DOMAIN DECOMPOSITION AND COMPUTATION OF TWO DIMENSIONAL DETONATION WAVES

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ABSTRACT. We present a hybrid domain decomposition numerical method for the computation of 2-D detonation waves. The numerical algorithm uses a multi-domain approach so that different numerical techniques and mesh resolution can be applied for different components of detonation waves. The detonation waves are assumed to undergo an irreversible, unimolecular reaction $A \to B$.

1. Introduction

In this paper, we present a hybrid numerical methods with domain decomposition technique for the computation of 2-D detonation waves. Previous work can be found in [8], [6] and [1] and the references therein. The motivation of our using domain decomposition is based on the special physical characteristics of detonation waves [5]. They include (1) a strong precursor detonation front; (2) Mach stem configuration of the "triple points" and transverse wave structures; (3) stiff chemical reactions. Thus, the flow field can be divided into regions of highly irregular and steep gradients near the detonation front and regions of strong but smooth pressure waves. Near the shock fronts, strong vorticity fields are expected from the roll-up of slip lines. The temporal changes of thermodynamic and chemical compositions also vary dramatically from region to

region. We construct our numerical schemes according to these characteristics of multi-dimensional detonation waves.

The reaction rate depends on the flow temperature exponentially through the Arrhenius relation. Accurate computations of the flow field are extremely important in producing the correct chemical reactions and thus the correct cellular structures. Traditional shock capturing schemes, designed to smooth shock and contact discontinuities, introduce a considerable amount of numerical viscosity near those discontinuities. They have been shown to have a tendency to distort the real chemical reaction processes. In [3], the widely used P.P.M. high-order Godunov scheme was found to produce nonphysical weak detonations. Also in [4], the ENO finite difference scheme was shown to yield wrong detonation speeds in one dimensional ZND simulations. All these facts point out the importance of designing numerical methods without excessive numerical viscosity.

2. Governing Equations

Consider two dimensional overdriven detonation waves in a channel moving from left to right into unreacted gas mixtures. The channel is denoted by Ω (Figure 2), $\Omega = (-\infty, \infty) \times [-\frac{W}{2}, \frac{W}{2}]$ where W is the channel width.

The governing equations for reacting detonation waves with one step $A \longrightarrow B$ reaction are the following nondimensionalized Euler equations,

$$(2.1) \qquad \frac{\partial \vec{u}}{\partial T} + \frac{\partial f(\vec{u})}{\partial x} + \frac{\partial g(\vec{u})}{\partial y} = \Phi(\vec{u}),$$

where

$$\vec{u} = (\rho, \rho u, \rho v, \rho e, \rho_A)^\top,$$

$$f(\vec{u}) = \left(\rho u, \rho u^2 + p, \rho u v, \rho u(e + \frac{p}{\rho}), \rho_1 \right)^\top,$$

$$g(\vec{u}) = \left(\rho v, \rho v u, \rho v^2 + p, \rho v(e + \frac{p}{\rho}), \rho_A v \right)^\top,$$

$$\Phi(\vec{u}) = (0, 0, 0, 0, \omega)^\top,$$

and $(u, v), \rho, p, e$ are velocity vector, density, pressure, and total specific internal energy. ρ_A is the mass density of the reactant A. The source term is $\omega = -K\rho\lambda\exp(-\frac{E^+}{T})$ where $\lambda = \frac{\rho_A}{\rho}$ and E^+ is the activation energy. If we assume an exothermic reaction, the specific internal energy is

$$(2.2) \qquad e = \frac{p}{(\gamma - 1)\rho} + \frac{u^2 + v^2}{2} + \lambda Q$$

where Q is the specific heat formation and $\gamma = 1.2$ is the ratio of specific heats. All quantities above have been non-dimensionalized by the initial states in the unreacted gas mixture in front of the detonation fronts.

3. Domain Decomposition and Hybrid Algorithm

The computational region is composed of the detonation front moving to the right and the rear piston boundary and upper and lower solid walls. In the computation presented in this paper, we take this region to be $[-150\ell^*, 0] \times [-\frac{W}{2}, \frac{W}{2}]$ where ℓ^* is the half reaction distance. $x = 0$ is the position of initial plane detonation front at $t = 0$ which will be curved as time progresses. The computational region is decomposed with the detonation front as the right most boundary. Method of lines will be used to discretize the Euler equations (2.1). Third order Runge-Kutta is used as time integrator while a combination of three spatial discretization techniques is applied in different parts of computational region. They are

- Shock tracking algorithm for the detonation front;
- High order ENO finite difference scheme in the subdomain which contains the reflected shocks and contact discontinuities along the detonation front;
- Chebyshev collocation method for the strong vorticity and pressure fields from the interaction of transverse waves along the detonation front.

We refer the reader to [2],[7] for the descriptions of those numerical techniques and will only describe here the implementation of interface condition between adjacent subdomains.

4. Interface Conditions between Subdomains

The idea underlying the treatment of the interface and the boundary conditions is the propagation of information along characteristics of the hyperbolic systems. On a typical interface between two subdomains, say Γ between Ω_l and Ω_r, $\vec{v} = (P, u, v, \rho, \lambda)^\top$ is the primitive flow variable, and $\vec{v}^l, \vec{v}^r$ denote the solutions computed for the time step t^{n+1} in Ω_l, Ω_r respectively. $S_{\Gamma,I}$ denotes the normal speed of the interface at point I with the normal direction $n = (n_x, n_y)$. The characteristic variables are

$$
(4.1) \qquad w_1 = p - \bar{a}\bar{\rho}u_n
$$

$$
(4.2) \qquad w_2 = u_t
$$

$$
(4.3) \qquad w_3 = p - \bar{a}^2\rho
$$

$$
(4.4) \qquad w_4 = \lambda
$$

$$
(4.5) \qquad w_5 = p + \bar{a}\bar{\rho}u_n
$$

where the overbar denotes an average state between $\vec{v}^l$ and $\vec{v}^r$.

In order to update $\vec{v}$ at point I for the time step t^{n+1}, we make the following correction on $w_i, 1 \leq i \leq 5$ based on the sign of the difference between the eigenvalues and the normal speed of the interface $S_{\Gamma,I}$, i.e.

$$
(4.6) \qquad w_i^{corrected} = \begin{cases} w_i^r & \text{if } \lambda_i - S_{\Gamma,I} < 0 \\ w_i^l & \text{if } \lambda_i - S_{\Gamma,I} \geq 0. \end{cases}
$$

Finally, we set $\vec{v}^r = \vec{v}^l = \vec{v}^{corrected} = T^{-1} w^{corrected}$.

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5. Numerical Results

We present one set of numerical results of 2-D detonation waves using the hybrid scheme. Consider a detonation wave with parameters $Q = 50, E^+ = 50, f = 1.6$, and channel width $W = 20\ell^*$, again ℓ^* is the half reaction distance. The domain of computation is chosen to be $[-150\ell^*, 0] \times [-10\ell^*, 10\ell^*]$ in (x, y) coordinate. Mesh convergence test [2] has shown that 13-15 points per half reaction distance is needed in the reaction zone, a uniform mesh based on this resolution will result in a mesh size $= 260 \times 1950 = 500,000$ points. By using domain decomposition, we can distribute most of the mesh points in the reaction region (in the right most subdomain) and the computational mesh consists of $\sum_{i=1}^9 (n, m) = (50, 250) + (34, 70) + (20, 40) + (20, 30) + (20, 30) + (10, 20) + (10, 10) + (10, 10) + (10, 10) = 17,380$ points, which is a saving of 20 times over the uniform mesh. The number of 'Marker Points' on the shock front is 300. Figure 1 shows a two cell pattern produced by the trajectories of four triple points (A, B, C and D) which is obtained by recording the pressure distribution along the detonation front at different times. There is a larger cell with width approximately $10\ell^*$ (half the channel width) and a smaller one with width $5\ell^*$. Figure 2 contains six snapshots of the detonation at time $t = 20.25t^*, 21.5t^*, 22t^*, 22.5t^*, 23t^*, 23.5t^*$, t^* is the half reaction time. A random perturbation with magnitude $\epsilon = 0.3$ is used to perturb the shock front at $t = 0$.

6. Conclusion

The multi-domain approach allows different numerical techniques and mesh resolutions to be applied for different components of detonation waves. The propagation of waves across the interfaces of subdomains is smooth and the order of accuracy of the whole numerical scheme is only limited by the accuracy of the time integrator. Tracking of the detonation front prevents differences across the detonation front, thus avoiding excessive numerical viscosity in shock capturing schemes. The adaptivity in numerical schemes makes accurate simulation of 2-D detonation waves possible while adaptivity in mesh resolution yields big saving in CPU time.

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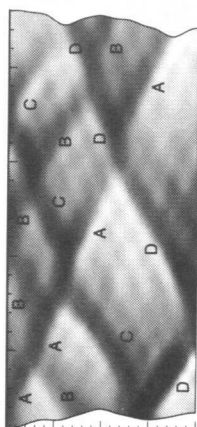

FIGURE 1. Cell pattern of detonation waves

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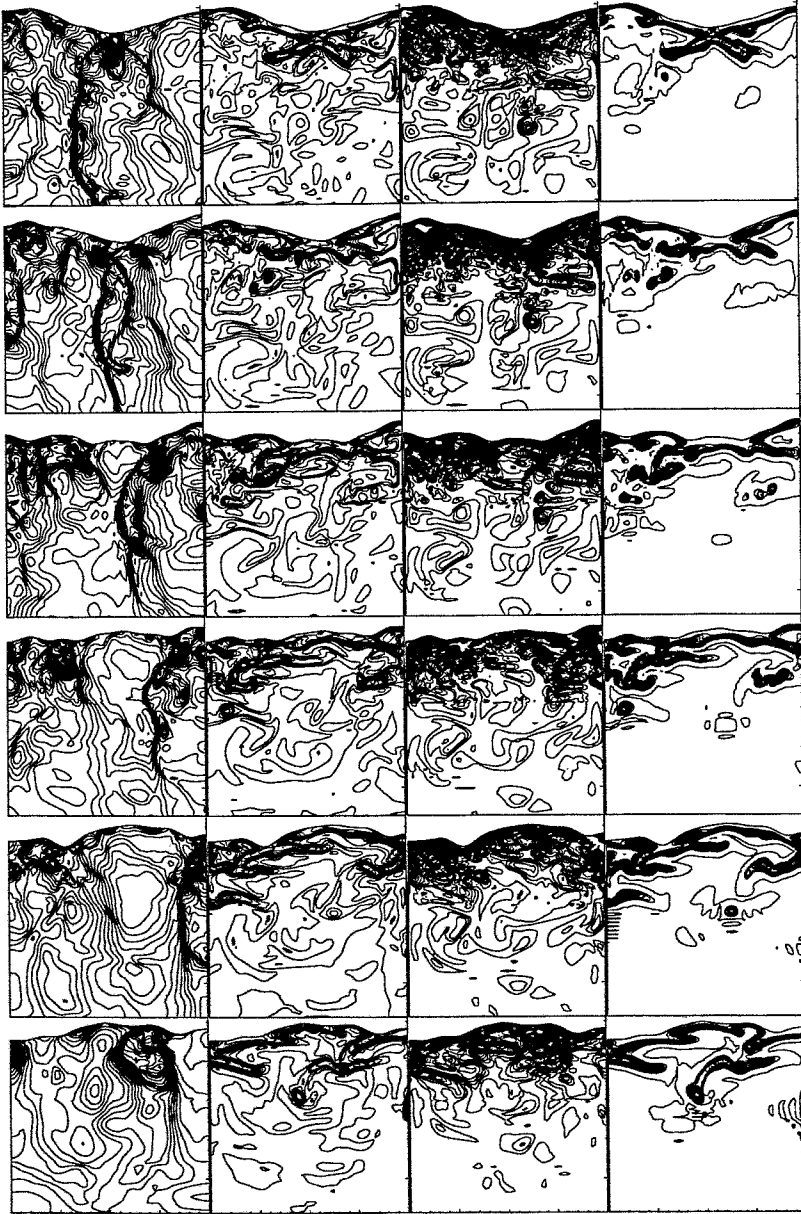
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FIGURE 2. Six snapshots of (from top to bottom) pressure, temperature, vorticity, and mass fraction of reactant at $t =$ $20.25t^*$, $21.5t^*$, $22t^*$, $22.5t^*$, $23t^*$, $23.5t^*$.