

Multiscale modeling and computation-intensive simulation of accidental fires on the Grid computing environment

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Time-accurate, full physics simulations of accidental fires require consideration of fundamental gas and condensed phase chemistry, structural mechanics, turbulent reacting flows, convective and radiative heat transfer, and mass transfer. It is also required to model the physical complexities from the molecular level of high energy materials, through millimeter-sized representations of the container, to the meter-sized representations of the fire spread. Due to the inherent multiple scales, the spatial requirements may exceed the terabyte range for the full simulation. The computation will also require 10^{10} time-steps. In this research we focused on providing science-based tools for the numerical simulation of accidental fires, comprising a problem-solving environment in which fundamental chemistry and engineering physics are fully coupled with visualization and experimental data verification. We are also investigating the coupling of the micro-scale and meso-scale contributions to the macroscopic application in order to provide full-physics accuracy and the effective utilization of the Grid computing environment and consisting supercomputers.