Adaptive Mesh Refinement Method Based on High Order Finite Difference WENO Scheme for Detonation Simulation

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1 Introduction

Detonation is a very complex hydrodynamic flow coupling with chemical kinetics. It consists of a shock wave followed by a zone in which the fuel is rapidly consumed. For direct numerical simulation of detonation, additional source terms modeling chemistry introduce extremely small scales into the flow. Due to multi-scale nature of detonation, the discretization of the flow domain needs to use properly grid system. Unless a very fine grid system is employed in reaction zone, the details of the detonation structure can not be revealed. Uniform mesh is a computationally expensive procedure due to the large separation of the characteristic scales. Adaptive Mesh Refinement(AMR) method refines the mesh locally to focus computational effort on reaction zone. As an efficient approach for detonation simulations, AMR method has become increasingly popular in recent years [1, 2].

We describe an AMR method based on high order finite difference Weighted Essentially Non-Oscillatory (WENO) scheme. The method combines the Berger–Colella [3] block structured AMR method with high order finite difference WENO scheme and Runge–Kutta method. The details of the method are outlined in the paper. We apply the method to solving Euler equations coupling with chemical reaction, which is an appropriate model for detonation. The performance of the method is analyzed by the instability [4] of low-overdrive detonations in high activation energy gaseous mixtures. One and two-dimensional test cases are performed. The results of the test cases demonstrate the advantages of the method from the view of accuracy and high efficiency.

The paper is organized as follows. Section 2 summarizes the governing equations for the detonation and the numerical method. Section 3 focuses on the implementation of AMR method based on high order finite difference WENO scheme. In Section 4, the results of one and two-dimensional numerical simulations are presented. The conclusions are summarized in Section 5.

2 Governing equations

The appropriate model for detonation propagation in premixed gases neglects the effect of viscosity, the heat transfer, diffusion and body forces. It can be written as the Euler equations with reactive source terms. In two-dimensional Cartesian coordinates these equations are given by:

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

$$\begin{aligned} U &= (\rho, \rho u, \rho v, \rho E, \rho Y)^T \\ F &= (\rho u, \rho u^2 + p, \rho uv, (\rho E + p)u, \rho uY)^T \\ G &= (\rho v, \rho uv, \rho v^2 + p, (\rho E + p)v, \rho vY)^T \\ S &= (0, 0, 0, 0, \omega)^T \end{aligned} \tag{2}$$

Here u and v are the components of the fluid velocity in x and y 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

$$E = p/(\gamma-1)\rho + (u^2+v^2)/2 + qY \tag{3}$$

Here q is the heat production by chemical reaction, and γ is the ratio of specific heats, the source term ω is assumed to have an Arrhenius form and written as

$$\omega = -K\rho Y e^{-(E_a/RT)} \tag{4}$$

Here E_a is the activation energy and K is a constant rate coefficient.

For perfect gas, the state equation is

$$p = \rho RT$$

The governing equations are discretized with fifth-order finite difference WENO scheme in space, and third-order TVD Runge-Kutta method in time.

3 Numerical method

A uniform Cartesian grid is used to discretize the domain $x \in [x_{\min}, x_{\max}]$, with N equally spaced nodes.The full discretization of the solution vector can be written as $U(x,t) \to U_i^n$. Here, i is the spatial node number corresponding to the location $x_i = x_{\min} + (i+1/2)\Delta x$, where $\Delta x = (x_{\max} - x_{\min})/N$,and n is the time level corresponding to $t_n = \sum_{m=1}^{n} \Delta t_m$ where Δt_m is the time step for each integration step. We define $C_i = [x_{i-1/2}, x_{i+1/2}], i = 1,...,N$ as uniform numerical grid with centers at x_i.

The uniform grid above is called 'root grid'. Finer grids, called the child of the root grid, are only created on parts of the domain. The 'root grid' and the child of 'root grid' can be organized into a tree/hierarchy structure.

For fixed mesh refinement ratio $r = 3$, a root grid C_i has three child grid which are defined as $C'_{i,j} = [x_{i-1/2} + (j+1)\Delta x/3, x_{i+1/2} + (j-3)\Delta x/3], j = 1,...,3$. The centers of the child grid are located at $x_i + (j-2)\Delta x/3$.

If k and $\Delta x'$ are defined as $k = 3i - j - 1$ and $\Delta x' = \Delta x/3$, respectively, child grid $C'_{i,j}$ can be expressed as $C'_k = [x'_{k-1/2}, x'_{k+1/2}]$, with $x'_k = x_{\min} + (k+1/2)\Delta x'$. The centers of grid located at x'_k. In order to ensure stability of explicit difference schemes, the time step need to be refined in the same refinement ratio.The time step on the child grid is defined as $\Delta t_{m'} = \Delta t_m/3$. The solution vector can be written as $U_k^{m'}$.

The criterion for refinement comes from the solution of root grid,such as small scale features,variable physical parameters and so on. Mass fraction of the reactant Y is employed as a criterion in this paper. The value of Y is between 0 and 1 in reaction zone.The grids with $0 < Y_i < 1$ are flagged. Two grids around the flagged grid form a buffer zone. The grid in buffer zone is alse flagged to ensure that discontinuities or other regions with large error does not propagate from a fine grid into coarser

regions. Bisection method[5]is used to organize the grids which is flagged into rectangular patch.All root grids in the patch need to be refined. Each patch can be consider as a new domain with finer mesh. On new domain, the numerical algorithm WENO-RK is implemented. Initial solutions and boundary conditions are necessary before we discretized the new domain.

Take time step $[t_n, t_n + \Delta t_m]$ for an example, the details of construction on the patch are as follows. The data on the new domain at t_n is defined as U_k^n. If C_i is covered by previously existing fine grids, then existing data of fine grid are copied directly into U_k^n. Otherwise U_k^n must be obtained from spatial interpolation of the root grid solutions U_i^n. The 5-th WENO interpolation is used in the paper.

$$U_k^n = WI(U_{i-2}^n, U_{i-1}^n, U_i^n, U_{i+1}^n, U_{i+2}^n) \tag{5}$$

All the finer grids on the patch get a solution in the initial stage.

Next step is to construct boundary conditions for the patch, not only at the initial stage, but also at intermediate fine grid time steps and their RK substages. We define Ub as the value of the grids on the patch boundary and employ Hermite interpolation[6] using the value of Ub^n, Ub^{n+1}, $D_t(Ub)^n$, $D_t(Ub)^{n+1}$. $D_t(Ub)$ is the temporal derivatives. $D_t(Ub)^n$, $D_t(Ub)^{n+1}$ are obtained from their spatial derivatives at both t_n and t_{n+1} as

$$D_t(Ub) = \frac{dUb}{dt} = -F(U)_x + S \tag{6}$$

Ub^n and Ub^{n+1} can be constructed by 5-th WENO interpolation. A third order polynomial $M(t)$ is constructed by Hermite interpolation as

$$M(t^n) = Ub_k^n, M(t^{n+1}) = Ub_k^{n+1}, M'(t^n) = D_t(Ub)_k^n, M'(t^{n+1}) = D_t(Ub)_k^{n+1} \tag{7}$$

Take time step $[t_n, t_n + \Delta t_{m'}]$ for an example, the first and second stages in third order TVD RK method are reconstructed as

$$\begin{aligned} &Ub(t_n) = M(t^n) \\ &Ub^{(1)}(t_n) = M(t^n) + \Delta t_{m'} M'(t^n) \\ &Ub^{(2)}(t_n) = M(t^n) + \frac{\Delta t_{m'}}{2} M'(t^n) + \frac{\Delta t^2{}_{m'}}{4} M''(t^n) \end{aligned} \tag{8}$$

$Ub^{(1)}(t_n)$ and $Ub^{(2)}(t_n)$ denote the boudary conditions on the first and second Runge-Kutta stages, respectively.

Based on the values of initial stage and boundary conditions, the solution U_k^n of the fine grids can be evolved to time t_{n+1}.We use the fine grid solution replace the root grid solution. One-dimension AMR method can be easily extended to multi-dimensional problems using a dimension by dimension approach.

4 Results and discussions

The AMR method is first tested by pulsating one-dimension detonation. It is well known that below a threshold in overdrive, one-dimension in high activation energy is unstable and a large number of unstable modes interact with each other in the finite-amplitude, and nonlinear regime. In the increasingly chaotic regime, small differences in truncation errors between algorithms eventually lead to large difference of solutions. In test case, the values of the heat release, activation energy, overdrive factor, and ratio of specific heats are fixed at $Q = 50$, $E_a = 50$, $f = 1.6$ and $\gamma = 1.2$. All one-dimension simulations in the paper are performed on the domain with $x \in [0,1000]$.

Fig.1 shows AMR results using three groups of grids with different sizes. The relative grid size is defined as n. The smaller n means that the size of the grid is smaller. With the decrease of the grid size, the numerical solutions of AMR show a good convergence. Fig.2 shows a comparison between AMR and corresponding uniform mesh. AMR has the same grid size in the reaction zone with the uniform mesh. In other regions, the grid size of AMR is three times that of uniform mesh. The numerical solutions of AMR are observed to match the uniform mesh solution very well.

The point tagged with 'Fickett&Wood' in Fig.3 is an theoretical solution with $Q = 50$, $E_a = 50$, $f = 1.6$ and $\gamma = 1.2$. The value of the point is 98.6. and it can be used to test our numerical method. The results of AMR converge quickly to the point. Fig.4 shows the pressure distribution near the detonation front at t=65. grid points in the reaction zone is finer than other area . resolution of pressure is well shown in Fig.4.

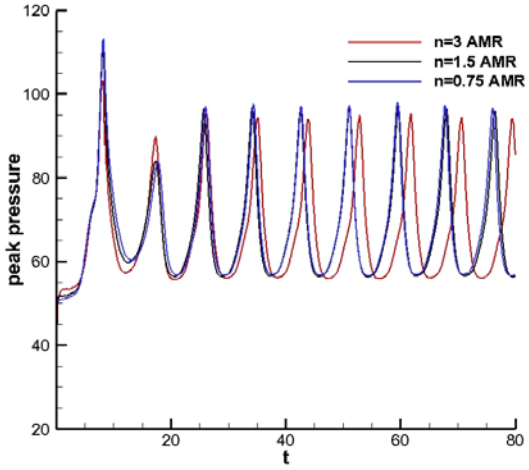


Figure 1. Pressure history at the perturbed ZND shock for one-dimensional plusting detonation. n is the relative grid size, and there is 5/n grids in half reaction.

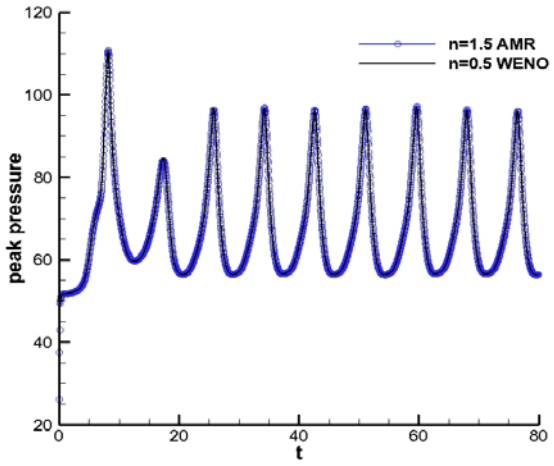
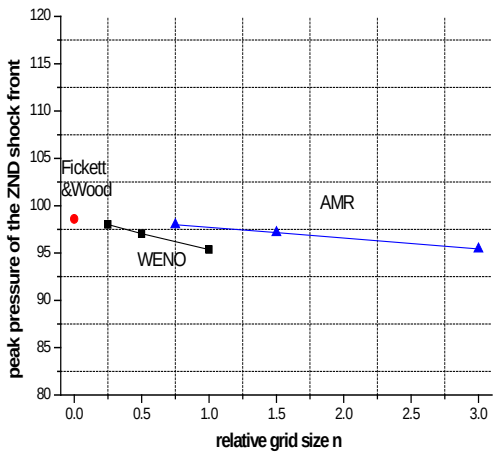


Figure 2. Pressure history at the perturbed ZND shock for one-dimensional plusting detonation of AMR and uniform meshes.



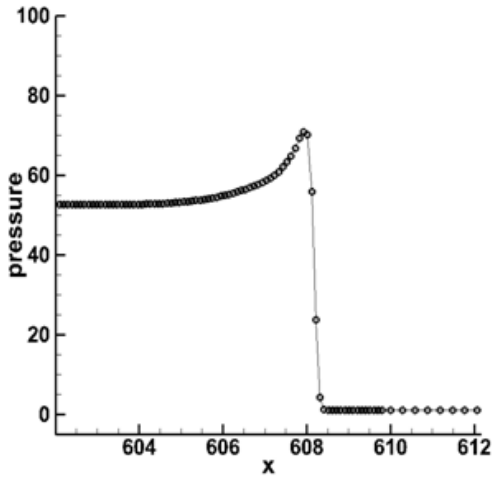


Figure 3. The peak pressure of the ZND shock front in the time domain

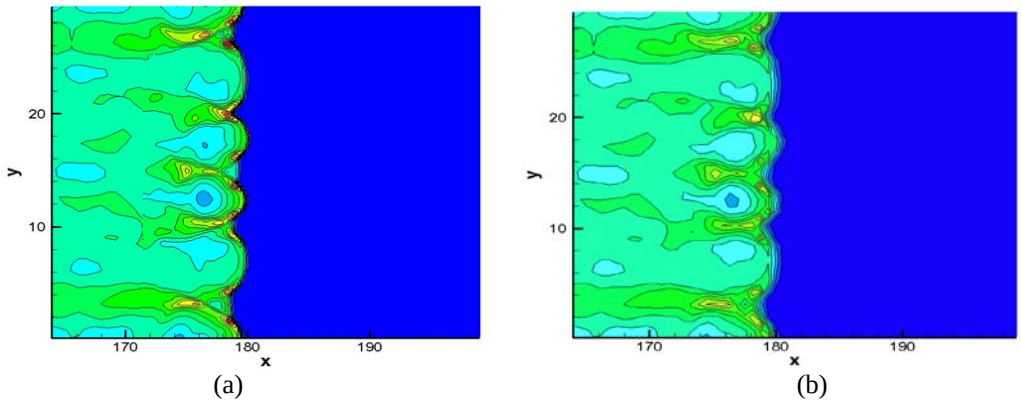
Figure 4. pressure distribution near the detonation front with t=65

Tab.1 outlines the CPU running times of AMR and corresponding uniform mesh. The terminal times of the simulation are both 80. Compared with the uniform mesh, we can find that CPU running time for AMR consumes only 9441 s, therefore AMR in the paper is more efficient.

Table 1: CPU running time Comparison between AMR and uniform mesh

One-dimension plusting detonation	AMR	Uniform mesh
points	3500	10000
CPU time(s)	9441	27755
relative grid size n	1.5	0.5

We extend AMR method to two-dimensional via a dimension by dimension fashion. In two-dimension detonation, the triple point trajectories form regular patterns called detonation cells. Cellular structure depends primarily on the energy release to the mixture. In this test case, the values of the heat release, activation energy, overdrive factor, and ratio of specific heats are fixed at $Q = 50$, $E_a = 50$, $f = 1.05$ and $\gamma = 1.2$. The results shown in Fig.5 are carried out in a channel with a size 30 $L_{1/2}$ × 300 $L_{1/2}$. The base mesh of AMR is 500×50 and the mesh of uniform mesh is is 500×50 too. It is easy to be found from the contour map of the pressure that the flow structure near detonation front is improved very well. The results shown in Fig.6 and Fig.7 are carried out in a channel with a size 30 $L_{1/2}$ × 300 $L_{1/2}$. The base mesh of AMR is 500×50 .The mesh of the uniform mesh is 1500×150. Fig.6 shows that the grids of AMR, the grids point in the reaction area is finer than other area. AMR has the same grid size in the reaction zone with the uniform mesh. In other regions, the grid size of AMR is three times that of uniform mesh. Fig.7 shows the numerical result of AMR. Compared with the result of corresponding uniform mesh in Fig.8, it is found that there are certain differences in the detials of the detonation cells. Because of the unsteadiness of the detonation with $E_a = 50$, small error can make the solution change dramatically. AMR method has minor loss of accuracy in two-dimension detonation. Future work will focus on the improvement of AMR method in three-dimension.The results in Tab.2 confirm the efficiency of AMR.



(a) (b)

Figure 5. (a) pressure distribution near the detonation front of AMR, the base mesh is 500×50
(b) pressure distribution near the detonation front of uniform mesh, the mesh is 500×50

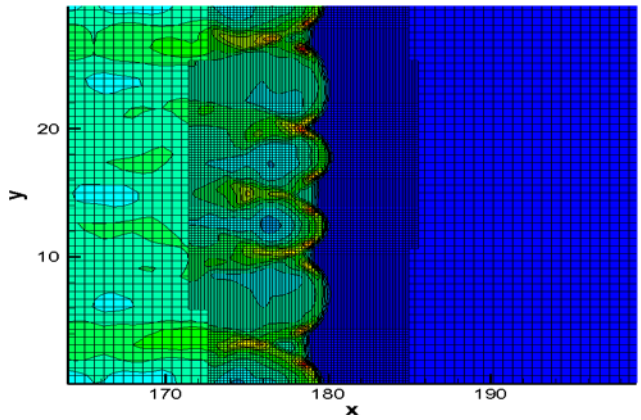


Figure 6. The grid map of AMR

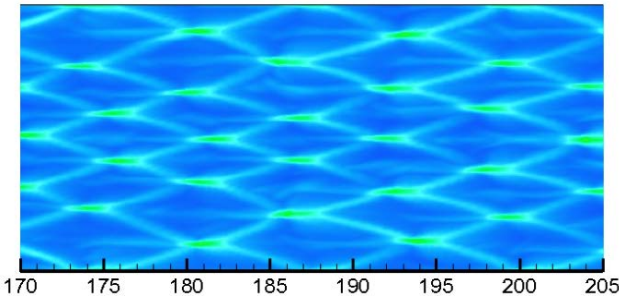


Figure 7. Cellular pattern for AMR method

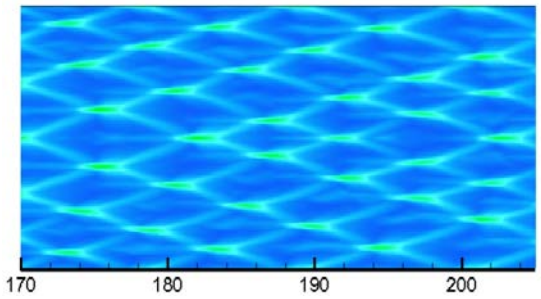


Figure 8. Cellular pattern for uniform mesh

Table 2: CPU running time Comparison between AMR and uniform mesh

Two-dimension detonation	AMR	Uniform mesh
points	500×50	1500×150
CPU time(s)	7116	44340
relative grid size n	1.5	0.5

5 Conclusions

We describe an efficient AMR method based on high order finite difference WENO scheme for numerical simulation of detonations. The performance of the method is analyzed by instability of low-overdrive detonations in high activation energy gaseous mixtures. It is well known that Low-overdrive detonations in high activation energy gaseous mixtures are unstable to both longitudinal and transverse modes. Small differences in truncation errors between algorithms eventually lead to dramatic change of solutions. We obtain one and two-dimensional results of the test case. In pulsating one-dimension detonation test case, the solution of AMR matches the corresponding uniform mesh solution very well. CPU running time of uniform mesh is three times that of AMR. In two-dimension detonation test case, there are some difference between the solution of AMR and corresponding uniform mesh, but CPU running time of uniform mesh is six times that of AMR. In general, the method performs very well in detonation simulations and it provides significant savings in CPU time with only minor loss of accuracy.

Acknowledgments

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