176c An E-Science Environment for Computation-Intensive Fire Modeling, Simulation and Research Collaborations

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Fire modeling can be accomplished through the use of experimental or mathematical techniques. Experimental methods include such methods as reduced and full-scale replicas of the situation or phenomenon being studied. Mathematical models are commonly divided into two groups: stochastic and deterministic models. 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 to compute the physical time scales ranging from microseconds to minutes or hours.

In this research we focused on providing science-based tools, and deploying them on the e-Sceince environment, for the numerical simulation of accidental fires, especially within the context of handling and storage of hydrocarbons. The objective is to provide a system comprising a problem-solving environment, operating on a government-supported e-Science infrastructure, in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, computational steering, 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. The Computational Grid and Access Grid/visualization module, composing key elements of the e-Science environment, provide a computational, visualization and collaboration infrastructure that can support multiphysics modeling, simulation and effective display of large-scale, complex phenomena. The ability of simulations using this system will help better evaluate the risks and safety issues associated with fires, through high speed network-based cooperations of collaborating researchers and organizations.