Hybrid Large-Eddy Simulation of Detonations in Reactive Mixtures

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Introduction

Accurate simulation of detonations and explosions presents severe challenges for numerical methods. The method must be able to capture strong shocks as well as to accurately compute the turbulent shear flows that frequently arise as a result of the explosion. Shock capturing methods have significant numerical dissipation to prevent generating unphysical oscillations near the shock, but this dissipation tends to smear out fine-scale turbulent structures in the flow. On the other hand, highly accurate numerical schemes developed to simulate smooth flow tend to produce unphysical oscillations in regions of strong gradients and/or discontinuities.

In order to solve this dilemma, a new hybrid method has been developed, that couples a high-resolution shock capturing method with a high-order finite-volume method. The shock capturing method is used only near discontinuities, while the high-order finite-volume method computes the remainder of the flow. The baseline code, LESLIE3D, is a well-established solver (1; 2; 3) used for LES and DNS studies for turbulent reacting single and two-phase flows. The baseline solver is second-order accurate in time and second or fourth-order accurate in space. For LES applications, it employs a localized dynamics model for the subgrid kinetic energy. Reaction-diffusion processes can be modeled with many approaches (depending upon applications), such as subgrid eddy break-up, flamelet models, and a new subgrid simulation approach called linear-eddy mixing (LEM) modeling (4). For multi-phase flows, the particle phase is included using a Lagrangian tracking scheme that tracks either individual particles or groups of particles (2). The gas phase is fully coupled to the particle phase. There is full two-way coupling in the LES model and both liquid and solid particles can be tracked in this solver.

This code's capability has been extended in order to allow for the simulation of strong detonations in reacting mixtures. Application to detonations in both single and two-phase reacting flows will be reported in this paper.

Governing Equations and Numerical Methods

Governing equations

The governing equations under consideration are the filtered conservative Navier-Stokes equations for mass, momentum, total energy and species densities with source terms due to the chemistry and to the coupling with the Lagrangian phase. The Large-Eddy Simulation closure is provided by a one-equation closure model based on the transport of the subgrid turbulent kinetic energy. A detailed description of the governing equations can be found elsewhere (2; 5).

Numerical Methods

In this section, a brief description of the hybrid method is presented. This scheme has been previously presented (6) and validated for both inviscid (6) and viscous, turbulent flows (5). It consists in coupling a high-order finite-volume method with a high-resolution shock-capturing algorithm. The shock-capturing technique is used only near shocks and contact discontinuities, while the high-order method handles the smooth regions of the flow.

We describe the hybrid method using the one-dimensional Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \tag{1}$$

where U is the vector of conserved quantities (density, momentum, energy, and species partial density) and F is the flux vector. Extension to multidimensional flows and more complex physics is straight forward.

The smooth-flow finite-volume solver is a predictor corrector method, which can be written as

$$U_i' = U_i^n - \frac{\Delta t}{\Delta x}\left(F^+_{i+\frac{1}{2}} - F^+_{i-\frac{1}{2}}\right) \tag{2}$$

$$U_i^{n+1} = \frac{1}{2}\left(U_i^n + U_i' - \frac{\Delta t}{\Delta x}\left(F^-_{i+\frac{1}{2}} - F^-_{i-\frac{1}{2}}\right)\right). \tag{3}$$

The quantity F_i can be evaluated using either a simple second-order approximation or a more complex extrapolation (7), which leads to fourth-order spatial accuracy. Alternating between forward and backward spatial differences of the flux derivatives between the predictor and corrector steps results in a central difference scheme.

The shock capturing technique used in the hybrid code is based on the Piecewise-Parabolic Method (PPM) (8). The PPM algorithm is a high-order extension of the method originally developed by Godunov (9) and as such, relies on the solution of Riemann's problem to compute fluxes through zone interfaces. In Godunov's original method, the flow variables were represented as piecewise-constant functions. In PPM, the flow variables are represented as piecewise-parabolic functions, permitting higher-order solutions. The method is able to accurately compute shocks and contact discontinuities that are only two zones wide with virtually no spurious oscillations.

In order to couple the two methods, it is necessary to compute a measure of the smoothness of the solution. For this purpose, we use an estimator similar to one proposed by Löhner (10) as a refinement criterion in adaptive mesh methods. We begin by defining a quantity S by

$$S_i = \frac{|Q_{i+1} - 2Q_i + Q_{i-1}|}{|Q_{i+1} - Q_i| + |Q_i - Q_{i-1}|}, \tag{4}$$

where Q can be any variable of interest. We use both density and pressure and take the maximum of the two values. For multidimensional flows, the maximum value of S_i for each coordinate direction is used. In any cell in which the value of S_i exceeds some threshold, typically 0.5, PPM is used to construct the fluxes through each face of that cell. For each cell bordering a cell in which PPM is needed, the average of the PPM flux and the smooth-flow solver flux is used. At the remaining grid points, the smooth-flow solver flux is used.

Results and Discussion

Here, we report on some of the validation studies conducted so far, and some of the preliminary results. Additional results will be reported in the final paper and presentation.

Detonation in a Gaseous Media

A 1-D simulation (using the full 3D code in a reduced capacity) of a blast wave in a shock-tube is used to investigate the ability of the new code to capture the formation of a detonation wave. The initial pressure jump is 50 and the shock tube is filled with H_2/air in stoichiometric proportions at 1 atm, and at 540 K. The present computation is performed in order to validate the 1-step mechanism developed by Marinov *et al* (11) for hydrogen/air chemistry, that reads:

$$H_2 \quad + \quad \frac{1}{2}\,O_2 \quad \rightarrow \quad H_2O \qquad\qquad k_{glob} = 1.8 \times 10^{13} exp\Big(-\frac{17614}{T}\Big) \tag{5}$$

The model was developed in such a way as to respect the flame structure, propagation, and ignition processes. Specifically, it has been shown (11) that the ignition delay times in a shock-tube problem are correctly simulated. The accuracy of the modeled mechanism was observed for equivalence ratios between 0.6 and 1.1.

As can be observed in Fig. 1, the Mach number reached behind the detonation front is 1, and a very slow decay of the shock front Mach number is observed in this simulation. After a transient period of time, the detonation follows the Chapman-Jouguet conditions. The same reaction mechanism is to be used in the circularly expanding detonations presented below.

Explosion in a Confined Medium

The initial conditions consist of a point explosion in a square building with a window in one wall. The shock generated by the explosion has an overpressure of 10^6. The results of the pressure field are shown in Fig. 2. This calculation shows the ability of the code to accurately capture shocks, reflections of shocks at solid walls, and complex shock-shock interactions. It also shows the turbulent nature of flows resulting from relatively simple initial conditions.

Solid Phase Tracking Procedure

A Lagrangian approach is used in order to track groups of particles. This method allows for an explicit and accurate two-way coupling between the gaseous and condensed phases. This method has been used in the past for the study of liquid-fueled engines (Diesel engines (12),liquid-fueled SCRAMJET (13)).

It has recently been used for the study of planar multiphase detonations with aluminum particles (5). The heat transfer and evaporation processes between gas and liquid phases are temporally resolved. One main assumption is that the aluminum oxide cap that has been observed to form by many researchers (see, *e.g.* (14)) does not occur in the present configuration. The justification for this assumption is the very high convective environment that should remove the oxide from the particles' close environment. The gaseous aluminum obtained from the evaporation then acts as a fuel to the oxygen and steam present in the flow. The reduced mechanism described by Beckstead (14) is used for the aluminum chemistry:

$$\begin{array}{lllllllll} Al_l & & & & & \rightarrow & Al_g & & \\ Al_g & + & O_2 & & & \rightarrow & AlO & + & O \\ AlO & + & O_2 & & & \rightarrow & AlO_2 & + & O \\ Al_g & + & H_2O & & & \rightarrow & AlO & + & H_2 \\ & & & & & & & & \\ O & + & O & + & M & \rightleftharpoons & O_2 & + & M \end{array} \qquad \begin{array}{ll} & \\ k_8 & = 9.76 \times 10^{15} e^{-80/T} \\ k_9 & = 4.63 \times 10^{14} e^{-10008/T} \\ k_{10} & = 1.90 \times 10^{12} e^{-443/T} \\ & \quad +1.60 \times 10^{10} e^{-2869/T} \\ k_{11} & = 6.17 \times 10^{15} T^{-0.5} e^{0/T} \end{array} \tag{6}$$

Multiphase Detonation

An explosion is considered in a reactive environment, composed of stoichiometric air/H_2. Initial over-pressure and temperature profiles are imposed according to

$$\begin{aligned} P(r) &= P_{atm}\left(1 + (P_{ratio} - 1) exp\Big(- \big(\tfrac{r}{1.4\ R}\big)^4 \Big)\right) \\ T(r) &= T_{atm}\left(1 + (T_{ratio} - 1) exp\Big(- \big(\tfrac{r}{1.4\ R}\big)^4 \Big)\right) \end{aligned} \tag{7}$$

The influence of aluminum particles on the overall detonative process is under consideration. A first case of pure simple detonation is used as a base case, in order to study the influence of particle loading and aluminum reaction on the overall detonation structure.

The initial conditions that were considered during this preliminary study are as follows. The post-explosion pressure was set to 300 atm, with a temperature of 800 K. The radius R of the initial over-pressure was set to 0.15 m, at the center of a domain measuring 3 $m \times 3$ m.

Three simulations are presented here. The first simulation considers the detonation as described above in a quiescent, particle-free environment. This is to be taken as a reference simulation. In a second simulation, 15 μm aluminum particles are initially placed inside the volume of high pressure with a loading of 170 g/m^3. The third simulation consists of a very high loading of 15 μm aluminum particles within five radii from the over-pressure center at a loading of 236 g/m^3.

First, it can be seen from the numerical shadowgraph represented in Fig. 3 (a) that the simplest case of the detonation without any particles already shows some non-axisymmetric features. This is a numerical

artifact due to the simulation of a circularly evolving feature on a rectangular grid. The locally aligned/misaligned fronts for an axisymmetric phenomenon results in numerical oscillations. They are however very small in amplitude, and will thus not interfere with the main simulation.

Particles initially located inside the explosion center have little influence on the evolution of the detonation front. The high temperature regions are at the edge of the moving front, and thus, the particles initially located inside the over-pressure region are contained in a moderately hot region. The evaporation of these particles is then slow compared to the velocity of the front, and the gaseous aluminum reaction plays little role on the overall propagation. Its evaporation and burning will, however, have an influence on the turbulence generation at the center of the domain.

In the third case, the very hot regions at the edge of the detonation front interact with the particles, thus significantly enhancing the evaporation rates. It can be seen from fig. 3 (c), which represents a numerical shadowgraph taken at the same physical time $t^* = 520\ \mu s$ as the two other shadowgraphs, that the friction of the particles results in a slower propagation of the detonation front. Furthermore, A different pattern is observed in this case, where two sharp fronts are observed. The first front is the actual detonation wave, and the second front is due to the aluminum combustion, which results in a steeper temperature gradient.

The presence of aluminum particles inside the explosion center does not change the temperature profile as shown in fig. 4, except for a very slight decrease in the propagation velocity. The high loading, on the other hand, shows a few changes from the particles-free case. The propagation velocity is slower, as already shown by the numerical shadowgraphs. Also, the heat losses due to the heating of the particles results in a lower peak temperature inside the reaction zone of the detonation. The temperature decay is, however, much stronger in the third case. This was observed to be the very sharp delimitation between the unburned/burned aluminum enriched region and the region that just reacted. Also, the final decay in temperature is smoother in the third case, when aluminum chemistry starts playing an important role.

Conclusion and Future Work

The goal of this paper is to understand the mechanism that results in the ignition of the reactive mixture and the propagation of a detonation wave. Physics of transition to detonation in turbulent shear flows will be analyzed. The influence of particle size, level of turbulence, and initial conditions on the detonation behavior will be investigated for the configuration described in this abstract.

References

[1] Kim, W.-W., Menon, S., and Mongia, H. C., "Large Eddy Simulations of a Gas Turbine Combustor Flow," *Combustion Science and Technology*, Vol. 143, 1999, pp. 25–62.

[2] Sankaran, V. and Menon, S., "LES of Spray Combustion in Swirling Flows," *Journal of Turbulence*, Vol. 3, No. 11, 2001.

[3] Génin, F., Chernyavsky, B., and Menon, S., "Large Eddy Simulation of Scramjet Combustion Using a Subgrid Mixing/Combustion Model." *AIAA Paper 2003–7035*, 2003.

[4] Sankaran, V. and Menon, S., "Subgrid Combustion Modeling of 3-D Premixed Flames in the Thin-Reaction-Zone Regime," *Proceedings of the Combustion Institute*, Vol. 30 (to appear), 2004.

[5] Génin, F., Fryxell, B., and Menon, S., "Simulation of Detonation Propagation in Turbulent Gas-Solid Reactive Mixtures," *AIAA Paper 2005–3967*, 2005.

[6] Fryxell, B. and Menon, S., "Large-Eddy Simulation of Richtmeyer-Meshkov Instability." *AIAA Paper 2005–0314*, 2005.

[7] Nelson, C. and Menon, S., "Unsteady Simulations of Compressible Spatial Mixing Layers," *AIAA-98-0786, 36th AIAA Aeropspace Sciences Meeting*, 1998.

[8] Colella, P. and Woodward, P., "The Piecewise-Parabolic Method for Hydrodynamics," *Journal of Computational Physics*, Vol. 54, 1984, pp. 174.

[9] Godunov, S. K., "A Finite Difference Method For The Computation of Discontinuous Solutions of The Equations Of Fluid Dynamics," *Mat. Sbornik*, Vol. 47, 1959, pp. 357–393.

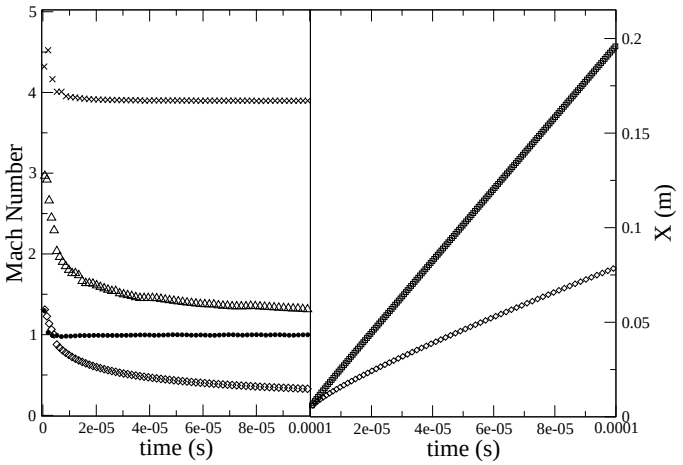


Figure 1: Detonation in a shock tube filled with a reactive mixture. Left panel: Shock front Mach number (triangles: non-reacting, Crosses: Reacting). Mach number behind the shock (Diamonds: non-reacting, solid circles: reacting). Right panel: Shock front location (Diamonds: non-reacting, squares: reacting).

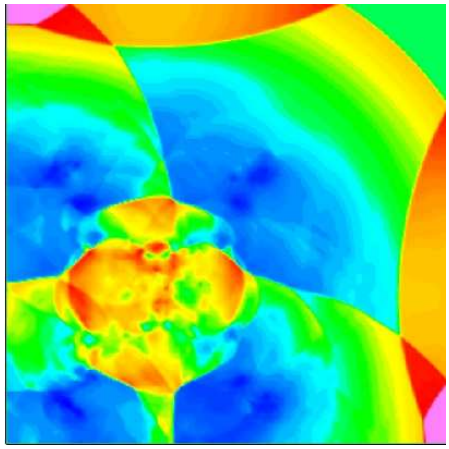


Figure 2: Pressure distribution due to an explosion in a confined cube with an opening in the left wall.

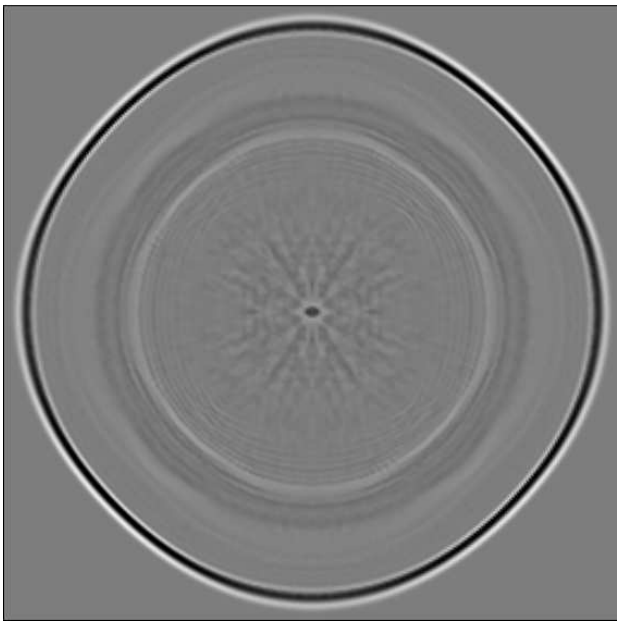
[10] Löhner, R., *Comp. Meth. App. Mech. Eng.*, Vol. 61, 1987, pp. 323.

[11] Marinov, N., Westbrook, C. K., and Piyz, W. J., "Detailed and Global Chemical Kinetics Model for Hydrogen," *Transport Phenomena in Combustion*, edited by S. H. Chan, Talyor and Francis, Washington, DC, 1996.

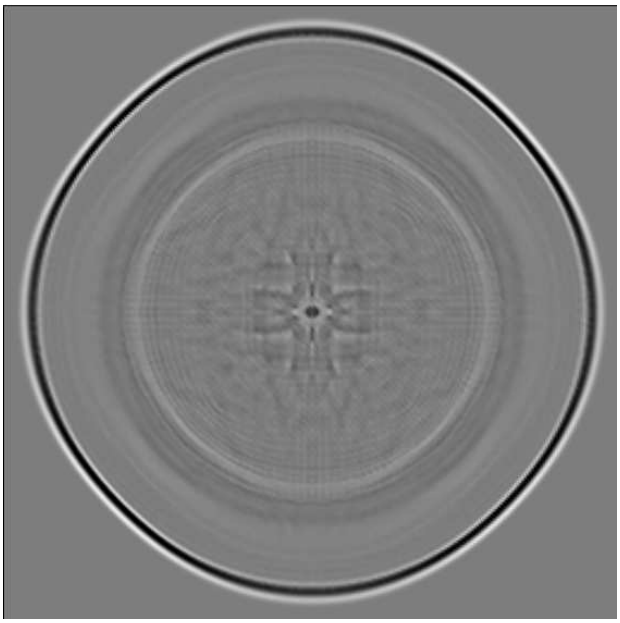
[12] Sone, K., Patel, N., and Menon, S., "Large-Eddy Simulation of Internal Combustion Engines," *Computational Combustion Lab Technical Report, CCL-TR-01-008, May, 2001*, 2001.

[13] Génin, F. and Menon, S., "LES of Supersonic Combustion of Hydrocarbon Spray in a SCRAMJET," *AIAA Paper 2004–4132*, 2004.

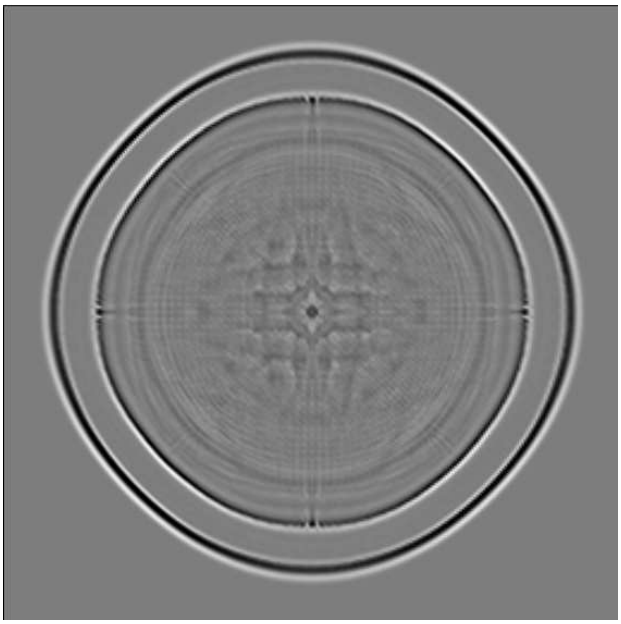
[14] Beckstead, M. W., "A Summary of Aluminum Combustion," *paper presented at the RTO/VTI Special Course on Internal Aerodynamics in Solid Rocket Propulsion, 21–23 May 2002*, 2002.



(a)



(b)



(c)

Figure 3: Numerical shadowgraphs of the detonations under different initial conditions. a) No particles in the flow. b) medium loading of particles, inside the over-pressurized region. c) high loading of particles surrounding the initial over-pressure region.

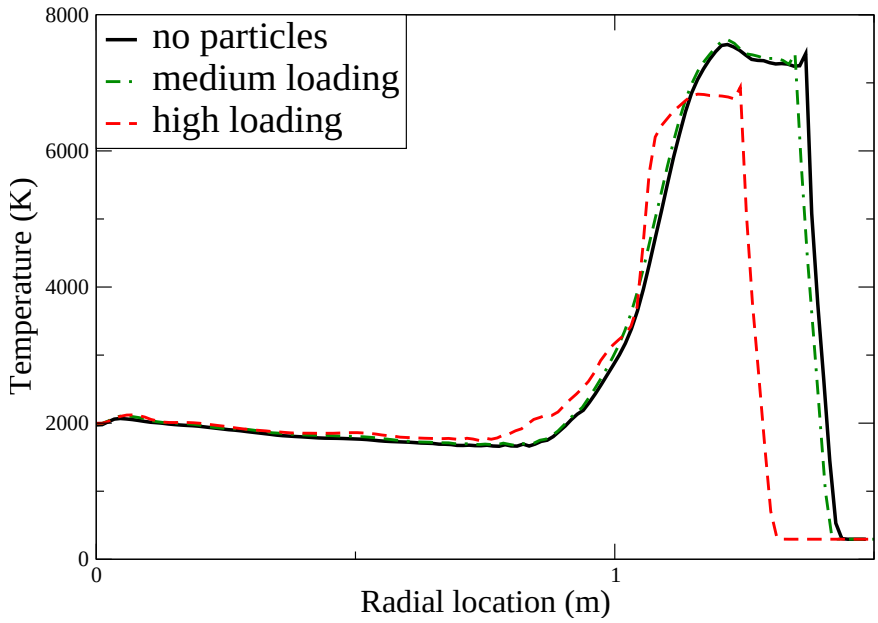


Figure 4: Comparison of the temperature profiles at the same physical time, for the three different initial conditions of detonative systems.