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Эффективное численное моделирование задачи о взаимодействии пузырька газа с ударной волной в трехмерной постановке с помощью численного метода RKDG и DiamondTorre алгоритма реализации

Аннотация. В данной работе рассмотрен метод RKDG для решения трехмерных уравнений Эйлера газовой динамики. Используется эффективная реализация численной схемы с помощью LRnLA алгоритма DiamondTorre. Рассматривается задача о взаимодействии пузырька с ударной волной в трехмерной постановке. Рассмотрены два случая: разреженного пузырька и плотного пузырька, соответствующие двум режимам — квазистационарному режиму с возникновением долгоживущих вихревых колец и неустойчивому режиму, при котором возникают нестабильные вихревые структуры. Полученные данные находятся в согласии с известными результатами экспериментов и численных расчётов. Отмечается, что результаты вычислений получены без использования дорогой суперкомпьютерной техники.

Ключевые слова: газовая динамика, RKDG метод, алгоритм DiamondTorre, вычисления на GPU, взаимодействие пузырька с ударной волной.

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Abstract. In this paper the RKDG method for solving three-dimensional Euler equations of gas dynamics is considered. For the scheme the effective implementation algorithm called DiamondTorre is used. The problem of the interaction of a spherical bubble with a shock wave is considered in the three-dimensional setting. Two cases are considered: the first is the rarefied bubble and the second is the dense bubble which corresponds to the two regimes, quasi-stationary regime with the emergence of stable vortex rings and unstable regime, in which unstable vortex structures appear. The obtained results are in agreement with the known results of experiments and numerical simulations. It is noted that the calculation results are obtained without the use of expensive supercomputer technologies.

Keywords: fluid dynamics, RKDG method, DiamondTorre algorithm, GPU computing, bubble-shock interaction problem.

1 Introduction

In this work the RKDG method (Runge-Kutta discontinuous Galerkin method) for the numerical solution of non-stationary equations of fluid dynamics is considered [1]. RKDG method is the high-order, non-oscillating and explicit method. It has some common features with the finite volume methods [2] and the finite element Galerkin method [3]. For the numerical fluxes construction, the exact or approximate Riemann solvers are used, which makes the RKDG closer to the Godunov methods [4].

The aim of this work is numerical simulation in the three-dimensional case with precise and detailed results. Moreover, encouraged by the progress of modern computer performance, it is desired to implement the numerical scheme using less number of computational units and obtaining more computational speed. As the attempt to partly resolve these difficulties, the numerical implementation algorithm called DiamondTorre is developed, which belongs to the family of LRnLA algorithms. The research of their use in various fields of computational physics like the numerical modeling of processes in the plasma physics [5] and the wave propagation [6, 7] show that LRnLA have the increased calculation speed, as well as the scalability and the parallel efficiency.

In this paper the application of the RKDG method and the LRnLA algorithms to the problem of interaction between the shock wave and the bubble of gas with the different density in the three-dimensional setting is investigated. This problem, which is thoroughly studied last years [8], is linked to the important tasks such as the description of turbulent combustion in the jet engines, interaction of fuel slurry with a shock wave of the piston in the internal combustion engines, the non-surgical removal of kidney stones (lithotripsy), the research of sonoluminescence, some problems in astrophysics and others. This problem is being numerically simulated with the use of high-performance computing [8, 9]. The works are known, where the RKDG method is used [10] for that. In this paper we introduce the RKDG method and the DiamondTorre algorithm to solve this problem with satisfactory accuracy without using the luxurious supercomputer technologies.[1]

[1]This doesn't mean that the authors alienate themselves from the supercomputers. The idea is that nowadays we might use them for significantly more harsh problems.

2 RKDG method

2.1 Governing equations

The system of Euler equations of fluid dynamics of the inviscid compressible flow can be written as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}_j(\mathbf{U})}{\partial x_j} = 0, \tag{1}$$

where $\mathbf{U} = (\rho, \rho u_i, E)^T$ is the vector of conservative variables, $E = \rho(\varepsilon + \frac{1}{2} u_i u_i)$ is the total energy, $\mathbf{F}_j(\mathbf{U}) = (\rho u_j, \rho u_i u_j + p\delta_{ij}, (E+p)u_j)^T$ are the convective or Eulerian fluxes.

We also should add the equation of state to make the internal energy, the pressure and the density functionally depended like $\varepsilon = \varepsilon(p, \rho)$.

This system is being solved in a three-dimensional domain $\Pi \in \mathbb{R}^3$ on a time interval $[0, T]$ with the given initial and boundary conditions

$$\mathbf{U}(x, 0) = \mathbf{U_0}(x),\ x \in \Pi,\ \mathbf{U}(x, t) = \mathbf{U_\Gamma}(x, t),\ x \in \partial\Pi,\ t \in [0, T]. \tag{2}$$

2.2 DG space discretization

The domain Π is divided into N non-overlapping elements or cells S_p, $p = \overline{1, \ldots, N}$, $\bigcup_{p=1}^{N} S_p = \Pi$, $S_p \cap S_q = \emptyset$, $p \neq q$. We will construct the approximate solution $\mathbf{U}_h$ for every S_p in form of the expansion

$$\mathbf{U}_h(x, t) = u_n(t)\varphi_n(x) \tag{3}$$

of the basis functions $V_p = \{\varphi_n(x_i)\}_{n=1}^{k}$. The coefficient $u_n(t) = [u_n^1(t), \ldots, u_n^5(t)]^{\mathbb{T}}$ is only time-dependent.

After inserting (3) into (1), we force the residual to be orthogonal to all basis functions. Therefore, after applying the divergence theorem, we get such an equality for the variables $u_n(t)$ in every S_p, $n = \overline{1, \ldots, k}$, $p = \overline{1, \ldots, N}$:

$$\dot{u}_n \int_{S_p} \varphi_n \varphi_m dV + \int_{\partial S_p} h_j(\mathbf{U}_h(x_{int}), \mathbf{U}_h(x_{ext}))\varphi_m n_j d\Sigma - \int_{S_p} \mathbf{F}_j(\mathbf{U}_h) \frac{\partial \varphi_m}{\partial x_j} dV = 0, \tag{4}$$

The values $\mathbf{F}_j(\mathbf{U}_h)$ at $x \in \partial S_p$ are redefined by the numerical flux $h_j(\cdot, \cdot)$, which depends on the variables according to the current cell side points x_{int} and the neighboring ones x_{ext}, and can be the exact or approximate Riemann solver [1]. The numerical flux used in this work is the HLLC flux [11].

Integrals in (4) are approximated with the quadrature rules. Therefore such an explicit system of the ordinary differential equations can be obtained

$$\dot{u} = Lu, \tag{5}$$
$$u(0) = u_0.$$

2.3 Time integration and limiting

The system (5) is solved by the TVD Runge-Kutta scheme [12]. On every stage the special limiter is applied.

1. $u^0 = \Lambda P(u_0)$
2. $\forall n = 0, \ldots, M-1$:
   - $u^{(0)} = u^n$,
   - $\forall i = 1, \ldots, K+1 : u^{(i)} = \Lambda\Big\{ \sum_{l=0}^{i-1} \alpha_{il} u^{(l)} + \beta_{il} \Delta t^n L(u^{(l)}) \Big\}$,
   - $u^{n+1} = u^{K+1}$.

P is the projection operator of the initial conditions on the discrete space. Coefficients α_{il}, β_{il} should provide the approximation order $k+1$ and satisfy the TVD condition [12]. The time step Δt^n is taken from the CFL condition [1].

Λ is the slope limiter, which manages to suppress the spurious oscillations near the discontinuities. The result of the work of the limiter depends on the values in the current cell and adjacent ones.

In this work the piecewise linear basis, the 2 order Runge-Kutta scheme and the *minmod* limiter [1] is used, so the scheme has the second order of accuracy in smooth regions.

3 The algorithm of implementation

For the effective GPU implementation algorithm of the numerical method the modified version of the DiamondTorre algorithm is used. In [13] it was previously applied to the PIC numerical method for the numerical simulation of Vlasov-Maxwell equations of plasma.

The DiamondTorre is of the family of locally recursive non-locally asynchronous algorithms (LRnLA). The LRnLA are applicable to the explicit numerical schemes, in particular, the RKDG method [14].

The DiamondTorre algorithm is adopted to the heterogeneous computer architecture and capable to solve the tasks with the numerical domain larger than the amount of GPU memory with high ratio of calculation speed to the theoretically possible. CUDA as the programming tool for GPGPU coding is used.

With the solver based on the RKDG method and the DiamondTorre algorithm the detailed numerical simulation and analysis of some actual three-dimensional problems can be performed, which is discussed further.

3.1 Limitations of the numerical experiments

The calculations in this work are performed using the PC having GTX Titan GPU and $32GB$ of CPU memory (DDR3). The maximum size of the numerical domain possible to deal with is less than $4 \cdot 10^8$ cells, which is limited by the memory (80B is needed for one cell). The reached calculation speed is less than $4.5 \cdot 10^7$ cells per second. Most of the simulations are made using the grid of $512 \times 512 \times 1024$ cells or smaller.

4 Bubble-shock interaction problem solution

4.1 Problem statement

The computational domain is a box filled with an ideal gas at rest with density $\rho = \rho_0$ and pressure $p = p_0$, the speed of sound there is equal to a_0. Inside this parallelepiped the spherical region of radius $R = R_0$ is defined, with the center at the point (x_0, y_0, z_0), where the pressure is equal to the external, and the density differs from the density of the ambient gas ($p_B = p_0$, $\rho_B \neq \rho_0$). On the left, at the coordinate $x = x_L$, there is a plane shock wave. Its front moves from left to right with the speed of $v_* > a_0$, behind the shock wave the unknown quantities are determined using the Rankine-Hugoniot conditions. Parameters of the shock waves are given by the Mach number $M = v_*/a_0$, the density of the bubble is characterized by the Atwood number $At = (\rho_B - \rho_0)/(\rho_B + \rho_0)$.

Due to the symmetry, to reduce the size of the computational domain, the task is set to the quarter, as shown at figure 1, planes xy and yz have the symmetry boundary condition, other planes have the boundary condition of the free flow.

4.2 Mesh-sensitive effects research

The numerical solution, as it proved in [8], has the mesh-sensitive features. To search for it and to define the proper parameters of the mesh to be used further, the following numerical experiment is set.

The same task is solved using the mesh with the width of $64, 128, 256$ and 512 cells. Results are compared with each other at the same specified time moment. At figures 2(a) —2(d) the part of the numerical solution in the diametrical cross-section of the bubble is shown at the same fixed time moment. It is easy to see

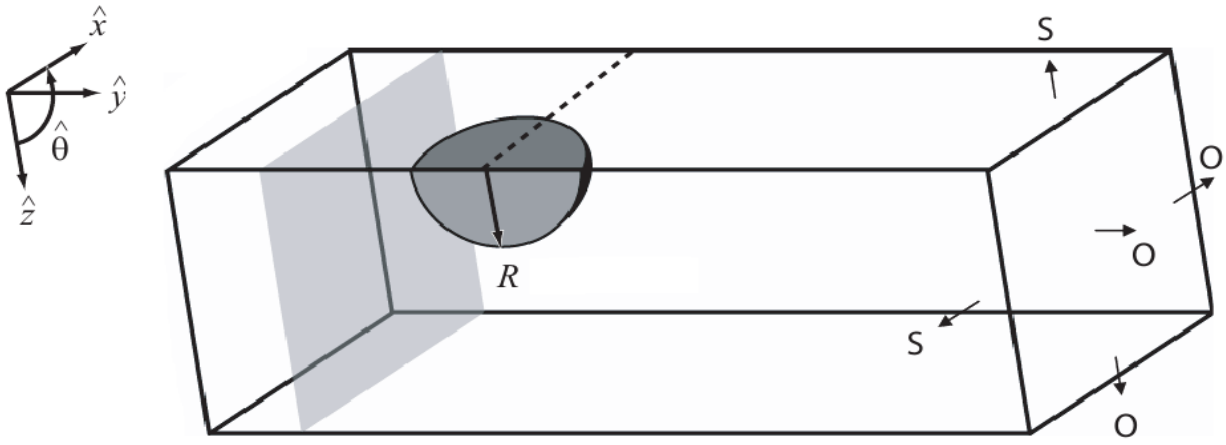
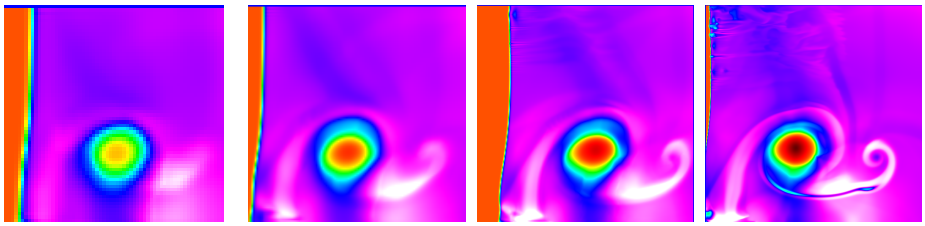


Figure 1: The computational domain at the initial time



(a) (b) (c) (d)

Figure 2: The dependence of the solution on the mesh. The mesh width (a) is 64 cells, (b) is 128 cells, (c) is 256 cells, (d) is 512 cells

that the mesh shredding leads to the display of new slight details of the solution, especially near the vortices.

Further the numerical experiments are held using the width of the grid equal to 256 or 512.

4.3 The case of a rarefied gas in a bubble

The figures show the results of modeling the interaction of helium bubble in air ($At = -0.757$) with a shock with Mach $M = 3$. In the papers [8] and [9] the similar setting is considered. The mesh used is $256 \times 256 \times 1024$ cells.

On the top half of each figure the vorticity is shown and density is shown on the bottom one in the diametrical cross-section. Scales for vorticity and density are at the top and bottom, respectively. At the initial stage of interaction, reflected at figure 3(a), the shock wave penetrates into the cavity, deforming the surface of the bubble, while the reflected rarefaction wave occurs. During the further evolution of the process, it could seen at figure 3(b) that the initial perpendicular wave, the wave-precursor and the Mach stem are connected to the so-called triple

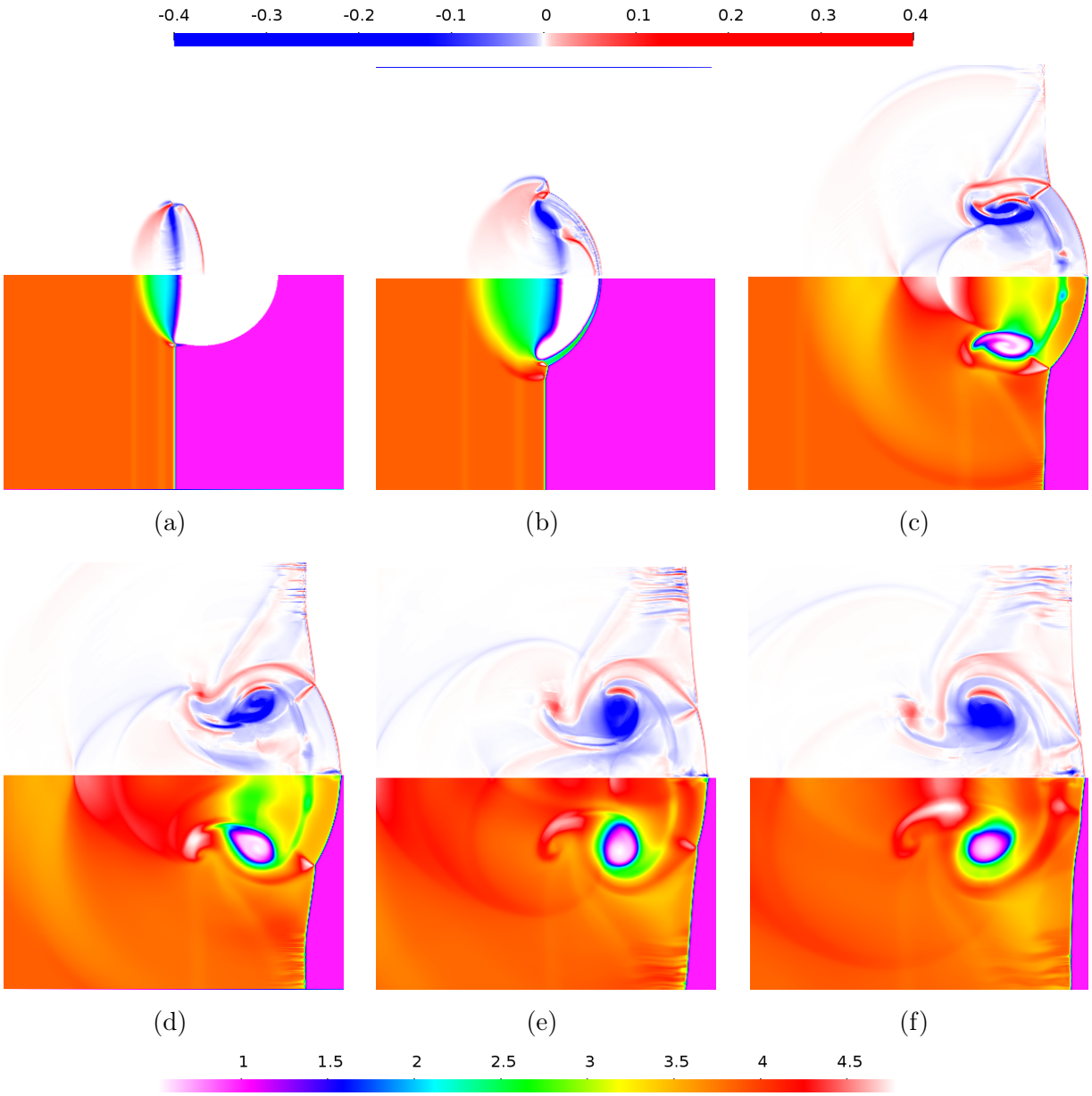


Figure 3: $At = -0.757$, $M = 3$; vorticity (top) and density (bottom) at the different time moments: (a) $\tilde{t} = 0.23$, (b) $\tilde{t} = 0.45$, (c) $\tilde{t} = 1.36$, (d) $\tilde{t} = 1.78$, (e) $\tilde{t} = 2.23$, (f) $\tilde{t} = 2.67$

point. After passing through the bubble, wave initiates the formation of the cylindrical-ring vortex structure, moving behind the shock wave, which mainly consists of low-density gas. The following process is shown at figures 3(c) — 3(f).

4.4 The case of a dense gas in a bubble

The series of drawings 4(a) – 4(k) show the results of modeling the interaction of the bubble with freon R12 ($At = 0.613$) in the air with a shock with Mach $M = 5$. In the paper [8] this statement is also considered. On the top half of

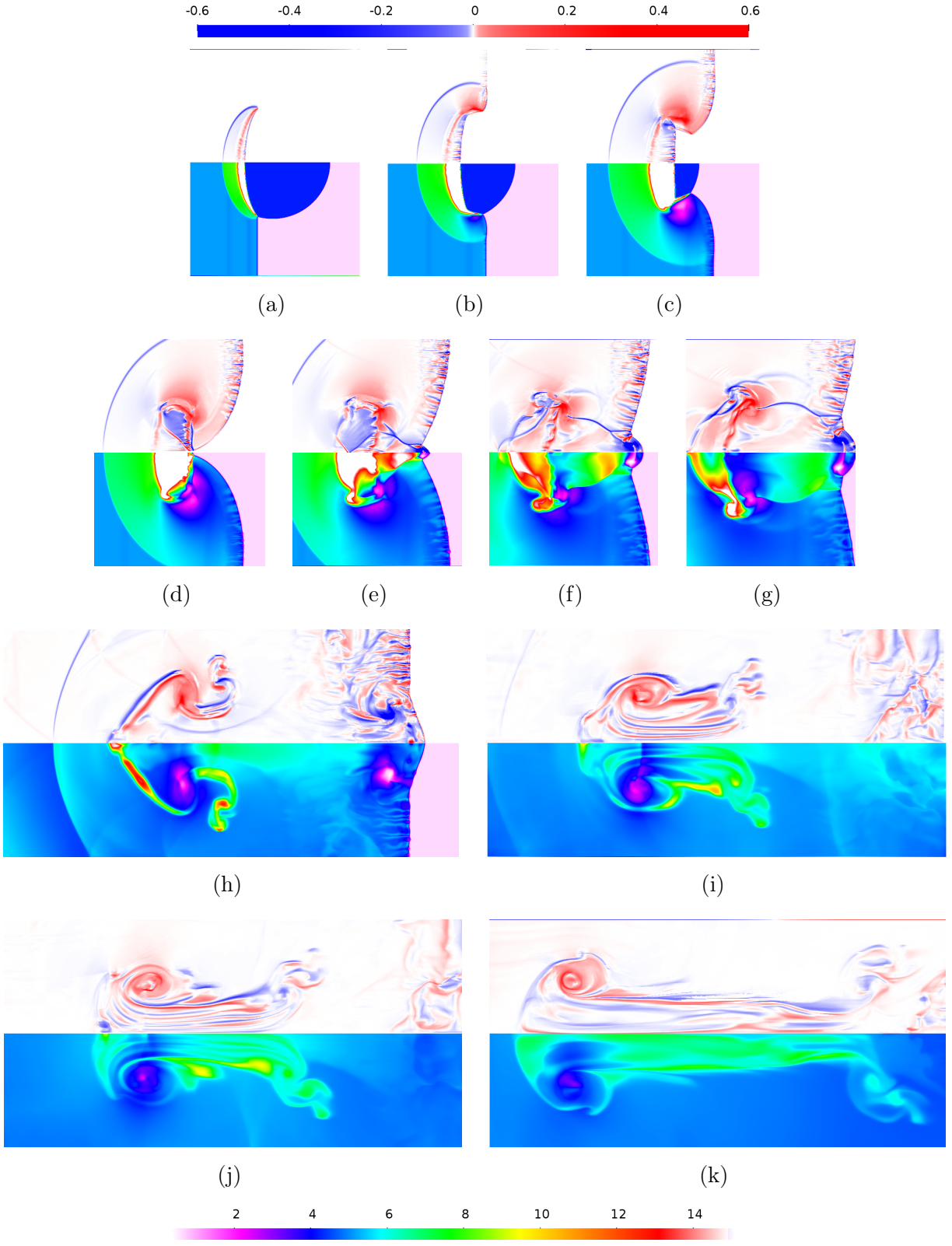


Figure 4: $At = 0.613$, $M = 5$; vorticity (top) and density (bottom) at the different time moments: (a) $\tilde{t} = 0.15$, (b) $\tilde{t} = 0.3$, (c) $\tilde{t} = 0.45$, (d) $\tilde{t} = 0.6$, (e) $\tilde{t} = 0.75$, (f) $\tilde{t} = 0.9$, (g) $\tilde{t} = 1.05$, (h) $\tilde{t} = 2.1$, (i) $\tilde{t} = 3.6$, (j) $\tilde{t} = 4.65$, (k) $\tilde{t} = 7.2$

each figure the vorticity is shown and density is shown on the bottom one in the diametrical cross-section. Scales for vorticity and density are at the top and bottom, respectively. The mesh size is $256 \times 256 \times 1024$ cells.

It should be noted that in this statement the process develops in the different way from the Air-He case. The profile of the shock wave becomes concave and focused while passing through the bubble. The bubble becomes deformed and pressured. In addition, the development of the unstable vortex structures behind the shock and exhausting from the bubble is obtained.

5 Concluding remarks

In this work the problem of bubble-shock interaction in fully three-dimensional statement is considered. Using the RKDG method, which is an explicit and high-order numerical method, and the DiamondTorre algorithm of implementation on GPU, the approach to simulate this problem numerically at the affordable computers, particularly, the PCs, is developed.

The mathematical model is rather simplified, for example, the multicomponentness is not taken into account. However, this statement is basic and its study is important for the extensions and applications. In the paper it is shown that this problem can be simulated on the PC, which means that dealing with more complex statements is also can be less difficult.

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6 References

[1] Runge-Kutta Discontinuous Galerkin Methods for Convection-dominated Problems : Rep. / NASA ; Executor: B. Cockburn, C. Shu : 2000.

[2] Caper J., Atkins H. A Finite-Volume High-Order ENO Scheme for Two-Dimentional Hyperbolic Systems // Computational Physics. — 1993. — Vol. 106. — P. 62–76.

[3] Reddy J. N., Gartling J. I. The finite element method in heat transfer and fluid dynamics // C.R.C. Press. — 1994.

[4] Van Leer B. Towards the Ultimate Cinservative Difference Scheme V. A second Order Sequel to Godunov's Method // Computational Physics. — 1979. — Vol. 32. — P. 101–136.

[5] Perepelkina A.Y., Levchenko V.D., Goryachev I.A. Implementation of the Kinetic Plasma Code with Locally Recursive non-Locally Asynchronous Algorithms // Journal of Physics: Conference Series / IOP Publishing. — Vol. 510. — 2014.

[6] Zakirov A.V., Levchenko V.D. The Effective 3D Modeling of Electromagnetic Waves Evolution in Photonic Crystals and Metamaterials // Session 3AP. — 2009. — P. 169.

[7] Use of 3D Computer Seismic Full Waveform Simulation for Validation of Porous-fractured Reservoirs Predictions / J.A. Titova, S.M. Glubokovskikh, V.E. Rok et al. // Saint Petersburg 2012. — 2012.

[8] A computational parameter study for the three-dimensional shock–bubble interaction / John H.J. Niederhaus, J.A. Greenough, J.G. Oakley et al. // Journal of Fluid Mechanics. — 2008. — Vol. 594. — P. 85–124.

[9] Hejazialhosseini Babak, Rossinelli Diego, Koumoutsakos Petros. 3D shock-bubble interactions at Mach 3 // arXiv preprint arXiv:1210.3822. — 2012. — URL: http://arxiv.org/abs/1210.3822.

[10] Gryngarten Leandro D, Menon Suresh. Shock-Bubble Interaction Simulations Using a New Two-Phase Discontinuous Galerkin Method // 49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, no. AIAA-2011-294, Orlando, FL. — 2011.

[11] Toro E.F. Riemann Solvers And Numerical Methods for Fluid Dynamics: A Practical Introduction. — Springer, 2009.

[12] Gottlieb Sigal, Shu Chi-Wang. Total variation diminishing Runge-Kutta schemes // Mathematics of Computation of the American Mathematical Society. — 1998. — Vol. 67, no. 221. — P. 73–85.

[13] Perepelkina A. Y., Levchenko V.D., Goryachev I.A. 3D3V plasma kinetics code DiamondPIC for modeling of substantially multiscale processes on heterogenous computers. — 2014.

[14] Korneev B.A., Levchenko V.D. A Locally Recursive non-Locally Asynchronous Algorithm to RKDG Methods for Gas Dynamics Equations // Preprints of Keldysh Institute of Applied Mathematics RAS. — 2013. — Vol. 28. — URL: http://library.keldysh.ru/preprint.asp?id=2013-28.

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