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# FY17 ASC L2 Milestone 6010: Demonstration of Effective Coupling between the SIERRA Low-Mach Module Fuego and the RAMSES Boltzmann Transport (Particle and Radiation) Code SCEPTRE

## Executive Summary

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### Introduction

This milestone campaign was focused on coupling Sandia physics codes SIERRA low Mach module Fuego and RAMSES Boltzmann transport code Sceptre(Scefire). Fuego enables simulation of low Mach, turbulent, reacting, particle laden flows on unstructured meshes using CVFEM for abnormal thermal environments throughout SNL and the larger national security community. Sceptre provides simulation for photon, neutron, and charged particle transport on unstructured meshes using Discontinuous Galerkin for radiation effects calculations at SNL and elsewhere. Coupling these ”best of breed” codes enables efficient modeling of thermal/fluid environments with radiation transport, including fires (pool, propellant, composite) as well as those with directed radiant fluxes. We seek to improve the experience of Fuego users who require radiation transport capabilities in two ways. The first is performance. We achieve this through leveraging additional computational resources for Scefire, reducing calculation times while leaving unaffected resources for fluid physics. This approach is new to Fuego, which previously utilized the same resources for both fluid and radiation solutions. The second improvement enables new radiation capabilities, including spectral (banded) radiation, beam boundary sources, and alternate radiation solvers (i.e. Pn). This summary provides an overview of these achievements.

### Milestone Description

As written in the ASC Implementation Plan, the milestone description is as follows:

The goal of this milestone is to demonstrate effective coupling between the Sierra low-Mach module Fuego and the RAMSES Boltzmann transport (particle and radiation) code Sceptre. This coupling is motivated by a variety of applications in which both fluid mechanics and participating media thermal radiation are significant contributors. To this end, coupling is achieved through the MPMD (multiple program, multiple data) methodology using an MPI split communicator. This approach alleviates the need to wrap all physics capabilities within the same executable. Distinct executables for each code do not require a consistent set of libraries, only an agreed upon pattern of communication and set of transferred data. This milestone will address both the feasibility of such a coupling through performance and scaling (weak and strong) and the additional physics capabilities that are made available through the coupling. A sample of problems of interest will be used to demonstrate both scaling and new physics capabilities.

### Impact Statement

We successfully demonstrated MPMD coupled Fuego/Scefire for each of 8 demonstration case’s specific needs, including both legacy and new capabilities. We also showed that additional resources can be leveraged to reduce radiation/fluid computation times when specific physics costs dominate. Finally, weak scaling for Fuego/Scefire was found to be on par or better than the current Fuego/Syrinx coupling.

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**Summary of Work Done**

MPMD methods were chosen for Fuego/Scefire coupling. Inter-program communication occurs through mostly sparse MPI calls. Programs do not require identical libraries (Trilinos, Nemesis, etc.) other than MPI. Both Fuego and Scefire required changes to communicate source terms needed by the other code. We developed a generalized MPMD library enabling coupled codes to geometrically determine the inter-processor communication pattern. Each code calculates source terms then communicates these to the other program. User execution of a Fuego/Scefire is instantiated as:

```
mpirun -n 8 fuego -i fuego.i : -n 16 scefire scefire.xml
```

Fuego/Scefire run on distinct processors. The order of executables in the above example is reversible. To demonstrate Fuego/Scefire coupling, we selected eight scenarios exercising a variety of physics. The first is an L-shaped domain with isotropic absorption and fixed wall/volume temperatures where comparison with our legacy PMR code (SIERRA Syrinx) was possible. The second is a complex DOE beaker fire. The third case added Lagrangian particles. Scenario 4 exercised isotropic scattering in a pseudo-1D domain, comparing to literature results. Case 5 demonstrated banded spectral radiation transport. Case 6 used beam boundaries for a solar furnace fire analysis. In scenario 7, we tested Spherical Harmonics for the scenario 4 domain. In the final example, we combined these capabilities for a large Aluminum propellant fire. Figure 1 is an image from scenario 8, the Aluminum propellant fire, at an intermediate time.

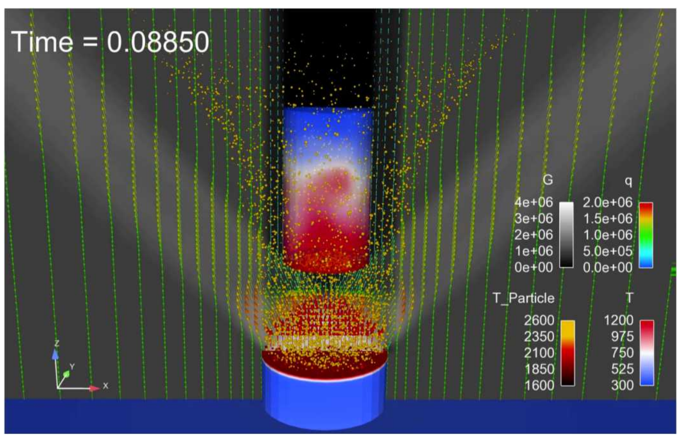


Figure 1: Scenario 8 - Al propellant fire with particle heat sources, scattering, beam boundary source, and spectral banding. Image shows evaporating/reacting Al particles birthed from lower propellant surface, shrinking during heating by chemical reaction and thermal radiation (particles colored by temperature). Cross sectional plane through propellant surface is shaded by scalar flux magnitude with radiative flux vectors shown as arrows (colored by magnitude). Side walls are colored by temperature.

**Path Forward**

As mentioned above, the successful completion of this effort has given Sandia significantly improved ability to simulate large scale, high resolution abnormal thermal environments where radiation transport plays a significant role. These improvements are twofold. The first is significant reduction of computational time for high order radiation calculations through independent selection of fluid and radiation computational resources. The second is the enabling of new capabilities made available to Fuego users including spectral radiation, directed beam sources, and alternate radiation solvers.