivity study around additional parameters
  - Heat transfer properties
  - Geometry
  - Kinetics
- Improve boundary conditions for cavity
- Quantitative comparisons with data

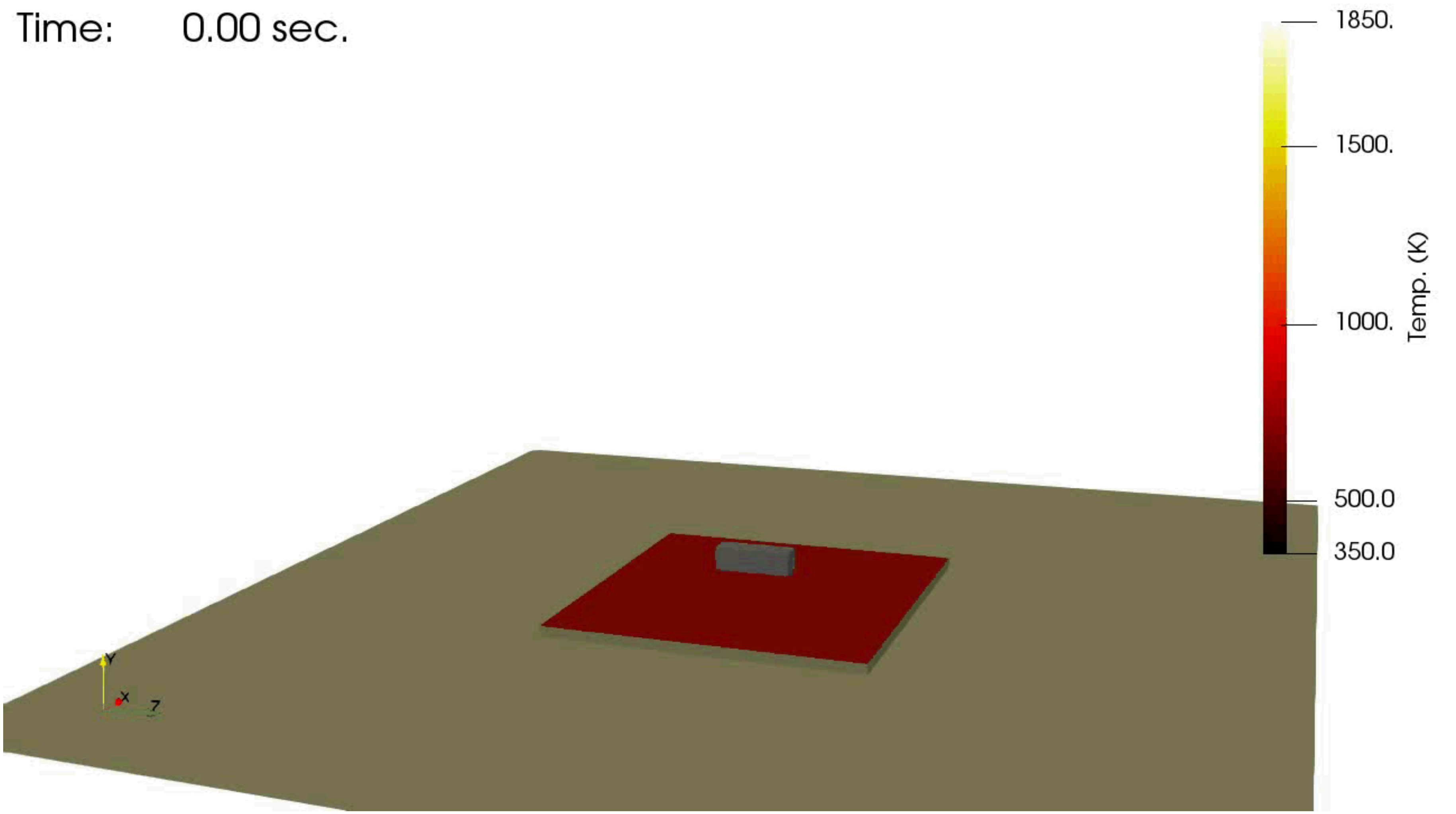
Summary

- A simulation exercise was performed to model thermal run-away for a cookoff scenario
- Methods utilize conjugate capabilities in SIERRA simulation tools
- Fire model mesh convergence was not particularly good
- Effect of convection and radiation approximations was relatively high
- These factors contribute to the uncertainty in the predicted behavior of a rocket motor exposed to fire conditions

Acknowledgements

- Heeseok Koo helped debug some input deck issues to enable this study
- The SIERRA/Fuego development team

Coarse Video



Medium Video