

# Computational sub-structure analysis of multidimensional detonation waves

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The propagation of self-sustained detonation waves in gaseous media is characterized by a fragile energetic balance between leading hydrodynamic shock wave and following chemical reaction. As a consequence, detonations exhibit inherently unstable behavior with transient shocks of considerable strength moving perpendicular to the detonation front. The transient shocks create evolving triple points with Mach reflection patterns in which pressure, temperature, and reaction rate are severely enhanced. While gaseous detonations propagate at supersonic speeds of 1000 m/s to 2500 m/s, the Mach reflection sub-structures are typically at the micrometer scale. One can fairly say that multiscale nature and hydrodynamic complexity make the accurate prediction of triple points a problem ranking in difficulty with fully turbulent compressible flow.

We report on recent advances in directly simulating detonations in hydrogen-oxygen-argon mixtures to understand transient triple point propagation. The computations reproduce all experimentally observed features such as “weak” and “strong” structures (which are identified uniquely as transitional- and double-Mach reflections by shock polar analysis), the transition between them, and triple point formation and decay. A detailed comparison for a single transverse wave uncovers considerable differences in the Mach reflection patterns exhibited in two and three space-dimensions.

Since it is vital for predictable detonation simulation to provide extraordinary high resolution in the induction zone only, all computations are done with a highly efficient adaptive finite volume method. Its key components, a high-resolution shock-capturing scheme of Roe-type, parallel block-structured Cartesian mesh adaptation, and operator splitting to handle stiff, detailed kinetics, will be briefly sketched [1, 2].

## References

- [1] R. Deiterding. Dynamically adaptive simulation of regular detonation structures using the Cartesian mesh refinement framework AMROC. *Int. J. Computational Science Engineering*, 2007, in press.
- [2] R. Deiterding. A parallel adaptive method for simulating shock-induced combustion with detailed chemical kinetics in complex domains. *Computers & Structures*, submitted.

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