Verification and Direct Numerical Simulation of Irregular Hydrocarbon Detonations

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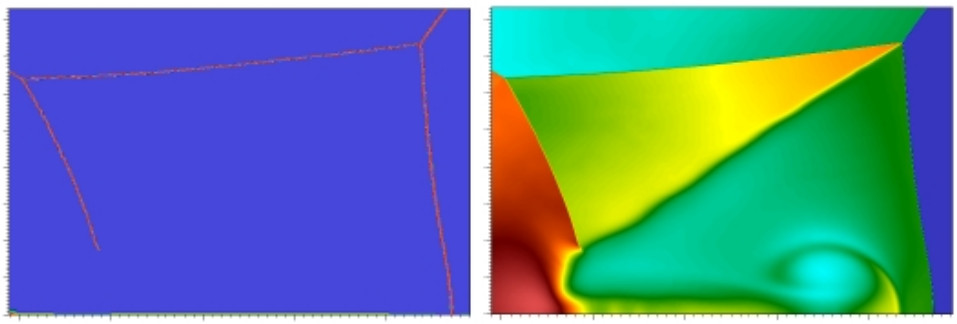
1 Simulation of the Reactive Navier-Stokes Equations

We describe direct numerical simulations of irregular hydrocarbon detonations using the multicomponent, compressible, reactive Navier-Stokes equations in two spatial dimensions. The simulations utilize a hybrid, WENO/centered-difference numerical method, with low numerical dissipation, high-order shock-capturing, and structured adaptive mesh refinement (SAMR) [1],[2], [3]. This enables the resolution of diffusive processes within reaction zones. A minimally reduced chemistry and transport model for a propane-air detonation is used to accurately capture the induction time, chemical relaxation, and the diffusive mixing within vortical structures evolving from the triple-point shear layers [1].



(a) Shock Detection (b) Density psuedocolor plot

Figure 1: Demonstration of shock-detection for WENO/CD scheme switch. (a) Shows in red where WENO is used and in blue where Centered-differences are used for a corresponding non-reactive double Mach reflection.

Our implementation includes new techniques for discontinuity flagging, scheme-switching, and high-order prolongation and restriction. In particular, the refined methodology does not require upwinded WENO at grid refinement interfaces for stability, allowing high-order prolongation and thereby eliminating a significant source of numerical diffusion within the overall code performance. Using Riemann problem based shock-detection, the coverage of the WENO scheme is precisely controlled, as is illustrated for a Double Mach Reflection test case in Figure 1.

The method has been extensively tested with a series of one- and two-dimensional steady and unsteady verification tests. These tests provide confidence in our simulations of the numerically unexplored topic of hydrocarbon detonations.

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2 Verification Study

Additionally, a series of one- and two-dimensional test problems are used to verify the implementation, specifically the high-order accuracy of the diffusion terms and the convergence of the whole implementation in an SAMR framework. These problems include; for 1D: a resolved viscous shock wave, unstable ZND detonation, and a laminar flame with detailed chemistry; for 2D: a decaying Lamb-Oseen vortex, and diffusive reactive and non-reactive double Mach reflections (DMR) with simplified and detailed chemistry models. For the decaying Lamb-Oseen vortex in Table 1, 6th-order-accurate convergence is shown, as there are no discontinuous shocks and the AMR levels were fixed in space. The reactive DMR convergence results are shown in Table 2 and Figure 2. Note that in this case, the convergence rates are lower, as the initial condition has a discontinuity and the incident shock and Mach stem are marginally resolved in the Navier-Stokes sense. These results demonstrate the resolution of reactive-diffusive processes for a non-steady, unstable, reactive problem including discontinuous shock waves.

Table 1: Convergence results for the decaying Lamb-Oseen vortex. Comparison of the WENO/CD method with 1st and 5th order-accurate prolongation and restriction with the equivalent uniform grid case.

Finest grid resolution	WENO/CD 2 levels L_1-error	rate	WENO/CD 2 levels higher order SAMR L_1-error	rate	MUSCL 2 levels L_1-error	rate	WENO/CD unigrid L_1-error	rate
0.1875	0.000282		0.000101		1.60		0.000102	
0.09375	5.80E-05	2.20	2.18E-06	6.82	0.409	1.97906	2.19E-06	6.81
0.046875	1.40E-05	2.03	4.72E-08	6.80	0.103	1.996228	4.75E-08	6.89
0.0234375	3.82E-06	1.92	1.31E-09	6.00	0.0248	2.036	1.01E-9	6.85

Table 2: Manufactured solution convergence results for the two-species, one-step, reactive double Mach reflection problem using SAMR.

Levels	Density L_1-error	rate	Y_1 L_1-error	rate
$t = 4.300$, domain: $[23.0, 30.0] \times [0, 5.0]$				
4	2.00432	-	0.216785	-
5	1.36915	1.21	0.160973	1.16
6	0.709029	1.40	0.0791281	1.43
7	0.329581	1.47	0.0360734	1.48
t = 4.608 domain: $[23.0, 30.0] \times [0, 5.0]$ (Mach stem/incident shock has left the domain)				
4	1.83941	-	0.226811	-
5	1.36174	1.16	0.170671	1.15
6	0.810797	1.30	0.104466	1.28
7	0.350756	1.52	0.0429677	1.56

The present convergence results for the non-reactive and reactive DMR simulations support the conclusion that, with our implementation and detailed simulations, diffusive processes within chemically reacting zones are resolved. A careful use of a hybrid method, where WENO is activated only at strong shock waves (using an approximate Riemann-problem based shock detection), allowed the sixth-order accurate centered difference stencils to be uniformly active on shear layers and surrounding regions [1].

3 Preliminary Hydrocarbon Results

With our two-species, one-step, diffusive, reactive DMR test case as a solid verification basis [1], we

have developed and simulated the DMR problem for hydrocarbon fuels. Shown in Figure 3 is a preliminary Propane-Air (C3H8-O2-N2) DMR. In order to control the computational expense in a detonation mechanism.

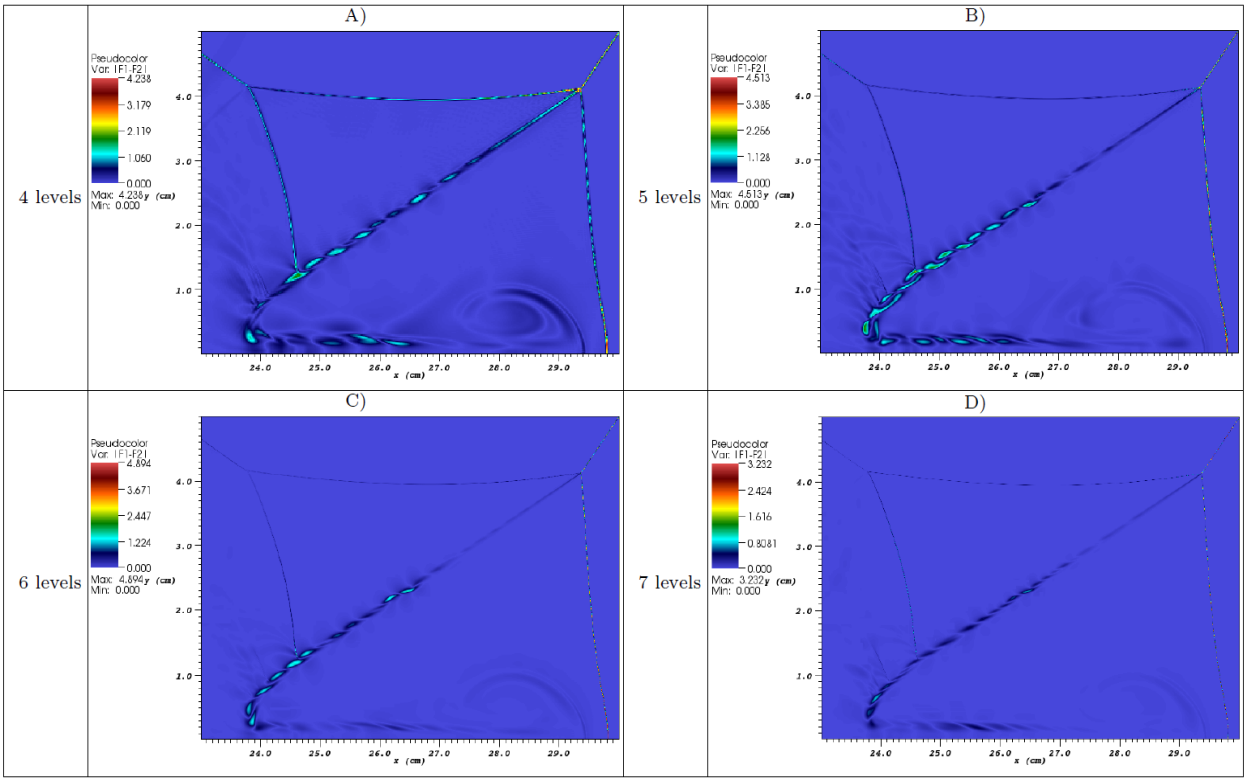

Figure 2: Visualization of the L1 density error norms for the reactive double Mach reflection problem.

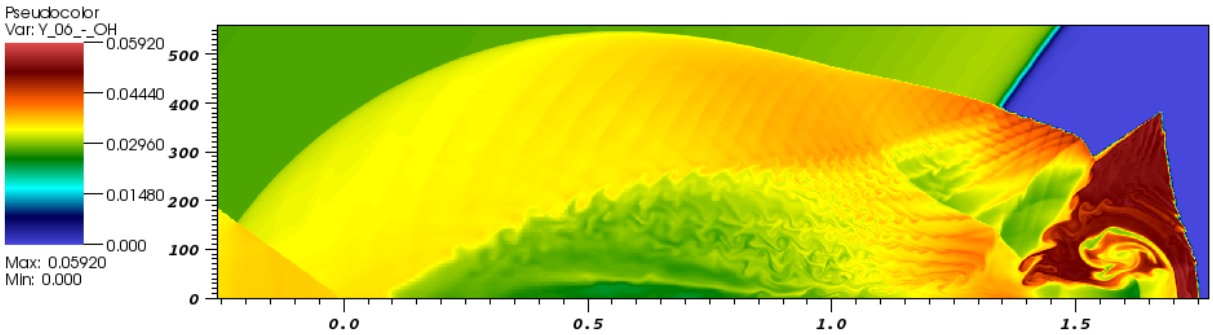

Figure 3. Pseudo-color plot of OH mass fractions for an C3H8-O2-N2 detonation double Mach reflection.

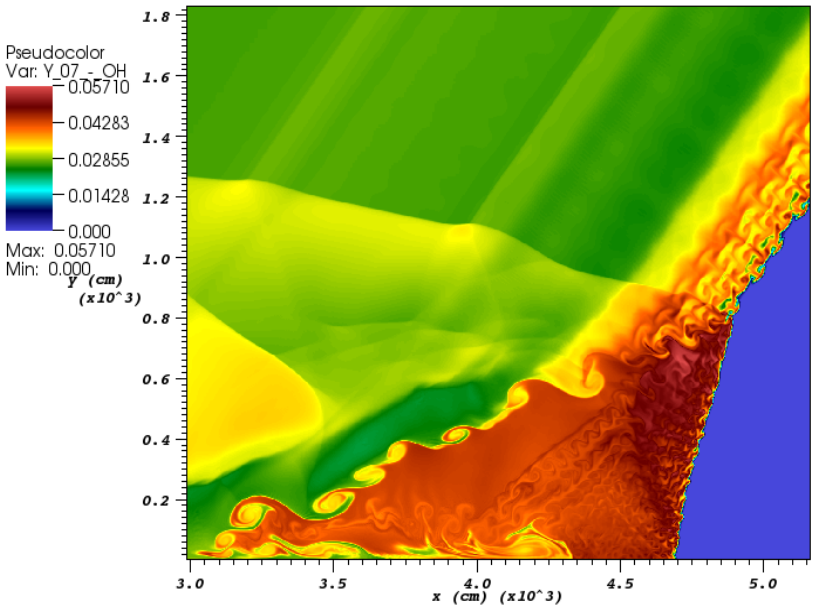

Figure 4. Pseudo-color plot of OH mass fractions for an C3H8-O2-N2 detonation double Mach reflection. This is at a later time step and with less resolution than that shown in Figure 3. Note that the incident shock has also gone unstable.

simulation which includes detailed chemistry and transport, we have developed custom reduced models which preserve the steady one-dimensional ZND solution. This was matched for the expected range of detonation speeds in an unsteady multi-dimensional detonation, as shown in Figure 5. The demonstration results are for a mechanism which has been reduced to 22 species and 53 reversible reactions. A comparison to experimental induction times is shown in Figure 6. Propane is of high interest as it is one of the most unstable fuels for which detonations have been studied experimentally in labs to date [3]. Our numerical simulations are investigating the mechanisms involved in the diffusive processes of irregular detonations. Here, the goal is to study highly unstable mixtures for which major effects along the shear layers can be expected; e.g., unreacted pockets transported downstream or highly irregular ignition. In this case, diffusive processes can be an integral part of the detonation mechanism.

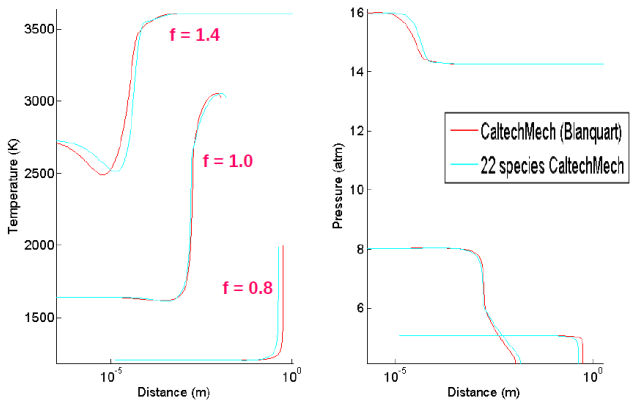

Figure 5. Comparing reduced and detailed mechanism (Blanquart) ZND solutions at dierent overdrive

values. The reduced propane mechanism neglects N2 chemistry and larger than C3 molecules to reduce 161 Species to 22 species and 1055 Reactions to 53 reactions. A few rates of sub-reactions for C2H5 were hand tuned to re-scale induction times.

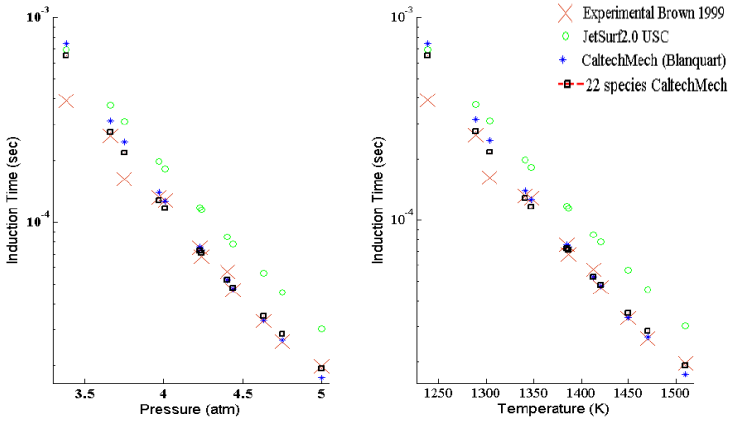

Figure 6: Detonation induction time comparisons for propane: comparing experimental vs. detailed and reduced mechanisms. The ambient conditions corresponds to T = 300 K, P = 20 kPa

References

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