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Detailed numerical simulation of shock-body interaction in 3D multicomponent flow using the RKDG numerical method and "DiamondTorre" GPU algorithm of implementation

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Abstract. Interaction between a shock wave and an inhomogeneity in fluid has complicated behavior, including vortex and turbulence generating, mixing, shock wave scattering and reflection. In the present paper we deal with the numerical simulation of the considered process. The Euler equations of unsteady inviscid compressible three-dimensional flow are used into the four-equation model of multicomponent flow. These equations are discretized using the RKDG numerical method. It is implemented with the help of the DiamondTorre algorithm, so the effective GPGPU solver is obtained having outstanding computing properties. With its use we carry out several sets of numerical experiments of shock-bubble interaction problem. The bubble deformation and mixture formation is observed.

1. Introduction
This paper studies the problem of interaction between a shock wave and an inhomogeneity in a gas. Being one of the basic topics in fluid dynamics, considered process has a lot of applications in industry, medicine, cosmology and other fields, and represents a complicated task both for analytical and numerical research.

The mathematical model of the dynamics of the mixture of fluids is the system of Euler equations. The issue of multicomponent flow is resolved in this work by using so called 4-equation model [1], which means that we introduce extra advection equation of volume fraction of mixture components. It is applied in the quasi-conservative form and does not require special treatment of the interface.

We use the RKDG method (Runge-Kutta discontinuous Galerkin method) for numerical solution of considered equations [2]. RKDG method is the high-order, non-oscillating and explicit method, based on the finite volume approach in symbiosis with the Galerkin method as the technique of increasing the local order of approximation. For the numerical fluxes construction, the exact or approximate Riemann solvers are used. The method is high-order, free from spurious oscillations, local and has clear logical structure simplifying its coding.

For the GPU implementation, a modified version of the algorithm called DiamondTorre developed by authors is used [3]. It uses the technique of special space-temporal tiling inside a 'window of computations', increasing the computational intensity of the algorithm. Specially
adjusted for large scale problems, the algorithm shows outstanding performance compared to the maximum possible, which finally allows to obtain results for sufficiently fine grids using only a single PC with GPU [4, 5]. Performance results for our solver are shown.

Numerical validation of obtained solver is made. First of all, we examine one-dimensional tests based on the Riemann problem. Due to existence of analytical solutions of such tests, it is easy to test solver accuracy and other properties of obtained numerical results, comparing them with exact solutions and numerical solutions made by other solvers [1]. Results for some commonly used test problems are presented, showing good quality of our solver.

Three-dimensional problem of interaction between a steady spherical bubble of gas put inside some gaseous medium, particularly, air and a planar shock wave is considered. The sphere is chosen as a simplest model of a body in the wider problem of shock-body interaction. For the numerical point of view, it can be treated as a hard-level test for the solver, as it is resource-consuming fully three-dimensional problem. The pattern of the solution behavior is known for the problem at early times. In this paper we show the numerical results for some set of initial parameters of the problem and compare them with some well-known works [1, 6, 7].

2. Governing equations

The dynamics of fluid mixture in space when viscous effects are negligible is described by the system of Euler equations shown below

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = 0, \tag{1}
\]

We use Cartesian coordinates \((x, y, z)\) here. \(\mathbf{U} = (\rho, \rho u, \rho v, \rho w, E)^T\) is a vector of conservative variables, \(E = \rho (\varepsilon + \frac{1}{2}(u^2 + v^2 + w^2))\) is full energy, \(\mathbf{F}(\mathbf{U}) = (\rho u, \rho u^2 + p, \rho uv, \rho uw, (E + p)u)^T\), \(\mathbf{G}(\mathbf{U}) = (\rho v, \rho vu, \rho v^2 + p, \rho vw, (E + p)v)^T\), \(\mathbf{H}(\mathbf{U}) = (\rho w, \rho uw, \rho vw, \rho w^2 + p, (E + p)w)^T\) are Eulerian fluxes.

2.1. Model of multicomponent flow

There are a lot of ways how to mathematically describe the multicomponent fluid flow. They can be defined into two groups. First are so called interface-tracking techniques, where the boundaries between two different fluids are taken into the account. Second is called volume-of-fluid (VOF) technique and it means that we do not pay special attention to the interfaces between different components, observing dynamics of every single component instead. We believe that for our case of gases the second approach is more appropriate, as it easily describes mixing and does not require numerically difficult interface tracing operations. In this paper the four-equation model of multicomponent flow is used [1]. Each component of the flow in every point of space is represented by the volume fraction \(\alpha_i, 0 \leq \alpha_i \leq 1, \sum_i \alpha_i = 1\). The advection equation for each volume fraction component is considered

\[
\frac{\partial \alpha_i}{\partial t} + u \frac{\partial \alpha_i}{\partial x} + v \frac{\partial \alpha_i}{\partial y} + w \frac{\partial \alpha_i}{\partial z} = 0, \tag{2}
\]

\(p = p(\rho, \varepsilon, \alpha_i)\) is equation of state which completes the system of equations. Further the EoS of the ideal gases mixture is used given by the following equations

\[
p = p(\rho \varepsilon (\gamma - 1)),
\]

\[
\frac{1}{\gamma - 1} = \sum_i \frac{\alpha_i}{\gamma_i - 1}
\]

\(\gamma_i\) is the adiabatic index of the \(i\) component of the mixture.
2.2. Quasi-conservative form of the system of equations
We transform the equations (1) and (2) to obtain the quasi-conservative form of the governing
system. As (2) is in non-divergent form, rewrite it the following way
\[
\frac{\partial \alpha_i}{\partial t} + \frac{\partial (v_j \alpha_i)}{\partial x_j} = \alpha_i \frac{\partial v_j}{\partial x_j}
\]
Now left-hand side is in the divergent form, and the right-hand expression can be treated as a
source term.

Introducing \( \mathbf{U} = [U, \alpha_i]^T \), \( \mathbf{F}_j = [F_j, v_j \alpha_i]^T \), \( \mathbf{S} = [0, \alpha_i \frac{\partial v_j}{\partial x_j}]^T \) we obtain the full system of
equations written in the divergent form with the source term in the right-hand side
\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} = \mathbf{S}
\]

3. RKDG method
3.1. DG spatial discretization
Let the domain is discretized with the cells \( L_j \).

Approximate solution \( \mathbf{U}_h \) at every cell \( L_j \) is written in form of the expansion in the specified
basis functions \( \{ \varphi_i(x) \} \)

\[
\mathbf{U}_h = \sum_{i=1}^{k} U_i(t) \varphi_i(x).
\]

Inserting it into the equation (4), requesting the result to be orthogonal to all the basis
elements and using the Divergence theorem we obtain
\[
\sum_{i=1}^{k} \frac{dU_i(t)}{dt} \int_{L_j} \varphi_i \varphi \, dV + \int_{\delta L_j} \varphi_i \mathbf{S}_j \, n \, dS = \int_{L_j} \left( \frac{\partial \varphi_i}{\partial x_j} \mathbf{F}_j + \varphi_i \mathbf{S} \right) \, dV,
\]

where \( \mathbf{S}_j = [F_j, v_j \alpha_i]^T \) is the numerical flux. We use HLLC flux \([8]\) flux for constructing \( \mathbf{F}_j \) and
Lax-Friedrichs flux \([9]\) for \( v_j \alpha_i \).

3.2. Time discretization and limiting
In the previous paragraph we obtained spatially discretized ODE system (5), where the highest
derivative is resolved. In terms of the RKDG method the explicit Runge-Kutta method is
supposed to apply with limiting the solution in a special way after each RK stage. It is necessary
to use the limiter for suppressing the spurious oscillations near big gradients. Various types of
limiters have been developed (minmod, ENO and WENO-type etc) \([2, 10]\). Reconstruction of
the coefficients is a local procedure, depending only on the values of the considered cell and the
cells which are adjacent to it.

3.3. Concluding remarks and specifications
The method has several significant features, including the explicit stencil, high-order accuracy
in time and space, and non-oscillation (TVDM) of the solutions.

Further in this work we use 3D Cartesian grid, second order in space and time RKDG method
on piecewise linear basis in every cell, HLLC numerical flux for the fluid dynamics terms and
Lax-Friedrichs flux for the volume fraction terms and the minmod limiter.

We would like to point out that the method combines both quite simplicity and high-order
accuracy. That makes it a suitable candidate for building on it the efficient solver for simulating
big three-dimensional problems. In the next section we consider the numerical algorithm of the
implementation on GPU.
4. **DiamondTorre algorithm of the implementation**

Here we suppose the approach called LRnLA to build the effective solver algorithm. LRnLA stands for "locally recursive non-locally asynchronous algorithms". Developed since 1990s, firstly published in [11], now this technique is used to construct various algorithms, including ones for GPU, for various physical codes [3, 4, 5, 12]. Stencil topology properties are used as a basis of the algorithm. Its structure is well-compatible with the computer architecture, having effective interaction between different levels of hierarchical computer systems (i.e GPU-CPU), resulting in the increased performance of the algorithm.

In this work the GPU algorithm called 'DiamondTorre’ is used [3, 12]. The main points of the algorithm are following: the DiamondTorre algorithm’s parts are associated with CUDA tools, while whole domain can be larger than the GPU memory amount because of 'computational window' using. The algorithm has the economic CPU-GPU exchange and is highly efficient.

4.1. **Performance results**

We use the domain with $512 \times 512 \times 1024$ cells (20 GB) for the performance tests. The solver is run on several GPUs with varying properties. The results of the testing are shown in figure 1. Performance gained is up to $5 \cdot 10^7$ cells per second. We note that using 32GB CPU DDR the task with the domain of dramatically big size of about $4 \cdot 10^8$ cells can be calculated.

Dealing with two-component problems, we get only one extra equation in addition to homogeneous fluid [3], so the performance stays practically the same in this case. Further we consider only one- or two- component flows.

5. **One-dimensional tests**

We provide a series of one-dimensional tests for validation of the solver. They basically represent the Riemann problem having known analytical solution. We show below the results of two well-known tests: Sod problem and Lax problem both in the two-component setting. The tests are taken from [1]. Initial conditions are given in the table 1, the discontinuity was located in the middle of the domain.

| Test # | $\rho_L$ | $v_L$ | $p_L$ | $\alpha_L$ | $\rho_R$ | $v_R$ | $p_R$ | $\alpha_R$ | $\gamma(\alpha)|_{\alpha=0}$ | $\gamma(\alpha)|_{\alpha=1}$ |
|--------|----------|-------|-------|------------|----------|-------|-------|------------|--------------------------|--------------------------|
| 1      | 0.445    | 0.699 | 3.527 | 0.9999     | 0.5      | 0     | 0.8565 | 0.0001     | 1.4                      | 1.6                      |
| 2      | 1        | 0     | 1     | 0.9999     | 0.125    | 0     | 0.1   | 0.0001    | 1.4                      | 1.6                      |

**Table 1. Initial conditions for the tests**

We show solutions for grids of 100 and 1000 cells in one graph. Results show quite good quality of numerical solutions expressing in very small spurious oscillations, excellent shock and good contact capturing.
6. Bubble-shock interaction problem

6.1. Problem statement

The bubble is a spheric region where density $\rho_B$ is different from the background one $\rho_0$ and pressures are equal. Shock wave moves and hits the bubble.

The dimensionless units of measure are chosen connected with the bubble size and the background gas condition as $x = R_0 \tilde{x}$, $y = R_0 \tilde{y}$, $z = R_0 \tilde{z}$; $u = a_0 \tilde{u}$, $v = a_0 \tilde{v}$, $w = a_0 \tilde{w}$; $t = t R_0 / a_0$; $\rho = \rho_0 \tilde{\rho}$; $p = \rho_0 \rho_0^2 \tilde{\rho} = \tilde{p} \rho_0 / \gamma$. The shock wave is characterized by the Mach number $M$ of its front moving velocity. The Atwood number $At = \frac{\rho_B - \rho_0}{\rho_B + \rho_0}$ is used for the characteristic of the density inside the bubble.

One quarter of the whole domain can be considered, introducing the boundary condition of symmetry on the diametrical cross-sections.

6.2. Results for $At < 0$

First case is considered when the bubble of He ($At = -0.757$) is hit by a shock at $M = 3$. This setting is known for long-living He vortex ring formation and is considered in various
works including [6, 7]. Figure 5 shows how He component (red) is distributed in the domain at different time moments. One can see the vortex ring appearance in 5(c)–5(f).

6.3. Results for $At > 0$

![Figure 6. Rendering of the freon component initially representing the bubble at different time moments: (a) $t = 0.0$, (b) $t = 1.0$, (c) $t = 2.0$, (d) $t = 3.0$, (e) $t = 4.0$; grid size is $600 \times 300 \times 300$](image)

Second case considered in the paper is when the bubble from heavy freon with $At = 0.613$ is hit with highly intensive shock at $M = 5$. The process is turbulent and a lot of vortices are created, tearing the bubble. We observe intense mixing of the bubble gas and air, which mainly has turbulent nature. The results have good coincidence with [6] and other known data.

7. Conclusion

In the paper the approach of studying the dynamics of multicomponent fluid using the Euler equations and 4-equation model is successfully applied. High-order numerical scheme is developed by the RKDG method and then validated. The solver having outstanding computing properties is constructed using the DiamondTorre algorithm of LRnLA class. The bubble-shock interaction problem with various initial conditions is resolved.

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