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Accelerated solution of problems of combustion gas dynamics on GPUs

B.P. Rybakin [*], L.I. Stamov, E.V. Egorova

SRISA RAS, Nahimovskiy Prospect, 36, 1, Moscow 117218, Russia
MSU, Leninskie Gory, GSP-1, Moscow 119991, Russia

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The paper deals with a solution of gas dynamics problems with chemical kinetics on graphic accelerators. To solve these problems, schemes are analyzed that combine high resolving power in the areas of small perturbations and monotony in areas of strong discontinuities. Problems are studied with consideration of chemical kinetics, which address the processes of transition from combustion to detonation. Parallel algorithms of the analyzed difference models are built for the purpose of calculations on graphic processors using the CUDA technology. The proposed algorithms and programs allow for 41.66 times faster acceleration on four graphic accelerators M 2090 than the CPU.

1. Introduction

The solution of 3D gas dynamics problems in consideration of combustion and detonation processes, gravitational and magnetic fields is of major practical interest. Such solutions are used in designing cars and airplanes, increasing the output of oil-bearing strata, studying galaxy formation, supernova explosions, weather forecasting, climate modeling, etc. High resolution difference schemes have been developed in recent years, which enable mathematical modeling of the above processes, but conducting 3D calculations on detailed grids require large computational resources. Therefore, the emergence of new program development technologies for working on a GPU (Graphical Processor Unit) allows for the use of new possibilities, in addition to existing ones, to conduct intensive computing.

As a result of increased GPU performance, the number of cores in such units reaches hundreds or even thousands. For example, Tesla C1060 has 240 cores, and the Fermi graphic processors has up to 512 cores. In the new Kepler technology, the number of CUDA cores exceeds 3000. At the moment, there are two main technologies of program development for working on GPU: CUDA and OpenCL. CUDA (Compute Unified Device Architecture) is a technology of programming graphic accelerators from NVIDIA [1]. This technology allows to work with C, FORTRAN and other programming languages. OpenCL (Open Compute Language) was developed jointly by several companies, and it enables the development of programs for graphic accelerators of NVIDIA, ATI and regular processors (CPU). This way, the possibility of intensive mathematical calculations on graphic accelerators is emerging.

2. High resolution difference schemes

Modeling of 3D gas dynamics flows is one of the complex nonlinear dynamic processes that place high demands on the utilized difference schemes. These schemes must reproduce the behavior of a substance in the vicinity of discontinuities and high gradient areas as accurately as possible, and reliably describe small perturbations away from shock wave fronts. To address such conflicting demands difference schemes are used that combine high resolving power in the areas of small perturbations and monotony in areas of strong discontinuities. Such schemes include TVD, ENO, WENO, PPM and other types of schemes. Such second-order-accurate non-linear schemes with limited overall variation enable to calculate shock waves with high resolution and to prevent non-physical oscillation in their fronts. Among these schemes, preference is given to schemes that allow to create good parallel algorithms, which enable calculations on heterogeneous computing systems using graphic accelerators.

Computation of gas dynamics flows in complex problems is not the only factor that requires the use of high-performance computers. Additional computation is needed to solve combustion and detonation problems, and to study gravitational and magnetic fields. Often, the time spent on these additional computations greatly exceeds the time for calculating the gas dynamics phase. This work provides solutions of several problems of computational gas dynamics, both in consideration of the influence of chemical kinetics [2,3], turbulence, and computations of pure gas dynamics flows.

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[*] Corresponding author at: SRISA RAS, Nahimovskiy prospect, 36, 1, Moscow 117218, Russia.

E-mail address: rybakin@vip.niisi.ru (B.P. Rybakin).

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The modeling of multidimensional processes of disturbances propagation in gas requires large computational resources. Gas flow equations can be represented conservatively as follows:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F_x}}{\partial x}+\frac{\partial \mathbf{F_y}}{\partial y}+\frac{\partial \mathbf{F_z}}{\partial z}=0, \qquad (1)$$

where **U** vector of conservative variables, $\mathbf{F_x}$, $\mathbf{F_y}$ and $\mathbf{F_z}$ – numerical threads. In Eqs. (1) for ideal gas equation, vector **U** is as follows:

$$\mathbf{U}=(\rho,\rho v_x,\rho v_y,\rho v_z,\rho E)^T, \qquad (2)$$

$$\mathbf{F}_x=(\rho v_x,\rho v_v^2,\rho v_x v_y,\rho v_x v_z,\rho E+p)^T. \qquad (3)$$

Here $\mathbf{v}=(v_x,v_y,v_z)^T$components of the speed vector, $E=\frac{|\mathbf{v}|^2}{2}+\frac{p}{(\gamma-1)\rho}$ energy, ρ – density and p – pressure. Threads $\mathbf{F_y}$ and $\mathbf{F_z}$ are determined analogously (3). In the equation of state γ was assumed to be $\gamma=5/3$.

Three high-resolution schemes were analyzed: (a) TVD scheme [4], (b) modification of TVD scheme, suggested by Jiang and Tadmor [5] and PPM scheme [6]. A program was written for each of these schemes, and a series of 1D, 2D [7] and 3D [8] tests were conducted. Testing of programs for 1D problems was conducted using Sod and Lax tests (Fig. 1). When testing have been used and other tests ([4]).

3. Testing of schemes

Fig. 1 demonstrates the results of testing obtained based on the TVD and PPM schemes for the Sod test problem, drawing (a,b) and Lax test problem, drawing (c,d). Density graphs are provided. On the top (diagram a,b) shows analytical (in red) and computational (blue line) solutions; diagram (c,d) shows solutions for the Lax problem in the same colors. In this case, computations were conducted based on the PPM scheme. It is noteworthy that the PPM scheme results in better correspondence of the analytical solution and numerical calculations. On the other hand, using the PPM scheme leads to considerable time expenditures and more complex algorithm used to work on graphic accelerators.

For 2D problem testing, test problems provided in [9] were used. Initial data for these tests are presented in Table 1. The rectangular computational domain was divided into four equal rectangles, and different initial conditions for pressure, density, energy and velocity components v_x and v_y were specified for each.

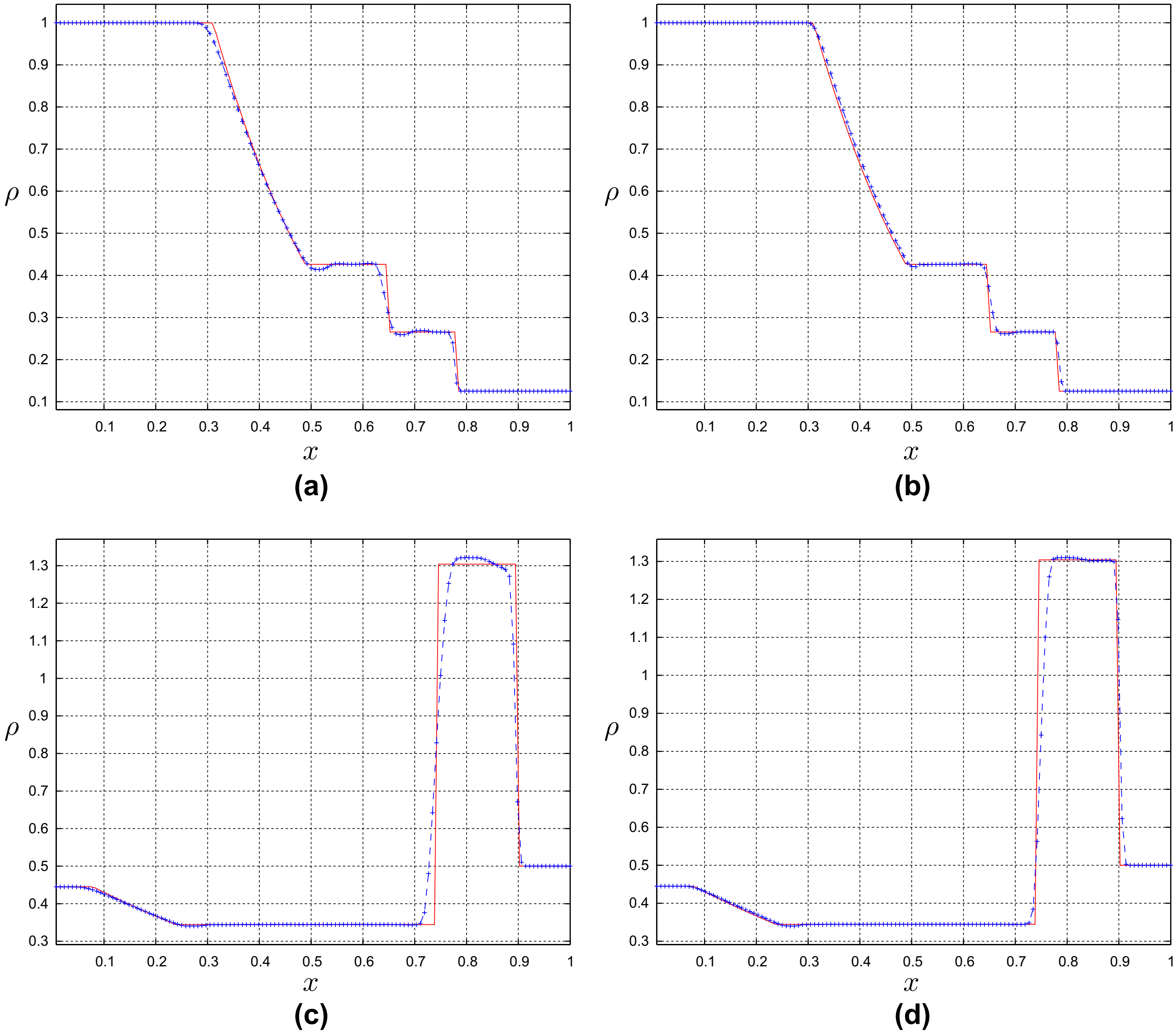

Fig. 1. Sod test problem for TVD-type method (a) and PPM method (b); Lax test problem for TVD-type method (c) and PPM method (d).