GPU-Accelerated High-Performance Numerical Simulation of Detonation Using Detailed Chemical Kinetics

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1 Introduction

Detonation is a complex phenomenon involving strong coupling between fluid dynamics and chemical reactions, making its numerical simulation highly challenging. For detonation engines, combustion instability significantly limits their engineering applications, primarily due to the complex propagation and interaction mechanisms of detonation waves within the combustor[1]. Therefore, it is of great importance to investigate the mode transition mechanisms of detonation. Although numerous studies have explored detonation phenomena, most of them rely on simplified chemical reaction mechanisms[2–5]. However, detonation is inherently a process tightly coupled with fluid dynamics and chemical reactions. Given that high-precision numerical schemes are already employed for fluid dynamics, the use of detailed chemical reaction mechanisms can help reveal the intricate structure and evolution of detonation waves more accurately.

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In computational fluid dynamics (CFD) simulations, chemical reaction calculations consume a significant portion of computational resources. Since the characteristic timescales of chemical reactions are much shorter than those of fluid dynamics, the point-implicit method can effectively address the numerical stiffness caused by this timescale disparity. However, the point-implicit method requires the inversion of the chemical reaction rate matrix, which is computationally expensive especially for detailed reaction mechanisms involving hundreds of species. In recent years, thanks to the rapid development of deep learning and the increasing demand for matrix operations, GPU acceleration has emerged as an efficient solution to this problem.

Against this background, this study develops a high-performance numerical simulation program that employs detailed chemical reaction mechanisms to conduct high-fidelity simulations of rotating detonation combustors. To balance grid resolution and computational cost, the program integrates adaptive mesh refinement (AMR) technology and graphics processing unit (GPU) acceleration for chemical reaction calculations. The results demonstrate that the program achieves approximately double the speed compared to central processing unit (CPU) calculations while accurately capturing the structure and evolution of detonation waves. This work provides a valuable numerical tool and theoretical foundation for the design and optimization of detonation engines.

This paper is arranged as follows. Section 2 introduces the detailed method of numercial methods. Section 3 briefly includes results. Finally, Section 4 concludes this work.

2   Methodology

In this study, the governing equations are the unsteady, compressible, multi-component conservation form of the Euler equations, which are solved for the continuous phase in Eulerian framework.

$$
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0
$$
$$
\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) + \nabla p = 0
$$
$$
\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho E \boldsymbol{v} + p \boldsymbol{v}) = \nabla \cdot \boldsymbol{q} \tag{1}
$$
$$
\frac{\partial}{\partial t}\left(\rho Y_k\right) + \nabla \cdot \left(\rho Y_k \boldsymbol{v}\right) = \nabla \cdot \left(\rho D_k \nabla Y_k\right) + \dot{\omega}_k
$$

Where ρ, p, E represents density, pressure, and total energy. The vectors $\boldsymbol{v}, \boldsymbol{q}$ represent velocity , and heat diffusion flux. $Y_k, D_k, \dot{\omega}_k$ represents the mass fraction, diffusion coefficient, and reaction rate of the k-th species. The equations is closed by the gas state equation.

In this work, the Euler equations are numerically solved using a finite-volume discretization approach. The convective fluxes are reconstructed through a modified second-order MUSCL scheme, with the min-mod limiter applied to ensure stability. The HLL Riemann solver is then used to estimate the fluxes at cell interfaces. Temporal integration is performed using a third-order Runge-Kutta method. For the chemical source terms, the reaction rates of individual species are determined based on the Arrhenius law. To mitigate stiffness issues caused by the short timescales of chemical reactions, the point-implicit method is implemented for the calculation of chemical source terms.

In terms of AMR and parallelization strategies, the model utilizes the AMReX library[6]. AMReX is a software framework designed for massively parallel, block-structured adaptive mesh refinement simulations. Additionally, we have developed a GPU-accelerated module within this framework specifically for updating the chemical reaction source terms. This acceleration is based on the NVIDIA HPC SDK. GPUs are equipped with numerous computational units and operate in a single-instruction,

multiple-thread (SIMT) mode, making them particularly suitable for accelerating tasks that are computationally intensive but logically simple. In this computational case, since the flow flux terms and chemical reaction source terms are updated sequentially, an heterogeneous computation approach is adopted. To minimize frequent data transfer operations, data is transferred in blocks aligned with AMReX's block structure. The schematic diagram of the proposed CPU-GPU heterogeneous computing algorithm logic is shown in Figure 1.
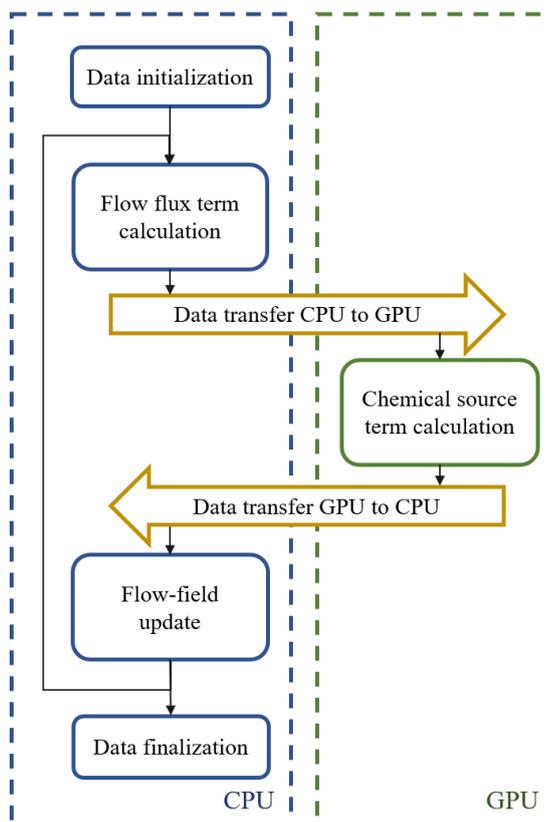

Figure 1: The schematic diagram of the proposed CPU-GPU heterogeneous computing algorithm used in current research

In the actual testing of this case, the hardware setup consisted of an Intel i7-13700F CPU and an NVIDIA GeForce 4090 GPU. Using 16 CPU cores and an initial grid size of 2×10^6, the computation time per time step was 2.04 s when using only the CPU. When utilizing both the CPU and GPU, the computation time per time step was reduced to 1.06 s. Despite the overhead associated with data transfer, the overall computational efficiency was significantly improved.

3   Results

This study conducted a calculation using a stoichiometric mixture of hydrogen and air in a two-dimensional detonation tube, with the initial pressures set to 3 MPa and 3000 K. This section presents only a brief overview of the results related to the detonation tube. Detailed results, including simulations of the detonation combustor, will be discussed in subsequent research. Figure 2 shows the results for the 2D cellular detonation. The results clearly distinguish the detonation wave and the cellular structure behind it. Figure 2 also illustrates the adaptive mesh refinement, showing that the grid structure is closely related to the detonation wave pattern.
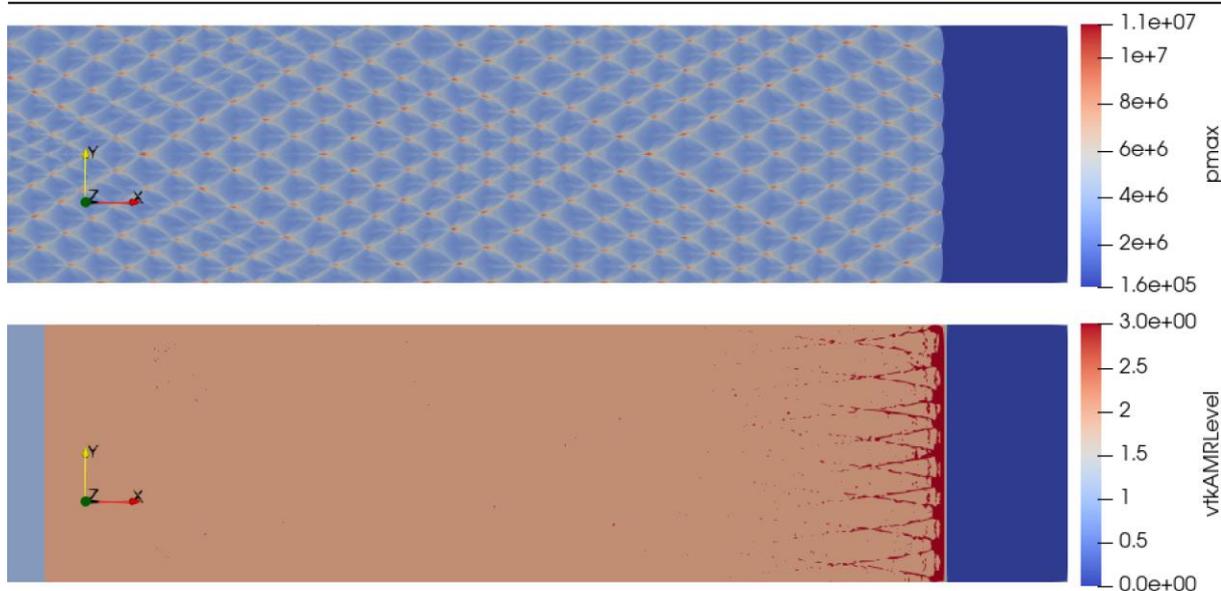
Figure 2: The contours of the maximum pressure (up) and mesh refinement level (down) for the detoantion tube.

4 Conclusion

In this study, we explored the application of GPU acceleration and AMR techniques in the numerical simulation of detonation tube with detailed chemical reaction mechanisms. The use of GPUs significantly improved computational efficiency, particularly in handling complex chemical kinetics, while AMR enabled precise resolution of detonation waves and other critical flow features. The integration of these advanced computational methods demonstrated their potential to enhance the accuracy and efficiency of detonation simulations, providing deeper insights into the underlying physics of detonation processes.

Furthermore, several directions can be pursued to further advance this research. First, optimizing asynchronous computing strategies can minimize idle times on CPUs and GPUs, maximizing their utilization and further improving computational efficiency. Second, extending the analysis to other working conditions will provide a more comprehensive understanding of the program's performances. By addressing these aspects, future research can pave the way for more efficient and practical detonation engines designs, contributing to the advancement of next-generation propulsion systems.

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