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Parallel adaptive mesh refinement method based on WENO finite difference scheme for the simulation of multi-dimensional detonation ☆

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ABSTRACT

For numerical simulation of detonation, computational cost using uniform meshes is large due to the vast separation in both time and space scales. Adaptive mesh refinement (AMR) is advantageous for problems with vastly different scales. This paper aims to propose an AMR method with high order accuracy for numerical investigation of multi-dimensional detonation. A well-designed AMR method based on finite difference weighted essentially non-oscillatory (WENO) scheme, named as AMR&WENO is proposed. A new cell-based data structure is used to organize the adaptive meshes. The new data structure makes it possible for cells to communicate with each other quickly and easily. In order to develop an AMR method with high order accuracy, high order prolongations in both space and time are utilized in the data prolongation procedure. Based on the message passing interface (MPI) platform, we have developed a workload balancing parallel AMR&WENO code using the Hilbert space-filling curve algorithm. Our numerical experiments with detonation simulations indicate that the AMR&WENO is accurate and has a high resolution. Moreover, we evaluate and compare the performance of the uniform mesh WENO scheme and the parallel AMR&WENO method. The comparison results provide us further insight into the high performance of the parallel AMR&WENO method.

1. Introduction

Detonation involves complex interactions between reactive chemical kinetics and fluid dynamics. It consists of a precursor shock wave that propagates into the unreacted medium at supersonic speed with a thin reaction zone immediately behind the shock. The research on detonation phenomena has lasted for more than one hundred years, yet even today many phenomena are still not very well understood. Because of the limited insight that experimental observations can provide, numerical simulations play a more and more important role in the investigation of detonation phenomena.

Detonation waves exhibit non-negligible multi-dimensional sub-structures. These sub-structures are in the millimeter range which is much smaller than the size of the physical geometry. The additional stiff source terms modeling chemical

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reactions introduce extremely small time scales into the flow field which are much smaller than the fluid-dynamical time scale. There is a requirement of a locally refined resolution for the numerical method, due to the separation in both time and space scales. The adaptive mesh refinement (AMR) method has an advantage for solving such problems with separation scales. It automatically refines the mesh locally where a fine resolution is needed. The AMR method was first developed by Berger et al. [1,2] to solve hyperbolic partial differential equations. Nowadays it is widely used in detonation simulation and has been validated to be an effective tool [3–11].

Recently, weighted essentially non-oscillatory (WENO) schemes have attracted increasing attention in the investigation of detonation owing to their advantage of high order accuracy, high resolution and essentially non-oscillatory shock resolution [12–14]. As is well known, WENO schemes can resolve complex solution structures with a relatively coarse numerical mesh. However, the mesh should still be refined enough to resolve detonation phenomena. High order conservative finite difference WENO schemes are very efficient in multi-dimensions in comparison with finite volume WENO schemes, yet they require uniform or smooth varying meshes. It is expensive in the investigation of detonation waves which would only need a locally refined resolution.

In order to develop an efficient method for detonation simulation, this paper aims to combine AMR methods with WENO schemes. The coupling of AMR methods and WENO schemes has been extensively studied. Li and Hyman [15] used a fifth order Lagrange interpolation for the prolongation in the space and a locked time step method in time. The locked time step method avoids time refinement, with the time step size limited by the CFL condition of the finest mesh. It may result in a waste of the computational effort. Baeza and Mulet [16] adopted the linear interpolation in time which would reduce the temporal accuracy of the scheme. Shen et al. [17] proposed an AMR method based on high order WENO schemes for hyperbolic conservation laws. High order prolongation is used in both space (WENO interpolation) and time (Hermite interpolation). The AMR method with high order prolongation is proved to be an accurate and robust method. However, due to the adoption of block-based data structure, the method in [17] may involve unprofitable refinement and is inflexible in dealing with complicated geometry. Also, the simulation is performed on hyperbolic conservation laws without considering possible complications from stiff source terms.

This paper focuses on developing an AMR method base on the fifth order WENO finite difference scheme for detonation problems, which is a generalization of the method in [17]. The outline of the paper is as follows. In Section 2, an appropriate model for gas detonation is proposed. The one-step Arrhenius chemistry model is utilized in this paper. Section 3 gives a description of the WENO scheme and introduces the detailed implementation of the parallel AMR&WENO method. In Section 4, the parallel AMR&WENO method is used to investigate a series of multi-dimensional detonation problems and a detailed analysis of the numerical results is provided.

2. Governing equations

The reaction mechanism adopted in this paper is the one-step reaction model. It is well known that one-step reaction models cannot reveal the detailed reaction chemistry of detonations and cannot give quantitatively correct description of detonation. However, it does have the practical advantage in terms of computational cost. In the investigation of detonation, detailed reaction models consume huge amount of computer resource. It is not realistic to use the detailed reaction model to simulate detonation in large domains or for high dimensional problems. In many situations, one-step reaction models are good choices as a compromise between cost and performance.

This paper aims to develop and test a numerical method, hence the simple one-step reaction model is a good testing model. This model for detonation propagation in premixed gases neglects the effect of viscosity, the heat transfer, the diffusion and body forces. It can be written as the Euler equations with reactive source terms. In three-dimensional Cartesian coordinates, these equations are given as follows

$$\begin{aligned}
&\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}+\frac{\partial H}{\partial z}=S\\
&U=(\rho,\rho u,\rho v,\rho w,\rho E,\rho Y)^T\\
&F=(\rho u,\rho u^2+p,\rho uv,\rho uw,(\rho E+p)u,\rho uY)^T\\
&G=(\rho v,\rho uv,\rho v^2+p,\rho vw,(\rho E+p)v,\rho vY)^T\\
&H=(\rho w,\rho uw,\rho vw,\rho w^2+p,(\rho E+p)w,\rho wY)^T\\
&S=(0,0,0,0,0,\omega)^T
\end{aligned}\tag{1}$$

where u, v and w are the components of the fluid velocity in the x, y and z directions, respectively. ρ is the density, p is the pressure, E is the total energy per unit volume, and Y is the mass fraction of the reactant.

The total energy E is defined as following

$$E=\frac{p}{\rho(\gamma-1)}+\frac{(u^2+v^2+w^2)}{2}+qY \tag{2}$$

where q is the heat production in the reaction, and γ is the ratio of specific heat.