"Adaptive High-resolution Simulation of Realistic Detonation Structures"

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Summary

The accurate approximation of realistic detonation waves in gaseous combustible mixtures is extremely demanding since a wide range of scales needs to be resolved. Combining block-structured mesh adaptation with high-resolution finite volume schemes for chemically reacting flows and parallel high performance computing has enabled the first systematic computational investigation of the transient behavior of regularly oscillating detonations in hydrogen-oxygen mixtures in realistic two-dimensional geometry.

A detonation is a shock-induced combustion wave that internally consists of a discontinuous supersonic shock wave followed by a smooth region of decaying combustion. The adiabatic compression due to the shock rises the temperature above the ignition limit of the chemical reaction. The reaction results in an energy release driving the shock wave forward. The energetic balance between shock and chemistry is inherently unstable and already early experiments uncovered that particular detonations in gaseous mixtures therefore never remain planar. The multi-dimensional instability manifests itself in instationary transverse shock waves propagating perpendicular to the detonation front. A complex flow pattern is formed around each *triple point* where the detonation front is intersected by a transverse shock. Pressure and temperature are increased remarkably enhancing the chemical reaction locally. Hence, the accurate representation of triple points is vital for safety analysis, but also in innovative technical applications, e.g., in pulse detonation engines. Under particular conditions, the trajectories of the triple points form very regular patterns, so called detonation cells, with characteristic length and width (compare Fig. 1).

Up to now, sufficiently resolved detonation structure investigations using detailed reaction networks have been carried out only for simplified periodic situations that can be simulated effectively with very fine, but geometrically small, uniform meshes attached to the moving detonation front. Discretizing realistic combustion devices in this manner would require several billion cells already in two space dimensions and is prohibitively expensive. Therefore, we have incorporated a time-explicit second-order-accurate shock-capturing scheme (approximate Riemann solver of Roe-type for thermally perfect gas mixtures) into a Cartesian block-structured adaptive mesh refinement algorithm that is parallelized for distributed memory machines. The stiffness of the reaction terms is handled by decoupling hydrodynamic transport and chemical reaction numerically with the method of fractional steps and employing a standard semi-implicit integrator for ordinary differential equations locally in each finite volume cell.

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The embedding of complex geometries with a level set approach allows for the computation of non-Cartesian problems.

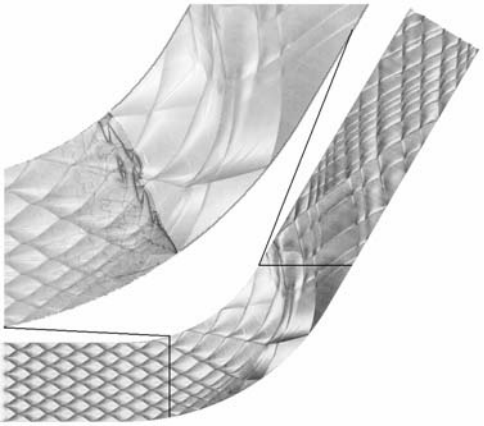

Figure 1: A trace of the maximal vorticity throughout the whole computation visualizes the triple point trajectories for a realistic 60º pipe bend (lower). The enlarged upper graphic displays a snapshot of the detonation front on the trajectory picture.

In order to demonstrate the enormous potential of the entire approach for combustion research, a series of computations has recently been carried out in which regularly oscillating detonation waves in low-pressure hydrogen-oxygen-argon mixtures propagate upwards through two-dimensional pipe bends. Such mixtures have been widely analyzed by experimental means and are a primary test case for numerical methods. The computations exhibit all experimentally observed features, such as detonation quenching and triple point decay at the outer, compressive pipe wall, and partial extinction and violent re-ignition by a transverse detonation wave at the inner wall. Specially, the multi-dimensional instability is captured accurately throughout the whole computations which can be inferred by the fact that amplitude and period of the triple point oscillation are recovered after the bend (see lower graphic of Fig. 1). To our best knowledge, this has never been achieved previously in numerical simulations.

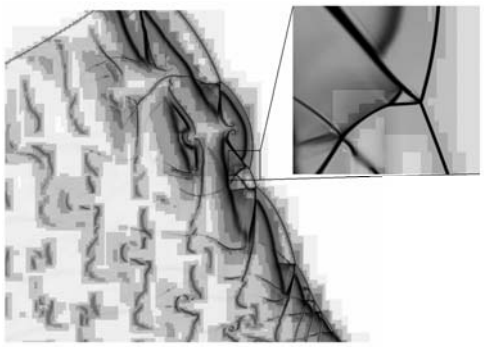

Figure 2: A Schlieren graphic of the detonation front snapshot overlying the domains of hierarchical mesh refinement (in different gray tones) visualizes the level of detail necessary for predictive detonation simulation.

The shown computation is carried out on a 1200x992 base grid with four additional levels refined isotropically by the factors 2, 2, 2, and 4. While using only around 5 million cells on average, the simulation is equivalent to a unigrid computation with more than 1.2 billion cells. Figure 2 visualized the domains of recursively finer mesh adaptation for the detonation front snapshot shown in the upper graphic of Fig. 1. An extreme enlargement (right graphic of Fig. 2) is necessary to display the evolving wave pattern around a single triple point at maximal detail. The calculations were run on 64 dual-processor nodes of the ASC Linux cluster at Lawrence Livermore National Laboratory and required approximately 70,000h CPU each.

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