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Verification and Validation of a Chemical Reaction Solver Coupled to the Piecewise Parabolic Method[1] NITESH ATTAL, PRAVEEN RAMAPRABHU, University of North Carolina at Charlotte, JAHED HOSSAIN, University of Central Florida, VARAD KARKHANIS, University of North Carolina at Charlotte, SUKESH ROY, Spectral Energies LLC, JAMES GORD, Air Force Research Laboratory, MESBAH UDDIN, University of North Carolina at Charlotte
— We present a detailed chemical kinetics reaction solver coupled to the Piecewise Parabolic Method (PPM [1]) embedded in the widely used astrophysical FLASH [2] code. The FLASH code solves the compressible Euler equations with a directionally split, PPM with Adaptive Mesh Refinement (AMR). The reaction network is solved using a library of coupled ODE solvers, specialized for handling stiff systems of equations. Finally, the diffusion of heat, mass, and momentum is handled either through an update of the fluxes of each quantity, or by directly solving a diffusion equation for each. The resulting product is capable of handling a variety of physics such as gas-phase chemical kinetics, diffusive transport of mass, momentum, and heat, shocks, sharp interfaces, multi-species mixtures, and thermal radiation. We will present results from verification and validation of the above capabilities through comparison with analytical solutions, and published numerical and experimental data. Our validation cases include advection of reacting fronts in 1-D and 2D, laminar premixed flames in a Bunsen burner configuration, and shock-driven combustion.
[1] P. Colella and P. R. Woodward, J. Comput. Phys. 54, 174-201 (1984). [2] B. Fryxell et al., Astrophys. J., Suppl. Ser. 131, 273 (2000).

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