# Investigation on Scaling Performance and Mesh Convergence with Sandia's ASC SIERRA/Fuego code for Fire Model Predictions of Heat Flux

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***Abstract*— Performance characteristics for coupled fire/thermal response prediction simulations are investigated using coarse, medium, fine and very-fine unstructured meshes on the Red Storm/XT3. These simulations have leveraged computationally demanding mesh convergence studies to obtain detailed timings of the various phases of the computation and will be helpful in performance tuning.**

***Index Terms*— Fire Model, Parallel Performance, Mesh Convergence**

## I. Introduction

The assessment of the thermal response of a weapon system to abnormal environments, like fire, for safety qualifications is an area of active investigation at Sandia National Laboratories. Fire is a fairly common occurrence and peak flame temperatures can exceed 2300K and have an average temperature above the melting, ablation and vaporization temperature of many materials in the weapon. Historically, weapon safety qualification was based on tests at both the component and system level. However, the scenario space that could be experimentally covered is quite limited. Accordingly, one of the goals of the DOE/NNSA Advanced Strategic Computing (ASC) programs [1] is to establish models of adequate geometric and physics fidelity to supplement the experiment-based qualification approach by providing additional qualification evidence through means of modeling and simulation. One approach to modeling used separate models for the fire computations and for the heat transfer calculations. The output from the fire model simulations were one-way coupled to the heat transfer model, mapping the thermal fluxes at the different time steps using spatial and temporal interpolations [2]. Recognizing the need for higher fidelity simulations, the ASC program has funded the fire environment simulation software development project, directed at providing simulations for both open large-scale pool fires and building enclosure fires. This project is an integral part of the SIERRA[3] multi-mechanics software development project at Sandia. Fuego represents the turbulent, buoyantly driven incompressible flow, heat transfer, mass transfer, combustion, soot and absorption coefficient model portion of the simulation software. Syrinx represents the participating-media thermal radiation mechanics. Calore represents the heat transfer within an object. Domino., et.al.[4] describe the details of the governing equations, discretization, decomposition and solution procedures. The general coupling strategy for the suite of abnormal-thermal environments is provided in Figure [1]. SIERRA/Fuego, SIERRA/Syrinx, SIERRA/Calore depend heavily on the core architecture developments provided by SIERRA for massively parallel computing, solution adaptivity, and mechanics coupling on unstructured grids.

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States National Nuclear Security Administration and the Department of Energy under contract DE-AC04-94AL85000.

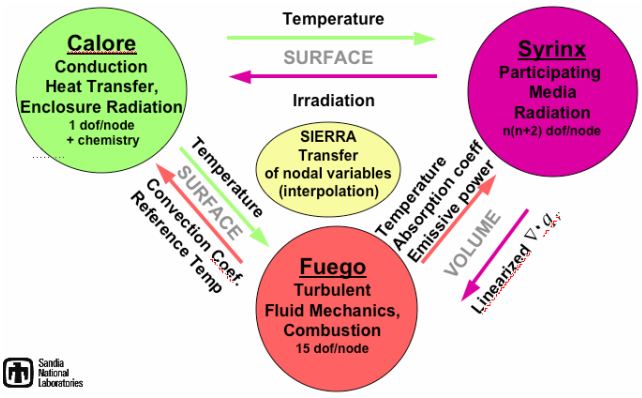


**Figure 1. Abnormal-thermal coupling strategy.**

Figure [2] shows an image from a parallel volume rendering of a 150 Million degrees of freedom cross-wind fire simulation using Fuego on 2048 processors of the Red Storm. This simulation was part of a qualification test plan for system testing to be conducted at the new Sandia's Thermal Test Complex Cross Wind Test Facility. This was one of the biggest fire simulations conducted to show case the capability class simulations needed at Sandia and the capability of the Fuego analysis package.

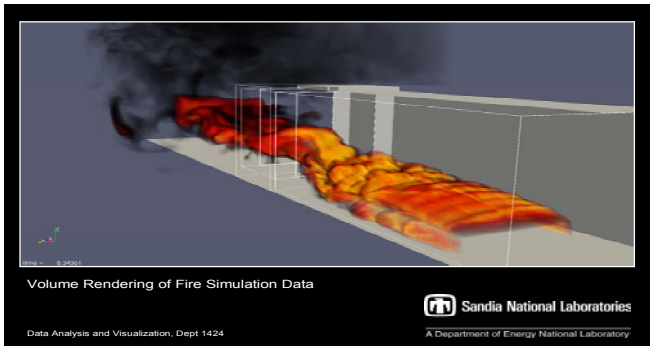


**Figure 2. Volume rendering of Fuego fire simulation data**

## II. The Model

In the application chosen for this paper, coupled fire/thermal response predictions for a weapon-like calorimeter is validated for a quiescent fire representative of a transportation accident scenario. The model constructed was used to compare numerical predictions against experimental data. Temperature measurements were used to validate the coupled Fuego/Syrinx/Calore predictions. The model consists of fluids (Fuego), radiation (Syrinx) and object heat transfer (Calore) meshes along with an output mesh. The main Fuego fluid mesh was constructed in three different sizes on the order of 500K, 1M and 2M nodes to investigate mesh convergence as part of a formal V&V solution verification study. Similar mesh sizes were used in the Syrinx radiation calculations. The Calore mesh size is much smaller, an issue that will be addressed later in this paper, and contains only the outer shell of the object. The output mesh is a vertical slice through the centerline of the fire that is only one cell thick. The simulations solve the governing set of complex coupled equations whose solution over a broad range of time and length scales is sought. This complexity in the model and the long run times to resolve the fire for 60-90 seconds could only be carried out on massively-parallel capability class supercomputers. These simulations were routinely conducted on the Red Storm computer. Figure 3 shows a cross section of the coarse mesh along the centerline of the FLAME burner and calorimeter geometry with instantaneous temperature contours overlaid.

## III. Mesh Convergence Investigation

A mesh convergence study using coarse (599K nodes), medium (1.1M nodes) and fine (2.4M nodes) meshes for the Fuego/Syrinx calculations was conducted. The Calore mesh (18K nodes) and the output mesh (43K nodes) sizes were held fixed. All three mesh calculations were run on Red Storm for 30 seconds of simulation time. The coarse mesh required ~3 days of computing time using 256 processors, the medium mesh required ~7 days using 512 processors and fine mesh required ~15 days using 1024 processors. All three mesh calculations required job restarts due to system down time. The output data generated per case ranged from 10-50 Gbytes. The output data was transferred to the Feynman visualization cluster using parallel data transfers.

The numerical results (coarse, medium and fine) used a time-filtered Navier Stokes (TFNS) turbulence treatment [5] which produces a time varying solution. The TFNS results were time averaged over the 10-30 second interval in order to produce average vertical velocities.

Figure 4 shows a comparison of the vertical velocity versus elevation for the three mesh results. The vertical distance shown is along the centerline between the burner surface and the base of the calorimeter. All three mesh results show similar values up to 2.8 m and reach peak velocity values at the same vertical location (3.31 m).

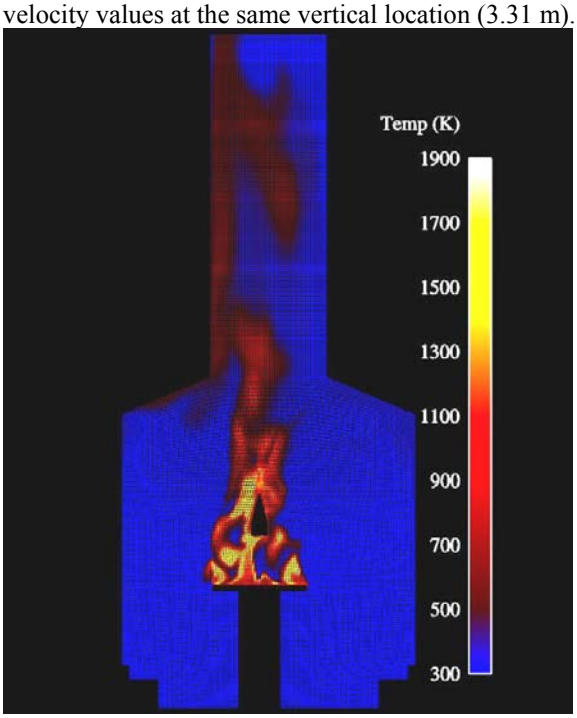


**Figure 3. FLAME Facility – Coarse Mesh Along the Burner Centerline with Temperature (K) Contours Overlaid**

Beyond a distance of 2.8 m, the coarse mesh result and medium mesh result are very similar and only differ by up to 8%; whereas, the fine mesh result differs by up to 25% in vertical velocity. As the mesh is refined, previous validation studies have shown that fine-scale turbulent features are better resolved [5]. Without the fine mesh result, which was only possible because of the availability of large computing resources, the numerical solution may have appeared to be converging. A finer mesh result is still necessary to confirm the grid independence of the solution but this will require substantially more computational resources and execution time.

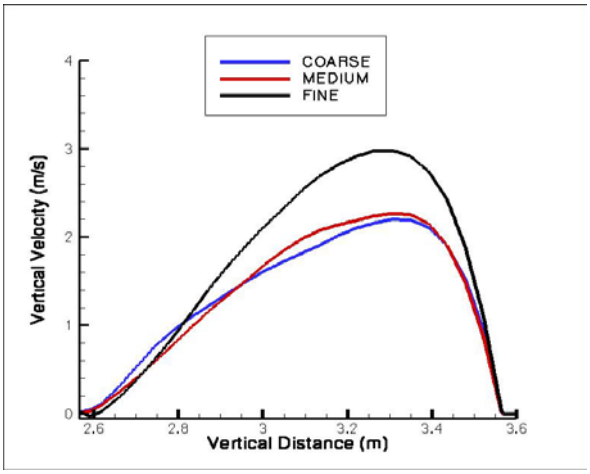


**Figure 3. Comparison of Three Mesh Results for Average Vertical Velocity along the Burner Centerline**

## IV. Performance Scaling Analysis

Ever since the seminal paper of Gustafson, et.al[6], when evaluating performance of applications on massively parallel computers, scaled speedup is often measured , This measure of scalability also referred to as 'weak scaling' minimizes the impact of the non-parallel portion of an application by linearly increasing the computational load as a function of the number of processors. Most fire simulations with Fuego use complex unstructured meshes for the targeted analysis and it is not practical to adapt such meshes to a weak scaling study. However, we have leveraged the availability of four different meshes, coarse, medium, fine, very-fine meshes used for mesh convergence studies, to evaluate the parallel performance of Fuego. For each mesh a 'strong scaling' analysis is undertaken by decomposing each mesh on increasing number of processors till no improvement in execution time is observed.

Fuego is an implicit multi-mechanics code. The model consists of three regions, Fuego, Syrinx, Calore regions with meshes defined for each region in addition to a mesh for the output. The output mesh is usually a simple plane mesh for tracking physical variables that may be compared to an experimental setup. The SIERRA framework code for each region manages the execution of each registered algorithm by each integrated code module. Transfers of specific coupling fields are managed by the transfer subsystem. Each equation set in the fire mechanics can specify a linear solver to be used. The solvers are selected from the Trilinos[7] package. Among the different solver choices available the ML solver [8] was used for the computationally demanding fluid region continuity equation solutions because of its speed and stability Aztec solver was used for other solutions like the momentum equations For an implicit code like Fuego time spent in the solvers account for a large percentage of the execution time.

The scaling study mesh sizes for the Fuego meshes and the time steps chosen for each mesh is shown in Table 1.

**Table 1. Scaling Study Mesh Parameters**

| | Coarse | Medium | Fine | VeryFine |
|---|---|---|---|---|
| Number of Elements | 574903 | 1029452 | 2382951 | 4190729 |
| Number of Nodes | 599156 | 1064089 | 2435869 | 4271179 |
| Time Step(secs) | 0.008 | 0.004 | 0.002 | 0.001 |

For the mesh convergence studies, each run, with a target simulation time of 30 seconds to resolve the fire, requires thousands of time steps and run time exceeding 48 hours. Such long runs are not needed for the scaling studies. However the scaling study must take into account time spent in different portions of the code such as setup and I/O. For the science runs, such as mesh convergence investigations, setup and I/O are typically small fractions of the run time, but they could be a significant fraction in scaling study runs as these overheads do not get amortized over many time steps. The scaling study timings were measured for 24 time steps, with a file I/O operation corresponding to the results file output (same as used for the mesh convergence studies) at the final time step. Restart I/O overhead was not included in the scaling study. For the purposes of measuring speed up and parallel efficiency, run times for each mesh was measured starting with a smallest number of processors on which the problem would fit in memory to some upper limit on the number of processors that produced only small reduction in execution time.

The objectives of the scaling study are: determination of the optimal number of elements per node, analysis of SIERRA Framework scaling separate from the linear solver scaling, and identification of opportunities for performance improvement. Fuego has an option to turn on detailed timer information that is useful in identifying the percentage of time spent in different regions and within each region. Figure 4 and Figure 5 shows the execution time and the parallel efficiency of the most compute intensive portion of these calculations, namely the computations associated with the Fuego/fluid region. In these simulations the time spent in the Calore region and the Syrinx region are less than 10%.

Figures 4 and 5 show the execution time and the parallel efficiency as a function of the number of processors. For the largest mesh, Red Storm gives a parallel efficiency of

75% for the Fluid Region execution and 68% efficiency for the whole application at 1024 processors. Looking for the knee of the curve in Figures 4, we can conclude that the optimal processor count for the coarse, medium, fine and very-fine meshes are: 128, 256, 512 and 1024. This is of course a conclusion based on the limited number of discrete processor configurations where we have measured the performance. At each of these configurations the execution time is close to one-half the execution time with half the number of processors. This corresponds to 4000 to 5000 elements per processor. These results also indicate that the maximum number of elements that would fit on 2GB node memory is 70,000 to 75,000. If the Syrinx and Calore meshes, are as large as the Fuego mesh (which was not the case in our study) then the number of elements per processor reduces to 25,000.

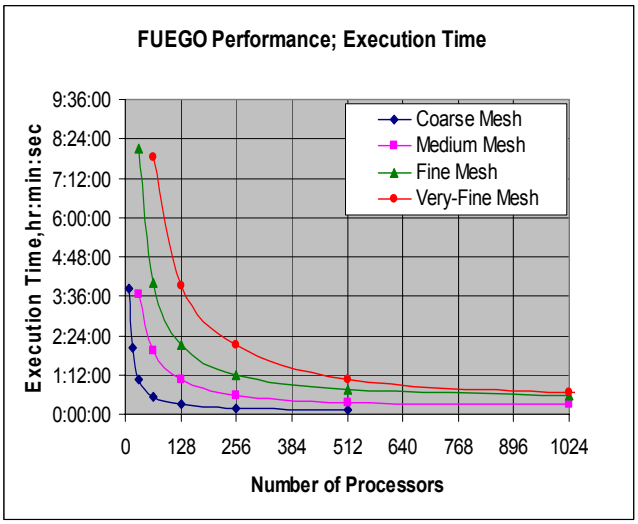


**Figure 4. Execution Times for the Fluid Region**

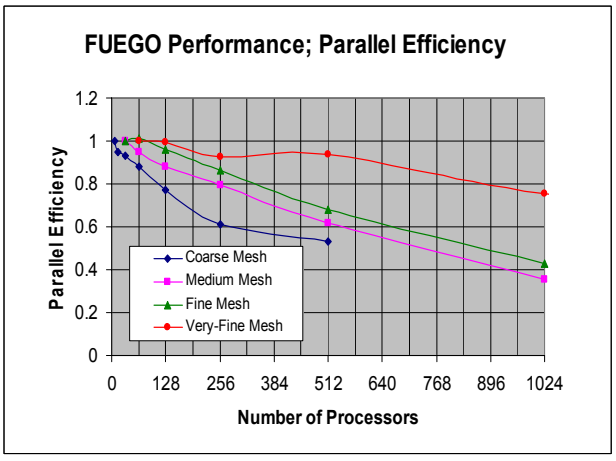


**Figure 5. Parallel Efficiency for the Fluid Region Computations**

Next we analyze the scaling characteristics of Fuego using the timing data from very-fine mesh runs. Figure 6 shows the parallel efficiencies of the full application, the most dominant component, the Fluid Region execution and for the Fluid Region the Matrix Assembly and the Matrix Solve portions of the computations. It is clearly seen from Figure 6, that the Matrix Assembly computations which involves the parallel gather/scatter operations to construct the coefficient matrix scales extremely well. This portion of the computations is a key component of the SIERRA framework. On the other hand the parallel efficiency of the Matrix Solve shows a linear decrease with close to 40% efficiency at 1024 processors. However this decrease in efficiency did not correlate with the average number of linear solve iterations for the continuity equation, with the number of linear solve iterations registering a slight increase from 40 iterations at 64 processors to 45 iterations at 1024 processors. Further instrumentation of the solvers is needed to understand the drop in efficiency. Red Storm has an option to use 'small_pages', which makes the page sizes 4K bytes instead of the default 2MB. Smaller page size was found to be beneficial in reducing the execution time by almost half in separate Trilinos solver tests. However, for the Fuego runs used in this scaling study, there was insignificant change in the execution time with the smaller pages.

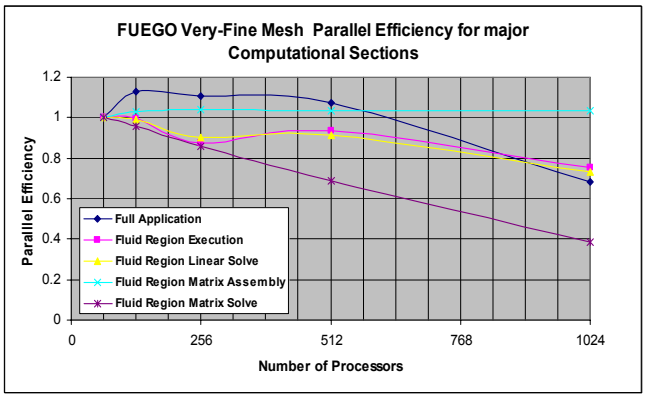


**Figure 6. Parallel efficiencies of key components for the Very-Fine Mesh**

It is instructive to look at significant other overheads from the execution timing results. Again using the Very-Fine mesh as an example, we list computations that registered a significant percentage of the overall execution time in Table 2. It is important to keep in mind that some of the items listed in Table 2 are an artifact of the very few time steps used in this scaling study. For example, the Initialize percentages would become insignificant in science runs that typically need two to three orders of magnitude larger number of time steps. However, it is presented here to explain the super linear speedup ( efficiency > 1) seen in Figure 6 for the full application.

**Table 2. Percentage of significant overheads for Very-Fine model run times**

| Item/ CPU | 64 | 128 | 256 | 512 | 1024 |
|---|---|---|---|---|---|
| Initialize | 14.7 | 7.67 | 4.74 | 5.82 | 10.5 |
| Mesh Output | 0.74 | 2.88 | 4.67 | 8.68 | 14.11 |
| Mesh Input | 1.78 | 2.75 | 1.23 | 2.12 | 5.04 |
| Fuego-Calore Xfer | 0.06 | 0.29 | 0.68 | 1.43 | 6.32 |
| Syrinx-Calore Xfer | 0.18 | 0.16 | 0.22 | 0.77 | 1.76 |

The calculations at 'Initialize' include a one-time setup for mesh association between the Fuego, Syrinx and Calore meshes, used to establish the spatial mapping for transfer of the physical variables. The item 'Mesh Input' is a startup overhead. Most interesting is the percentages observed for the 'Mesh Output'. While the absolute percentages are likely to be much smaller in science runs, the increase from less than a percent at 64 CPUs to 14% at 1024 CPUs is a cause for concern. All input/output was directed to a Lustre file system on 32 I/O servers and 64 storage targets. The output consisted of 4 files per processor with a total output of approximately 1.6GB per run. Preliminary testing of the Lustre file system with user accessible selection of files with different stripe count and stripe size attributes suggests that if the I/O was directed to a file set up with a stripe count of 1-8 instead of 64, there would be substantial improvement in the performance. Table 2 also suggests that Fluid-Conduction transfer is not scaling optimally. The reasons for this may likely be related to the disparity in element count between the fluids and conduction region. Specifically, at 1024 processors the Calore mesh has only $O$(50*nodesPerElement) sends per processor.

## V. Conclusion

Mesh convergence studies, requiring large number of processors and long simulation times, have been carried out on Sandia's Red Storm. The study identified the need for even finer mesh than the 2M element simulations completed so far, to confirm the grid independence of the solution. This will require substantially more computational resources and execution time. Further we have begun a process to investigate scaling characteristics of this important Sandia application to optimally use Red Storm. Work is in progress to measure its performance all the way up to the full Red Storm system with 10,360 processors because of its importance in planned capability class simulations. Our investigations indicate that Fuego will scale well for an appropriately sized mesh consisting of at least 4000 elements per processor. The most time consuming portion of the simulations registered an impressive 78% efficiency at 1024 processors. The challenge in scaling implicit codes is in using solvers with good scaling characteristics. While the ML solver used in this investigations shows good scaling based on the very slow growth in the number of solve iterations required, its parallel efficiency as measured by the time spent in the solver, should be improved. Factors limiting the solver scalability has not yet been identified. The SIERRA framework under which the bulk of the computations setting up the matrix for the solver, showed near perfect scaling for the range of processors considered. Other computational portions, such as the mesh transfers, needs to be investigated further.

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