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COMPUTATIONAL MODELING OF MULTISCALE FLOWS

T. Grenga[1] and S. Paolucci[2]

[1] University of Notre Dame, 117 Cushing Hall, 46556 Notre Dame IN, USA, tgrenga@nd.edu
[2] University of Notre Dame, 117 Cushing Hall, 46556 Notre Dame IN, USA, paolucci@nd.edu

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The *p*arallel *W*avelet *A*daptive *M*ultiresolution Representation (pWAMR) method is particularly suited for solutions of challenging multi-dimensional continuum physics problems having strong multi-scale character. Since the amplitudes of the wavelet transform implemented in the method provide a direct measure of the local error at each collocation point associated with a wavelet, the method is able to efficiently capture to any desired accuracy a wide range of spatial scales using a relatively small number of degrees of freedom by evolving the dynamically adaptive grid. Subsequently, high resolution computations are performed only in the regions where near-singularities or sharp transitions occur. In an effective fashion, the multilevel structure of the algorithm provides a simple way to adapt computational refinements to local demands of the solution, thus automatically producing verified solutions. The parallel algorithm utilizes an MPI-based domain decomposition approach and a load-balancing algorithm that exploit a Hilbert space-filling curve data structure. The use of these techniques, in conjunction with the wide availability of distributed memory parallel computers, enables the simulation of challenging problems, such as unsteady, compressible, reactive flows.

The algorithm is demonstrated through the problem of a three dimensional reactive shock-bubble interaction (RSBI). The problem is modeled using the reactive Navier-Stokes equations for a multi-component gas mixture, including detailed chemical kinetics, multi-component diffusion, Soret and Dufour effects, and state dependent thermodynamic and transport properties. In the problem, a bubble, filled with a mixture of hydrogen, oxygen and nitrogen and in an air environment, is impacted by a planar shock wave. Depending on the shock strength and mixture composition, the bubble is potentially ignited. The transmitted shock wave in the bubble is observed to be slower or faster than that outside the bubble according to the sign of the Atwood number. Either situation generates complex interactions between the shock and reacted and unreacted regions, and lead to intricate shock-wave diffractions and reflections. The hydrodynamic and reactive phenomena, and their reciprocal influence, are investigated by resolving all physically relevant spatial scales. It is found that a minimum grid spacing of O(0.1 μm) can capture the smaller physical structures, such as the intricate coupling between fluid dynamics and chemistry.