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Multi-Dimensional Adaptive Simulation of Shock-Induced Detonation

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This paper describes an efficient strategy for solving the Euler gas dynamics equations for mixtures of thermally perfect gases with non-equilibrium reaction chemistry using high resolution versions of Godunov's scheme available in the CLAWPACK suite. The approach uses the Berger–Colella block structured adaptive mesh refinement technique for explicit time-dependent finite volume schemes to overcome the stiffness problem arising from the wide time scales. One- and two-dimensional detonation simulation for the oxyhydrogen reaction mechanism in Cartesian geometry was performed and the strategy for non-equilibrium reaction terms has been outlined.

Keywords: Berger–Colella; CLAWPACK; adaptive mesh refinement; detonation; shock tube

Introduction

In the Zel'dovich–von Neumann–Döring (ZND) model,[1] a detonation is a reacting flow mechanism wherein a strong shock wave, coupled with a chemical reacting zone, propagates at supersonic speed. While the ZND model and the predecessor Chapman–Jouguet model have been instrumental in the study of detonations, they are one-dimensional only. Thus, they are unable to truly capture the three-dimensional nature of detonations. Lately, three-dimensional modeling of detonations has been attempted.[2–6]

Numerical simulations can be used to provide an understanding of the multi-dimensional nature of detonation waves. But accurate simulations require methods that can resolve a wide range of length and time scales of the fluid flow and the chemical kinetics that cause numerical stiffness. The Berger–Colella block-structured adaptive mesh refinement (AMR) technique, which is designed specifically for explicit time-dependent finite volume schemes, is able to overcome the stiffness problem by dynamic grid adaptation.[7] A three-level schematic of the concept is shown in Fig. 1. Regions with a sharp gradient, say of density, are packed with more grids which enhances the local resolution.

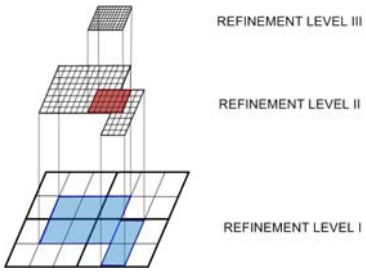

Fig. 1 A three-level patch refinement strategy

Numerical Method

The need to resolve the chemical kinetics so as to properly capture the ZND structure creates enormous numerical difficulties.[8,9] In this paper, the Euler equations with chemically reacting source terms are solved with a finite volume scheme. The chemical reactions introduce small scales which lead to numerical stiffness, requiring grids of high resolution. In particular, the shock front in the detonation wave is extremely sensitive to the reaction zone and the Riemann problem at the detonation front is changed remarkably leading to incorrect detonation speeds, should the grids fail to resolve the reaction detail accurately. On the other hand, the physical geometry may be of the order of meters. The wide range of scales can be treated by AMR techniques.

This paper describes the application of the **C**onservation **LAW**s **PACK**age[10] with a Runge–Kutta time operator splitting technique to account for temporal stiffness.[11] This approach enables the homogenized Euler equations to be solved separately and introduces the source terms as ordinary differential equations.

Governing Equations

The set of time-dependent, coupled, partial differential equations for gas-phase, inviscid reactive flows is given by

$$\frac{\partial \vec{Q}}{\partial t}+\frac{\partial \vec{F}}{\partial x}+\frac{\partial \vec{G}}{\partial y}=\vec{S} \tag{1}$$

where

$$\vec{Q}=\begin{bmatrix}\rho_i\\ \rho u\\ \rho v\\ \rho E\end{bmatrix},\quad \vec{F}=\begin{bmatrix}\rho_i u\\ \rho u^2+p\\ \rho uv\\ (\rho E+p)u\end{bmatrix},$$
$$\vec{G}=\begin{bmatrix}\rho_i v\\ \rho uv\\ \rho v^2+p\\ (\rho E+p)v\end{bmatrix}\quad \vec{S}=\begin{bmatrix}W_i\dot{\omega}_i\\ 0\\ 0\\ 0\end{bmatrix} \tag{2}$$

In the above equations, $i=1,\ldots,N_s$ where N_s denotes the number of species assumed to be ideal gases in thermal equilibrium, ρ_i is the density of species i, u and v are the x and y velocity components respectively, and E is specific total energy. The hydrostatic pressure is obtained from the thermal equation of state $p=\sum_i^{N_s} RT\rho_i/M_i$ where R is the universal gas constant, T is the temperature and M_i is the molecular weight, the evaluation of which necessitates the previous calculation of the temperature. This is accomplished by solving an implicit equation

$$\sum_{i=1}^{N_s}\rho_i h_i(T)-E=RT\sum_{i=1}^{N_s}\rho_i/W_i \tag{3}$$

Source term evaluation

The elementary reaction mechanism for an oxyhydrogen mixture is obtained from Chemkin,[12] which uses the GRI-Mech database and consists of eight species, H, O, H_2, O_2, HO_2, H_2O and H_2O_2, and 27 reactions. The chemical production rate for each species is derived from a reaction mechanism of J chemical reactions as

$$\dot{\omega}_i=\sum_{j=1}^{J}\left(\frac{\rho_l}{M_l}\right)^{\nu_{ji}^r} \tag{4}$$

where $i=1,\ldots,K$ is the number of species, and ν_{ji}^f and ν_{ji}^r are the forward and reverse stoichiometric coefficients of the i^{th} species in the j^{th} reaction. The forward and reverse reaction rates of each chemical reaction are given by k_j^f and k_j^r, respectively. The reaction rates are calculated by the Arrhenius law

$$k_j^f(T)=A_j^f T^{\beta_j^f}\exp\left(-E_j^f/RT\right) \tag{5}$$

The reverse reaction rates can be calculated by assuming the corresponding chemical reaction to be in chemical equilibrium, though detonation simulations require mechanisms that utilize non-equilibrium reaction rates for some of the reactions.[9]

Numerical Method

The **C**onservation **LAW**s **PACK**age[10] was used to discretize the governing equations. It is a finite volume method which uses the integral form of the equations, thus ensuring correct treatment of discontinuities. The general solution approach as proposed by Godunov [13] uses the wave structure determined by the Riemann solution, thus allowing shock waves to be handled properly. The methods used are finite volume on uniform rectangular grids in one dimensional Cartesian coordinates given by

$$Q_i^{n+1}=Q_i^n-\frac{\Delta t}{\Delta x}\left(F_{i+1/2}^n-F_{i-1/2}^n\right) \tag{6}$$

The value of Q_i^{n+1} is an approximation to the cell average of $\vec{Q}$ over the ith cell and F is the numerical flux function.

Godunov's method can be extended to a high-resolution scheme by taking the modified form of Eq. (6) as

$$Q_i^{n+1}=Q_i^n-\frac{\Delta t}{\Delta x}\left(A^- Q_{i+1/2}^n+A^+ Q_{i-1/2}^n\right)-\frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+1/2}^n-\tilde{F}_{i-1/2}^n\right) \tag{7}$$

where $A^{\pm}Q_{i\mp1/2}^n$ are the fluctuations corresponding to Godunov's method and the flux $\tilde{F}_{i\pm1/2}^n$ is the high resolution correction. By this approach, it becomes easy to extend the scheme to second and higher orders using CLAWPACK, which has the built-in functionality to select the required scheme for the problem to be solved.

Linking the chemical kinetics model with the finite volume model requires numerical integration of stiff ODEs. The rate equation has to be integrated first before the evaluation of the reaction rates. Integration of reactive source terms requires the solution of the ODE

$$\frac{\partial\rho_i}{\partial t}=M_i\dot{\omega}_i(\rho_i,T),\quad i=1,\ldots,N_s \tag{8}$$

The total density ρ, the specific energy E and the velocities (u,v) in a cell remain unchanged during the integration, meaning that the chemical reaction is adiabatic. Detailed chemical kinetics are stiff ODE which are solved within CLAWPACK with a semi-implicit second-order Runge–Kutta method which has good accuracy

The chemical reaction rates and thermodynamic constants are evaluated based on the Chemkin-II library.[12] The Jacobian of the rate function $\dot{\omega}_i(\rho_i,\ldots,\rho_{N_s},T)$ required by the ODE solver is approximated using standard difference quotients.

The accurate simulation of detonation waves require computational meshes which can correctly represent local

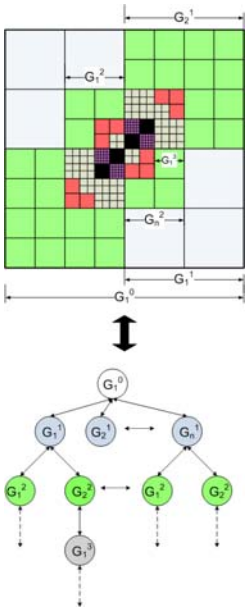

Fig. 2 Berger-Oliger AMR scheme – Adaptive grid hierarchy in 2D [14]

flow changes occurring due to chemical reactions. Specifically, the region between the shock and the head of the chemical reaction zone requires high resolution because the shock is sensitive to the changes in the reaction zone. The Berger–Colella[14] block-structured dynamic mesh refinement strategy was implemented here for capturing the rapid changes within the detonation wave. A patch-wise refinement strategy is adopted rather than replacing individual cells by finer ones as illustrated in Fig. 2. The cells being flagged by an error estimator are clustered into boxes. Thus the refinement regions are described in a geometric pattern. Refined grids are recursively generated from coarser meshes and an entire hierarchy of grid patches is therefore constructed. Since all grid patches are logically rectangular, the adaptive algorithm calls a single integrator routine automatically. This method ensures proper transfer of the cell values between coarse and refined grids using conservative interpolation functions. When compared to the usual unstructured AMR approaches, this AMR strategy is more efficient due to the application of refined time-steps on finer subgrids. This is important because application of the same refinement factor in space-time will result in the CFL number staying the same.

Results and Discussion

Preliminary code validation to estimate the accuracy of the shock-capturing algorithm is the Sod shock tube problem.[15] Here, a reactive Sod's problem is reported where a 30 cm long driver section is filled with high-pressure helium and a 50 cm long driven section is filled with a stoichiometric oxyhydrogen mixture initially at STP. An initial, uniform, 500 cell distribution for the entire tube and a five-level refinement are used for this simulation. Closed boundary conditions are imposed at the left end.

Depending on the driver conditions, either a deflagration or a detonation is propagated in the reactive mixture. With the helium driver at 10 atm, a detonation wave is sustained in the driven tube. Also, the results show that the propagation is initially overdriven, but decreases to CJ values rapidly.

The density gradient profiles in Fig. 3 shows an undulating wave-front in contrast to other simulations of detonation waves. The use of highly refined grids at the shock front has captured triple shear phenomena which would have not been possible with uniform grids in a reasonable amount of time.

One-dimensional simulations under the same conditions (Fig. 4) show a distinct von Neumann spike and defined Taylor rarefaction waves, characteristic of detonations. The detonation velocity of 1120 m/s, a CJ temperature of 3110 K compare well against theoretical results. The velocity behind the shock front is sustained at almost 450 m/s as the high-pressure helium is exhausted.

Conclusions

An efficient numerical framework for numerical simulation of detonations using AMR was implemented that can resolve all spatial and temporal scales. High-resolution shock capturing schemes using CLAWPACK were employed to reduce the number of grid cells. The AMR algorithm provided the required resolution dynamically and eliminated the use of inefficient uniform meshes. One-dimensional simulations of a reactive Sod's problem showed that both shock-induced deflagrations and detonations can be captured.

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Fig. 3 Density-gradient plots of a propagating detonation wave

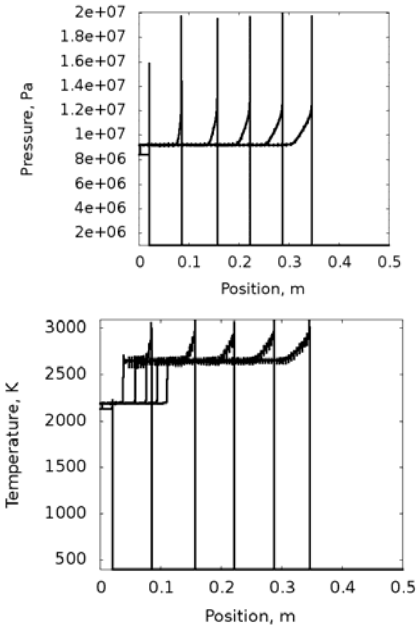

Fig. 4 One dimensional pressure and temperature profiles of a propagating detonation wave

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