Simulation of Continuous Detonation in H₂-O₂ Mixture Using Adaptive Mesh Refinement

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Abstract:
The Internal flow of a Continuous Detonation Wave Rocket Engine (CDWRE) is characterized by a large spectrum of scales, both spatial and temporal. The necessity to have a fine resolution within a relatively large computational domain represents an important difficulty especially for 3D simulations. To cope with this problem, the method of Adaptive Mesh Refinement (AMR) can be used. This paper presents some simulations performed with an Euler solver integrated in an AMR code. Results obtained for a model problem of detonation propagation in a layer of stoichiometric H₂-O₂ mixture are used to evaluate the AMR code efficiency. Examples of 2D and 3D simulations of CDW are presented.

Key words: continuous detonation engine, H₂-O₂ mixture, 3D numerical simulation, adaptive mesh refinement.

1 Introduction

During the last decade, the interest in the use of CDW in aerospace propulsors has been growing quickly. Both experimental and computational studies are under way in different countries. In France, ICARE-CNRS closely collaborates with MBDA France and contributes to the numerical studies of the CDW process. At the moment, the main effort is focused on the hydrogen-oxygen mixture, which is suitable for space launchers. A parametric study of a CDWRE chamber has been already carried out using a high-resolution 2D Euler solver [1, 2]. This study permitted to characterize numerical requirements to the spatial and temporal resolution. The obtained results allowed to analyze the flow structure, to identify problem scaling factors, and to determine trends for some important characteristics of the CDW process.

The periodic flow structure in the CDWRE chamber is shown in Fig. 1. The chamber geometry is defined by the length of the constant-area section, \(L\). The main geometric parameter and scaling factor characterizing the flowfield is the period between two consequent CDW, \(l\). The \(h\) size corresponds to the detonation front height, which is proportional to \(l\). The propellant injection is characterized by the relative injection area, \(A_j/A_w\), the total injection pressure, \(P_{ij}\), the total temperature, \(T_{ij}\), and the injected mixture composition. For the present study, it is supposed that \(T_{ij} = 300\) K and the injectant is represented by a homogeneous stoichiometric mixture of H₂ and O₂.

Simulation of the CDWRE chamber operation is connected with several issues. The compression and combustion processes within the detonation waves are extremely rapid, whereas the overall convective motion of the flow is several orders of magnitude slower. As the detonation propagation simulation requires fine spatial and temporal resolution, the simulation of the entire flowfield necessitates a very large number of mesh points and time steps. This represents an important difficulty especially for 3D simulations because the use of a uniform fine mesh is prohibitively expensive. It is evident that the flow zones that need a fine resolution are around the detonation waves and the free surfaces of the fresh mixture layer. One can see from Fig. 1 that these zones represent a small fraction of the combustion chamber volume. Hence it is possible to reduce the computational cost by using a local mesh refinement, which must dynamically adapt to the flowfield evolution. The Adaptive Mesh Refinement (AMR) is a suitable technique, whose application to the CDW simulation will be considered in the following sections.
2 AMR fundamentals and present implementation

According to the original works of Berger and Collela e.g. [3], AMR consists in obtaining a numerical solution on block structured meshes that constitute a mesh hierarchy. Starting from a base-level mesh, which is the coarsest one and covers the whole computational domain, the mesh hierarchy is composed of rectangular blocks of different levels so that higher level blocks are nested within lower level ones. A schematic illustration of a 2D mesh hierarchy is presented in Fig. 2. For a 3D mesh, the refinement is applied to the three directions, however the 3D case is difficult to illustrate. Each new level, identified by the $i$ index, corresponds to a refined mesh and is characterized by a constant refinement factor, $r_i$, with respect to the parent level $i-1$. Within a global time step, $\Delta t_0$, the number of time steps on level $i$ is defined as $\prod_{j=1}^{i} r_j$.

Thus the spatial and temporal resolutions are proportionally increased. The boundary conditions are treated using the ghost cell/point method. More details concerning the AMR method can be found in [3, 4].

Being initially proposed for the finite volume method, AMR has also been successfully used with a high-order finite difference scheme [5]. There exist many AMR implementations available through the Internet, e.g. AMRCLAW, Dagh, AMROC, CHOMBO, PARAMESH. Among these codes, AMROC is the most suitable one for our purposes. Initially developed by R. Deiterding from the Dagh code [6], AMROC is currently realized with different Euler solvers, based on TVD and WENO schemes, and integrated in the VTF software [7]. This is a powerful code that can be run on parallel computational platforms.

For the present study, a new WENO-based Euler solver has been developed and implemented in the VTF framework. It uses a high-resolution WENO scheme for the numerical flux approximation and a semi-implicit Runge-Kutta integration scheme. Efficiency and robustness of these numerical methods have already
been proved in the previous study [1, 2]. New FORTRAN modules for the numerical fluxes, time integration, thermodynamics and chemical kinetics have been created by the authors.

3 Tests of computational efficiency of the AMR code

To test the parallel efficiency of the AMR code, a model problem of detonation propagation in a layer of fresh mixture is considered. A schematic of the computational domain is shown in Fig. 3 and the initial conditions are specified in Table 1. Zones 1 and 2 are initially filled with fresh mixture whereas zone 3 is initialized with equilibrium combustion products. Due to the high pressure and temperature in zone 2, the fresh mixture explodes and initiates a detonation that propagates in zone 1. The base-level mesh is composed of $56 \times 22 \times 3$ cells correspondingly along the length, height, and width of the domain. Two refinement levels with $r = 3$ are allowed. The mesh refinement criteria are based on local gradients of flow density and temperature. The mesh refinement-derefinement is done every time step whereas the load balancing and domain partitioning between the parallel processors is performed every 10 time steps.

![3D domain schematic](image)

**FIG. 3 – Schematic of the 3D domain for numerical tests.**

<table>
<thead>
<tr>
<th>Zone</th>
<th>$P$, MPa</th>
<th>$T$, K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>300</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>3000</td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>3000</td>
</tr>
</tbody>
</table>

**TAB. 1 – Conditions for the simulation of detonation propagation.**

The instantaneous field of flow temperature is presented in Fig. 4 for the physical time $t \approx 13 \mu s$. The corresponding distribution of the mesh blocks is shown in Fig. 5. Comparing Figs. 4 and 5, one can note that the mesh is refined around the zones of notable temperature variation: the interface between the fresh mixture and combustion products; the detonation wave; the shock attached to the detonation; the slip surface behind the shock. A complex structure and an important number of mesh blocks are due to two main requirements: efficiency of the mesh adaptation to the flow structure and load balancing between the parallel processors.

![Temperature field](image)

**FIG. 4 – Instantaneous field of flow temperature for $t \approx 13 \mu s$.**
The computational efficiency of the AMR code is evaluated in terms of parallel speed-up and total runtime. The parallel speed-up is defined as a ratio of runtimes obtained for a single processor and for parallel code execution. The AMR efficiency can be measured with respect to computations on a fine mesh (504×198×27) without AMR. The plots in Figs. 6 and 7 indicate the computational speed-up and the total runtime versus the number of processors used, $N_p$. The speed-up without AMR is almost proportional to $N_p$, whereas the speed-up with AMR is significantly reduced for $N_p = 16$ and 26. This speed-up reduction is explained by the fact that the domain partitioning with AMR is limited to a certain extent, beyond which the processor load balancing becomes less effective or even impossible.

The total runtime is estimated for a physical time period of 17 μs, during which the detonation wave propagates to the end of the domain. In spite of the loss of parallel efficiency, the use of AMR provides runtime reduction by a factor of 2 or more (see Fig. 7) and an important memory saving as the total number of computational cells is lesser by 60%. With AMR, the runtime cannot be reduced to the same ratio as the number of cells because the AMR realization is linked to a significant computational overhead, which can vary from 10% to 50% of the total computational cost.
4 2D and 3D simulations of the flowfield in a CDWRE combustion chamber

To test the newly developed code, a 2D simulation of continuous detonation has been performed using the same approach as in the previous study [1, 2]. The domain dimensions are \( l = 50 \text{ mm} \) and \( L = 20 \text{ mm} \), the relative injection area is \( A_j/A_w = 0.133 \), and the injection pressure is \( P_{ij} = 1 \text{ MPa} \). One refinement level with \( r = 3 \) is used. The minimum cell size is \( 99 \mu\text{m} \times 101 \mu\text{m} \). The computation has been done on 32 processors.

Instantaneous temperature field, representing the flow structure, is shown in Fig. 8 together with the refined grid structure and the domain partitioning between parallel processors. One can see that the refined mesh, represented by the black area, covers the zones of high gradients: the fresh mixture layer, the detonation wave with the attached oblique shock, and the slip line behind the shock. The refined area is much smaller than the entire domain providing that AMR is computationally efficient. Concerning the domain partitioning, one can note that the regions treated by different processors have complex configurations that result from the load balancing. The load balancing algorithm [4] provides some minimization of boundaries between the neighboring parallel regions.

![FIG. 8 – Instantaneous temperature field from 2D simulation using AMR. The underlying fields illustrate the structure of the refined mesh zone (on the left) and the domain partitioning between parallel processors (on the right).](image)

Main features of the flow structure can be easily distinguished in Fig. 8. The detonation wave is almost normal to the injection boundary and becomes oblique toward the edge of the mixture layer. The detonation results in a strong increase of pressure (by a factor of 20) and temperature (by a factor of 13). Combustion products expand behind the detonation. At a certain distance from the detonation wave, the wall pressure, \( P_w \), is greater than the injection pressure, \( P_{ij} \), hence the injection is blocked in that zone. From the point where \( P_w = P_{ij} \), the layer of fresh mixture continuously grows to \( h \approx 4.5 \text{ mm} \) before the next detonation arrives. The mixture layer edge is clearly marked in the temperature field. Interaction between the high-pressure flow generated by this detonation and already expanded flow from the previous one results in three waves: an expansion fan centered at the top of the detonation front, an oblique shock that recompresses the flow from the previous detonation, and a slip line that separates the two flows having different velocities and static temperatures. These three waves are originating from the point where the detonation front meets the edge of the fresh mixture layer. One can note a Kelvin-Helmholtz instability developing along the slip line. The development of vortex structures is governed by the flow shear and the numerical viscosity that depends on the mesh resolution. In the present study, we do not try to correctly simulate the observed instability. Nevertheless, the present result shows that, for a proper simulation of turbulent structures, the mesh resolution must be further increased.

A 3D simulation has been performed for the same domain dimensions as in 2D. The third dimension, representing the domain width, is 2.5 mm. The fresh mixture is injected through a longitudinal slot with \( A_j/A_w = 0.06 \) and \( P_{ij} = 1 \text{ MPa} \). Two refinement levels with \( r = 3 \) are allowed. The minimum cell size is \( 99 \mu\text{m} \times 101 \mu\text{m} \times 8.3 \mu\text{m} \), the last dimension is smaller in order to resolve the slot injection. The total cell number during the simulation is of the order of \( 20 \times 10^6 \). The computation has been done on 128 processors. Illustrations of instantaneous pressure and temperature fields are presented in Fig. 9. In the background, the adapted mesh structure is shown corresponding to the chamber wall. In the pressure field, the detonation and shock fronts are clearly depicted. The temperature field illustrates several flow features, especially the development of the mixture layer (blue surface). With respect to the 2D case, the mixture layer in front of the detonation is higher but it does not fill the cross section in width. The flowfield demonstrates important instabilities related to the mixture layer fluctuations.
FIG. 9 – Instantaneous fields of pressure (on the left) and temperature (on the right) from 3D simulation using AMR. The adapted mesh is shown for the chamber wall.

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References