Accelerated GPU simulation of the gaseous detonation cell structure

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Abstract. The aim of the present paper is to report on our recent results for GPU accelerated simulations of the gaseous detonation structure. Reactive Euler equations with a one-step Arrhenius chemistry model have been used for numerical simulation. And the NND space discretization scheme combined with Steger-Warming split method has been used. For time discretization we have applied the explicit third order Runge-Kutta method. We have obtained a speedup of 8 times (in comparison to 30 threads openmp program) for the gaseous detonation simulation on a structure grid of 320 million points.

1. Introduction
A gaseous detonation is a combustion-driven, compressible wave propagating as supersonic speeds. Many experiments and numerical simulations had confirmed that detonation waves have a complex cellular structure generated by various gas dynamic interactions. Research on the detonation proved the detonation cell structure to have a significant influence on the gaseous detonation propagating process.

As for simulations of normal detonations, a sufficient level of numerical resolution is generally required to correctly reveal the transverse wave structure and various sources of instability [1]. As shown in [2], the lack of numerical resolution in the simulation can prohibit the correct appearance of transverse waves and various hydrodynamic instabilities within the flow. Moreover, it takes a huge computation consumption to completely evolve a detonation propagating process to the point when the regular detonation cell structure is formed.

Since the introduction of CUDA by Nvidia in 2007, many scientific algorithms have been successfully ported to GPUs. Examples include the molecular dynamics simulations [3-4] and the analysis of financial market data [5] to name just a few. Application of the GPU for multidimensional flow problems has also been advanced for the Euler equations [6-8].

In this paper, we port the openmp parallel program to the GPU using cuda language. By doing so, we are able to speed up the gaseous detonation cell structure simulation, resulting in an eight fold speedup (GeForce RTX 2080 Ti versus Intel Xeon CPU E5-2640 v4 2.40GHz) of the overall computation process.
2. Mathematical model

The present simulation of gaseous oblique detonation is based on the inviscid, reactive two-dimensional Euler equations. The governing equations with a single-step, irreversible chemical reaction are of the form [9]:

\[
\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = S(U)
\]

(1)

where the conserved variable \( U \), the convective fluxes \( F \) and \( G \), and reactive source term \( S \) are, respectively,

\[
U = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho e \\
\rho \lambda
\end{pmatrix},
\quad
F(U) = \begin{pmatrix}
\rho u \\
\rho u^2 + p \\
(\rho e + p)u \\
\rho \lambda \\
\rho \mu
\end{pmatrix},
\quad
G(U) = \begin{pmatrix}
\rho v \\
\rho v^2 + p \\
(\rho e + p)v \\
\rho \nu \\
\rho \nu \lambda
\end{pmatrix},
\quad
S(U) = \begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
\omega
\end{pmatrix}
\]

(2)

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

(3)

where \( \rho, u, v, p \) and \( e \) are density, particle velocities in \( x \) and \( y \) directions, pressure, temperature and total energy respectively. \( \lambda \) is the reaction progress variable, which varies between 1 (for unburned reactant) and 0 (for product).

The reaction rate is a one-step Arrhenius type given by the following Eq. (4):

\[
\dot{\omega} = -k \rho \lambda \exp\left(-\frac{E_a}{\kappa \Theta}\right)
\]

(4)

3. Results and discussion

Figure 1. shows the detonation cell structure in the detonation wave propagating process and Figure 2. shows the density distribution at the same time. As seen in the figure, the flow field behind the detonation front involves vortices of different scales generated from the Mach and other shock reflections, Kelvin-Helmholtz instabilities along the shear layers and Richtmyer-Meshkov instabilities by different gasdynamic interactions. The transverse wave along with the detonation wave generate multiple triple points and these triple points that periodically moving perpendicular to the detonation wave direction form the regular detonation cell structure.

The computation result verified the GPU program and the detonation cell structure is clearly captured in the figure. Simulation on GPU costs nearly 12 hours for detonation cell structure to evolve to the steady state and it would cost several days on CPU with 30 threads since we achieved a speedup of 8 times.
4. GPU implementation and accelerating efficiency

The main procedure of the numerical simulation contains Steger-Warming split process, NND scheme discretization process and Runge-Kutta time evolve process. All these subprogram can be calculated in parallel on both CPU and GPU.

Table 1 shows the comparison of the execution times of the program running on different devices. We use 30 threads by openmp sharing memory parallel method on two Intel(R) Xeon(R) CPU E5-2640 at 2.40GHz and port the code to cuda using two different GPU device. The result shows that we can achieve at most 8 times speedup using GPU parallel program using GeForce RTX 2080ti graphic card. Comparison between two graphic cards shows us that GPU capability has a huge influence on the acceleration.

| Device         | Intel(R) Xeon(R) CPU E5-2640 | GeForce RTX 2080ti | Quadro M4000 |
|----------------|-------------------------------|---------------------|---------------|
| Running time   | 4.02                          | 0.49                | 3.51          |
| Cores used     | 30                            | 4352                | 1664          |
5. Conclusion
In the present paper we reported on our recent results for a GPU accelerated implementation of the Euler equations for gaseous detonation research. We use NND scheme combined with Steger-Warming split method for space discretization and the explicit third order Runge-Kutta method for time integration. Compared with 30 threads openmp program, we can achieve a significant speedup of 8 times, with a potential for further optimization of the cuda code.

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