An Infrastructure for Parallel Multi-Physics Mechanics Simulations

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We describe the Uintah Computational Framework (UCF), a set of software components and libraries that facilitate the simulation of PDEs on Structured Adaptive Mesh Refinement (SAMR) grids using hundreds to thousands of processors. We employ a component-based framework based on the Common Component Architecture (CCA). Through these mechanisms, we have coupled a particle-based mechanics technique (the Material Point Method, or MPM) with an Eulerian hyrodynamics algorithm (a cell-centered ICE method). This simulation software is being developed within the University of Utah's Center for Simulation of Accidental Fires and Explosions (C-SAFE) [1,3], a DOE sponsored ASCI ASAP Center.

The UCF [2] employs a non-traditional approach to achieving parallelism. Instead of explicit MPI calls placed throughout the program, applications are cast in terms of a *taskgraph*, a construct that describes the data dependencies between various steps in the problem and communication between those tasks. Computations are expressed as directed acyclic graphs of *tasks*, each of which produces some output and consumes some input (which is in turn the output of some previous task). These inputs and outputs are specified for each patch in a structured AMR grid. Tasks form a UCF data structure called the *taskgraph*, which represents imminent computation.

This flexible approach helps accomodate multi-physics integration. These two simulation components, MPM and ICE, were developed separately, but both used the same underlying mesh and infrastructure. Using the UCF, a bridge component was created that facilitates the fine-grained coupling of the MPM and ICE algorithms. The taskgraph facilitates this integration by allowing each application component (MPM and CFD in this example) to describe their tasks independently. The scheduler connects these tasks where data is exchanged between the different algorithm phases.

The taskgraph approach can also accomodate performance and scalability on complex large-scale parallel architectures. It forms the basis for a flexible load-balancing strategy, and facilitates the combination of traditional MPI-based parallelism with thread-based shared memory execution. The component-based approach facilitates development of pieces of the simulation that evolve independently; typically implemented in a basic form at first, and evolving as the technologies mature. Most importantly, the UCF allows the aspects of parallelism (schedulers, load-balancers, parallel I/O, and so forth) to evolve independently of the simulation components.

References

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