

Modeling of Hydrodynamics Processes with Phase Transition

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Моделювання Процесів Гідродинаміки з Фазовими Переходами

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Abstract—A new method of modeling for heterogeneous fluid dynamics processes with take of phase transitions like graphite-diamond will be presented. The method is based on a discretization of conservation laws for masses, momentums, and energies in integral and differential forms. The combination of Harlow's particle-in-cell method and Belotserkovskii's large particles method is used for computing by the method simulation.

Анотація—Новий метод моделювання процесів динаміки неоднорідної рідини з урахуванням фазових переходів графіт-алмаз буде представлено. Метод ґрунтується на дискретизації законів збереження маси, моментів і енергії в інтегральній і диференціальній формах. Комбінація методів частинок у комірках Харлоу та методу крупних частинок Білоцерківського використовується при чисельній реалізації цього методу.

Keywords—*modeling; hydrodynamics processes; phase transitions; conservation laws; graphite-diamond transition.*

Ключові слова—*моделювання; процеси гідродинаміки; фазові переходи; закони збереження; перехід графіт-алмаз.*

I. INTRODUCTION

A new method of direct parameter computing for some processes of heterogeneous fluid dynamics with take of phase transitions like graphite-diamond will be presented. It is supposed that the fluids are compressible and inviscid (non-viscous). Heterogeneities of the fluids are considered as small drops or particles of one fluid within other fluid. Total number of the drops may be large enough and the drops may have phase transitions. Thus simulations of the main fluid (or gas) with small transited drops dynamics are discussed. These are dynamics of multiphase flows really. Therefore it is possible

to use general multiphase flow models in the case. However, relevant equations are not complete as a rule. For example, there is a problem as to distribute energies between the phases in the model dynamics. Various physical experiments are necessary for solving of the problem in concrete cases. The situation is more difficult whenever phase transitions like graphite-diamond are possible.

Presented method is based on a discretization of conservation laws for masses, momentums, and energies in integral and differential forms. The discretization is natural and numerical simulations are realized as direct computer experiments for dynamics of main fluid together with transited drops without use multiphase flows approach. The method seems to be much more adequate to the physical and mathematical essence of the dynamics because conservation laws are correct on the discrete level at least.

The presented method is a combination of the Harlow's particle-in-cell method and Belotserkovskii's large particles method (see [1] and [2], for example). Let us recall some background of the methods before to give more details on the method combination.

Euler's and Lagrange's approaches are used simultaneously in the particles in cells method for homogeneous fluid (or gas). The method is based on a discretization of conservation laws for masses, momentums, and energies of the fluid in the following integral forms

$$\int_{V(t)} \rho'_i d\tau = - \int_{S(t)} (\rho W) \cdot N ds, \\ \frac{d}{dt} \int_{V(t)} \rho W d\tau = - \int_{S(t)} p N ds, \quad (1)$$

$$\frac{d}{dt} \int_{V(t)} \rho E d\tau = - \int_{S(t)} (pW) \cdot N ds,$$

where $V(t)$ and $S(t)$ are volume and surface of some Lagrange's domain in the fluid, N is an exterior normal to the domain, $p = p(\rho, E)$ and ρ, W, E are unknown density, velocity, and full energy. For example, the case of three dimension space may be discussed and therefore by definition ones have $W = (u, v, w)$.

II. MODELING METHOD

It is known [1] that the conservation laws are equivalent to conservation laws for masses, momentums, and energies of the fluid in the following differential forms

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \text{div}(\rho W) &= 0, \\ \frac{\partial \rho W}{\partial t} + \text{div}(\rho W \otimes W) + \nabla p &= 0, \\ \frac{\partial \rho E}{\partial t} + \text{div}(\rho E W) + \text{div}(pW) &= 0, \end{aligned} \quad (2)$$

where $W \otimes W$ is the tensor square of vector function $W = W(t, x, y, z)$ and x, y, z is a point of some domain Ω , which is filled by the heterogeneous fluid under consideration.

The time discretization in the method is natural. Simulations are conducted step by step with a small enough time interval Δt that starting from an initial configuration. The space discretization in the method is more complicated and dynamics are taking into consideration. The fluid region Ω is divided into cells with the small size Δx and the fluid filling every such cell is considered as a collection of a few particles or drops. Every such particle have own mass, volume, energy, and coordinates that are specified at an initial moment. In addition the density, velocity, and full energy $\rho^n, u^n, v^n, w^n, E^n$ are specified for every such cell with number i, j, k at the time moment $t = n\Delta t$.

Corresponding time step of the simulation is split up to three stages so the discrete conservation laws are faithful. For example, the total mass of particles under consideration is saved at every time step of such discretization.

On the first stage of the time step, the intermediate velocities $\bar{u}^n, \bar{v}^n, \bar{w}^n$ and the energy \bar{E}^n of particles from the sell with number i, j, k are calculated by the following formulas

$$\bar{u}_{i,j,k}^n = u_{i,j,k}^n - \frac{p_{i+1,j,k}^n - p_{i-1,j,k}^n}{2\Delta x} \frac{\Delta t}{\rho_{i,j,k}^n},$$

$$\begin{aligned} \bar{v}_{i,j,k}^n &= v_{i,j,k}^n - \frac{p_{i,j+1,k}^n - p_{i,j-1,k}^n}{2\Delta y} \frac{\Delta t}{\rho_{i,j,k}^n}, \\ \bar{w}_{i,j,k}^n &= w_{i,j,k}^n - \frac{p_{i,j,k+1}^n - p_{i,j,k-1}^n}{2\Delta z} \frac{\Delta t}{\rho_{i,j,k}^n}, \\ \bar{E}_{i,j,k}^n &= E_{i,j,k}^n - \\ &\frac{p_{i+1/2,j,k}^n u_{i+1/2,j,k}^n - p_{i-1/2,j,k}^n u_{i-1/2,j,k}^n}{\Delta x} \frac{\Delta t}{\rho_{i,j,k}^n} - \\ &\frac{p_{i,j+1/2,k}^n u_{i,j+1/2,k}^n - p_{i,j-1/2,k}^n u_{i,j-1/2,k}^n}{\Delta y} \frac{\Delta t}{\rho_{i,j,k}^n} - \\ &\frac{p_{i,j,k+1/2}^n u_{i,j,k+1/2}^n - p_{i,j,k-1/2}^n u_{i,j,k-1/2}^n}{\Delta z} \frac{\Delta t}{\rho_{i,j,k}^n}, \end{aligned} \quad (3)$$

where

$$\begin{aligned} p_{i+1/2,j,k}^n &= \frac{p_{i+1,j,k}^n - p_{i,j,k}^n}{2}, \quad p_{i-1/2,j,k}^n = \frac{p_{i,j,k}^n - p_{i-1,j,k}^n}{2}, \\ u_{i+1/2,j,k}^n &= \frac{u_{i+1,j,k}^n - u_{i,j,k}^n}{2}, \quad u_{i-1/2,j,k}^n = \frac{u_{i,j,k}^n - u_{i-1,j,k}^n}{2}, \\ v_{i,j+1/2,k}^n &= \frac{v_{i,j+1,k}^n - v_{i,j,k}^n}{2}, \quad v_{i,j-1/2,k}^n = \frac{v_{i,j,k}^n - v_{i,j-1,k}^n}{2} \end{aligned}$$

and similar formula is used for $p_{i,j+1/2,k}^n, \dots, w_{i,j,k-1/2}^n$.

This is the Euler's stage for approximations of transport free momentums equations in (1) by the pressure forces for every sell. On the second stage, motions of the particles by the velocities are taking into account. This is the Lagrange's stage for an approximation of masses equation that is modeling of mass transports from a sell to surrounding sells. On the third stage, moving of the momentums and energy are calculated. This is the concluding stage for approximations of pressure free momentums and energies equations in (1) that are modeling of the momentums and energy transports by the dynamics from a sell to surrounding sells.

The approximations are rationale from physical and mathematical point of view since conservation laws are correct on the discrete levels during the courses of corresponding numerical simulations. Therefore the particle-in-cells method is effective enough for numerical evaluations of homogeneous fluid (or gas) dynamics by boundary conditions and external forces. Concrete types of fluid are defined here by a form of state equation $p = p(\rho, J)$, where $J = E - W^2 / 2$ is a notation for interior energy.

An essential problem is only that total number of particles may be very large. Indeed total number of cells must be large enough for best approximations and the number of particles at every cell must be large enough also. Moreover every such particle must have own mass, volume, energy, and coordinates. Thus there is massive data and the data is recalculated from step to step.

In order to avoid the problem it is possibly to use the large particles method. The time discretization in the method is similar to the discretization in the particles in cells method. The space discretization in the method is following. Fluid region is divided into cells with small size and the fluid filling every such cell is considered as a large particle or drop. Every such particle have own mass, volume and energy that are specified at an initial moment. In addition the density, velocity, and full energy are specified for every such cell at the moment. But the volume of particle is coincided with the volume of cell now. Therefore the mass and energy of particle are defined by the density and full energy. Thus the data is not so massive in the method.

Corresponding time step of the simulation is split up to three stages also and so the discrete conservation laws are faithful. The stages are similar to the stages of the particles in cells method, for example, formulas (3) are used on the first stage. Modifications are need only for modeling of the mass and momentums transports by the dynamics. For example, the mass transports are calculated as moving of corresponding share of large particle mass from the cell to corresponding surrounding sell by the following formulas

$$\begin{aligned}
M_{i+1/2,j,k}^n &= \bar{\rho}_{i+1/2,j,k}^n \bar{u}_{i+1/2,j,k}^n \Delta y \Delta z \Delta t, \\
M_{i-1/2,j,k}^n &= \bar{\rho}_{i-1/2,j,k}^n \bar{u}_{i-1/2,j,k}^n \Delta y \Delta z \Delta t, \\
M_{i,j+1/2,k}^n &= \bar{\rho}_{i,j+1/2,k}^n \bar{v}_{i,j+1/2,k}^n \Delta x \Delta z \Delta t, \\
M_{i,j-1/2,k}^n &= \bar{\rho}_{i,j-1/2,k}^n \bar{v}_{i,j-1/2,k}^n \Delta x \Delta z \Delta t, \\
M_{i,j,k+1/2}^n &= \bar{\rho}_{i,j,k+1/2}^n \bar{w}_{i,j,k+1/2}^n \Delta x \Delta y \Delta t, \\
M_{i,j,k-1/2}^n &= \bar{\rho}_{i,j,k-1/2}^n \bar{w}_{i,j,k-1/2}^n \Delta x \Delta y \Delta t,
\end{aligned} \tag{4}$$

where $\bar{u}_{i+1/2,j,k}^n, \bar{u}_{i-1/2,j,k}^n, \bar{v}_{i,j+1/2,k}^n, \dots, \bar{w}_{i,j,k-1/2}^n$ are calculated as in (3) and we use the equalities

$$\begin{aligned}
\bar{\rho}_{i+1/2,j,k}^n &= \begin{cases} \rho_{i,j,k}^n, & \text{if } \bar{u}_{i+1/2,j,k}^n \geq 0, \\ \rho_{i+1,j,k}^n, & \text{if } \bar{u}_{i+1/2,j,k}^n < 0, \end{cases} \\
\bar{\rho}_{i-1/2,j,k}^n &= \begin{cases} \rho_{i-1,j,k}^n, & \text{if } \bar{u}_{i-1/2,j,k}^n \geq 0, \\ \rho_{i,j,k}^n, & \text{if } \bar{u}_{i-1/2,j,k}^n < 0, \end{cases} \\
\bar{\rho}_{i,j+1/2,k}^n &= \begin{cases} \rho_{i,j,k}^n, & \text{if } \bar{v}_{i,j+1/2,k}^n \geq 0, \\ \rho_{i,j+1,k}^n, & \text{if } \bar{v}_{i,j+1/2,k}^n < 0, \end{cases} \\
\bar{\rho}_{i,j-1/2,k}^n &= \begin{cases} \rho_{i,j-1,k}^n, & \text{if } \bar{v}_{i,j-1/2,k}^n \geq 0, \\ \rho_{i,j,k}^n, & \text{if } \bar{v}_{i,j-1/2,k}^n < 0, \end{cases} \\
\bar{\rho}_{i,j,k+1/2}^n &= \begin{cases} \rho_{i,j,k}^n, & \text{if } \bar{w}_{i,j,k+1/2}^n \geq 0, \\ \rho_{i,j,k+1}^n, & \text{if } \bar{w}_{i,j,k+1/2}^n < 0, \end{cases}
\end{aligned} \tag{5}$$

$$\bar{\rho}_{i,j,k-1/2}^n = \begin{cases} \rho_{i,j,k-1}^n, & \text{if } \bar{w}_{i,j,k-1/2}^n \geq 0, \\ \rho_{i,j,k}^n, & \text{if } \bar{w}_{i,j,k-1/2}^n < 0. \end{cases}$$

On the third stage, moving of the momentums $u^{n+1}, v^{n+1}, w^{n+1}$ and the energy E^{n+1} on the step $n+1$ are calculated by the following formulas

$$\begin{aligned}
\rho_{i,j,k}^{n+1} &= \rho_{i,j,k}^n - \\
&\quad - O_{xyz}^{-1} \{ M_{i+1/2,j,k}^n - M_{i-1/2,j,k}^n + M_{i,j+1/2,k}^n - \\
&\quad - M_{i,j-1/2,k}^n + M_{i,j,k+1/2}^n - M_{i,j,k-1/2}^n \}, \\
u_{i,j,k}^{n+1} &= \frac{\rho_{i,j,k}^n}{\rho_{i,j,k}^{n+1}} u_{i,j,k}^n - \\
&\quad - O_{xyz}^{-1} \{ \bar{u}_{i+1/2,j,k}^n M_{i+1/2,j,k}^n - \bar{u}_{i-1/2,j,k}^n M_{i-1/2,j,k}^n + \\
&\quad + \bar{u}_{i,j+1/2,k}^n M_{i,j+1/2,k}^n - \bar{u}_{i,j-1/2,k}^n M_{i,j-1/2,k}^n + \\
&\quad + \bar{u}_{i,j,k+1/2}^n M_{i,j,k+1/2}^n - \bar{u}_{i,j,k-1/2}^n M_{i,j,k-1/2}^n \}, \\
v_{i,j,k}^{n+1} &= \frac{\rho_{i,j,k}^n}{\rho_{i,j,k}^{n+1}} v_{i,j,k}^n - \\
&\quad - O_{xyz}^{-1} \{ \bar{v}_{i+1/2,j,k}^n M_{i+1/2,j,k}^n - \bar{v}_{i-1/2,j,k}^n M_{i-1/2,j,k}^n + \\
&\quad + \bar{v}_{i,j+1/2,k}^n M_{i,j+1/2,k}^n - \bar{v}_{i,j-1/2,k}^n M_{i,j-1/2,k}^n + \\
&\quad + \bar{v}_{i,j,k+1/2}^n M_{i,j,k+1/2}^n - \bar{v}_{i,j,k-1/2}^n M_{i,j,k-1/2}^n \}, \\
w_{i,j,k}^{n+1} &= \frac{\rho_{i,j,k}^n}{\rho_{i,j,k}^{n+1}} w_{i,j,k}^n - \\
&\quad - O_{xyz}^{-1} \{ \bar{w}_{i+1/2,j,k}^n M_{i+1/2,j,k}^n - \bar{w}_{i-1/2,j,k}^n M_{i-1/2,j,k}^n + \\
&\quad + \bar{w}_{i,j+1/2,k}^n M_{i,j+1/2,k}^n - \bar{w}_{i,j-1/2,k}^n M_{i,j-1/2,k}^n + \\
&\quad + \bar{w}_{i,j,k+1/2}^n M_{i,j,k+1/2}^n - \bar{w}_{i,j,k-1/2}^n M_{i,j,k-1/2}^n \}, \\
E_{i,j,k}^{n+1} &= \frac{\rho_{i,j,k}^n}{\rho_{i,j,k}^{n+1}} E_{i,j,k}^n - \\
&\quad - O_{xyz}^{-1} \{ \bar{E}_{i+1/2,j,k}^n M_{i+1/2,j,k}^n - \bar{E}_{i-1/2,j,k}^n M_{i-1/2,j,k}^n + \\
&\quad + \bar{E}_{i,j+1/2,k}^n M_{i,j+1/2,k}^n - \bar{E}_{i,j-1/2,k}^n M_{i,j-1/2,k}^n + \\
&\quad + \bar{E}_{i,j,k+1/2}^n M_{i,j,k+1/2}^n - \bar{E}_{i,j,k-1/2}^n M_{i,j,k-1/2}^n \},
\end{aligned} \tag{6}$$

where $O_{xyz} = \Delta x \Delta y \Delta z$ is the volume of the cell under consideration and the values $\bar{u}_{i+1/2,j,k}^n, \bar{u}_{i-1/2,j,k}^n, \dots, \bar{E}_{i,j,k-1/2}^n$ are calculated as in formulas (5).

Thus total mass of the fluid under consideration is saved at every time step of such discretization if there are no external mass sources under the simulation of course. For example, the

mass sources may be induced by boundary conditions and external forces that leads to corresponding modifications of conservation laws in (1) and on the discrete level also. The momentums and energy transports are modeling in similar manners. The approximations are rationale also. Thus large particles method is effective enough for numerical evaluations of homogeneous fluid dynamics also and the recalculated data is not very massive as in particle-in-cell method.

Let us return to presented method. The method is designed to numerical modeling of the main fluid with small transited drops dynamics. The time discretization in the method is as in above methods. The space discretization in the method is following. Heterogeneous fluid region is divided into cells with small size. The main fluid filling every such cell is considered as a large particle while the transited drops are considered as the collection of a few "small" particles in the cell. Every large particle have own mass, volume and energy that are specified at an initial moment. Every small particle have own mass, volume, energy, and coordinates that are specified at the moment. In addition the density, velocity, and full energy are specified for every such cell. This is a combination of above methods at the initial moment. Corresponding time step of the simulation is split up to three stages with additional preliminary stage.

On the preliminary stage, energies of large particle and small particles in every cell are distributed between the particles so that a pressure in the cell is uniform. Indeed the large particle induce some pressure by own state equation and the small particles induce some pressure by own state equation and it is natural to distribute energies of the particles so that the first pressure coincides with second pressure. Moreover on the stage, it is possible to observe phase transitions of the small particles by the pressure, for example. The phase transitions are realized if the pressure is more than critical pressure by the corresponding phase diagram. In the case the small particles may change own volume, energy, and state equation. Thus the heterogeneous fluid may have three or more phases. Thus, we use formulas (3) on the stage to calculate the intermediate velocities $\bar{u}^n, \bar{v}^n, \bar{w}^n$ and the energy \bar{E}^n of particles from the sell with number i, j, k at the time moment $t = n\Delta t$. The remaining stages are similar to the stages of above methods. For example, the mass transports are calculated as moving of corresponding share of large particle mass and small particles masses from the cell to corresponding surrounding sell by formulas (5), which are used in (6).

Thus total mass of the heterogeneous fluid under consideration is saved at every time step of such discretization. The momentums $u^{n+1}, v^{n+1}, w^{n+1}$ and the energy E^{n+1} on the step $n+1$ are modeling in similar manners by formulas (6). Thus, this is a combination of above methods from step to step during the courses of corresponding numerical simulations. The method seems to be reasonable for numerical evaluations of such heterogeneous fluid (or gas)

dynamics and the recalculated data is not very massive. On the other hand it is possible to use the particles in cells method with the preliminary stages for modeling of the dynamics. But the recalculated data is very massive in the case.

The presented method is designed to numerical modeling of following physical processes. Let consider graphite drops distributing uniformly in some fluid. More exactly, there is heterogeneous medium with graphite particles and the medium may be considered under high pressure as "fluid" with corresponding state equation. For example, we consider a cylinder of the medium that consist of copper with graphite particles. Let the cylinder be in an outside explosive tube device. Inducing detonation shock waves in the outside explosive tube device, we can observe dynamics of such shock waves in computer experiments by the method.

Results of the computer experiments may be found in [3]. The results were in agreement with known results of physical experiments. More details of the presented method and other modifications may be found in papers [4,5].

The presented method was applicable to numerical simulations of plasma dynamics according to [6]. The plasma may be considered as gas with ionized particles. The gas and particles were defined by corresponding state equations. Equations (2) were coupled with Maxwell's equations and on the discrete level also. Inducing motions of the heterogeneous plasma in some region it was possible to observe absorption of the ionized particles on relevant boundaries in computer experiments by the method coupling with appropriate method for Maxwell's equations [3, 6]. Alternative methods and corresponding references for the problem may be found in [7].

Nevertheless, the presented method seems to be perspective for numerical simulations of other absorption and diffusion processes in complex fluid and plasma dynamics.

REFERENCES

- [1] O. M. Belotserkovskij, Yu. M. Davidov, The large particles method in gas dynamics. Nauka, Moscow, 1982. (in Russian)
- [2] G. Shirkov, "Particle-in-cell method for numerical simulation of beam and plasma dynamics," *Nuclear Instruments and Methods in Physics Research. Section A: Accelerators, Spectrometers, Detectors and Associated Equipment.* no. 1 (558), pp. 317–324, 2006.
- [3] S. V. Boyko, G. V. Sandrakov, "Parameter computing of hydrodynamics processes with phase transitions," *Bulletin of Taras Shevchenko National University of Kyiv, Series: Physics & Mathematics*, Special no. , pp. 11–16, 2013.
- [4] S. V. Boyko, G. V. Sandrakov, "Mathematical modeling of complex heterogeneous fluid dynamics," *Journal Num. and Appl. Math.*, no. 1 (104), pp. 109–120, 2011. (in Russian)
- [5] S. V. Boyko, G. V. Sandrakov, "Mathematical modeling of phase transitions graphite-diamond dynamics," *Journal Num. and Appl. Math.*, no. 2 (108), pp. 88–109, 2012. (in Russian)
- [6] S. V. Boyko, V. V. Mischenko, G. V. Sandrakov, "The numerical investigation method for evaporated plasma," *Journal Num. and Appl. Math.*, no. 2 (95), pp. 3–12, 2007.
- [7] G. R. Liu, M. B. Liu, Smoothed particle hydrodynamics. A meshfree particle method. World Scientific Publishing, New Jersey, 2003.