Modeling of Hydrodynamics Processes with Phase Transition

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Моделювання Процессів 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 методмоделювання процесів динаміки неоднорідної рідини з урахуванням фазових переходів графіт-алмазбуде презентовано. 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;перехідграфіт-алмаз.

I. INTRODUCTION

A new method of direct parameter computing for some processes of heterogeneous fluiddynamics with take of phase transitions like graphite-diamond will be presented. It is supposed that the fluids arecompressible and inviscid (non-viscous). Heterogeneities of thefluids are consideredas small drops or particles of one fluidwithin other fluid. Total number of the drops may be largeenoughand the drops may have phase transitions. Thus simulations of themain fluid (or gas) with small transited drops dynamics arediscussed. These are dynamics of multiphase flows really.Therefore it is possible to use general multiphase flow models inthe case. However, relevant equations are not complete as a rule. Forexample, there is a problem as to distribute energies between thephases in the modeldynamics. Various physical experiments arenecessary for solving of the problem in concrete cases. Thesituation is more difficult whenever phase transitions like graphite-diamond arepossible.

Presented method is based on a discretization of conservation lawsfor masses, momentums, andenergies in integral and differential forms. Thediscretization is natural and numerical simulations are realizedas direct computer experiments for dynamics of main fluid togetherwith transited drops without use multiphase flows approach. Themethod seems to be much more adequate to the physical andmathematicalessence of the dynamics becauseconservation laws arecorrect 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 moredetails on the method combination.

Euler's and Lagrange's approaches are used simultaneously in theparticles in cells method for homogeneous fluid (or gas). Themethod is based on a discretization of conservation laws formasses, momentums, and energies of the fluid in the following integralforms

$$\int_{V(t)} \rho'_t \, d\tau = -\int_{S(t)} (\rho W) \cdot N \, ds,$$

$$\frac{d}{dt} \int_{V(t)} \rho W \, d\tau = -\int_{S(t)} p \, N \, ds, \quad (1)$$

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

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

II. Modeling method

It is known [1] that the conservationlaws are equivalent to conservation laws formasses, momentums, and energies of the fluid in the following differentialforms

$$\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho W) = 0,$$

$$\frac{\partial\rho W}{\partial t} + \mathrm{div}(\rho W\otimes W) + \nabla p = 0, \qquad (2)$$

$$\frac{\partial\rho E}{\partial t} + \mathrm{div}(\rho EW) + \mathrm{div}(pW) = 0,$$

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 areconducted step by step with a small enough time interval Δt that startingfrom an initial configuration. The space discretization in themethod is more complicated and dynamics are taking intoconsideration. The fluid region Ω is divided into cells with the small size Δx and the fluid filling every such cell is considered as acollection of a few particles or drops. Every such particle haveown mass, volume, energy, and coordinates that are specified at aninitial 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 $t = n\Delta t$.

Correspondingtime step of the simulation is split up to three stages so thediscrete conservation laws are faithful. For example, the total massof particles under consideration is saved at every time step of suchdiscretization.

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

$$\bar{u}^n_{i,j,k} = u^n_{i,j,k} - \frac{p^n_{i+1,j,k} - p^n_{i-1,j,k}}{2\Delta x}\frac{\Delta t}{\rho^n_{i,j,k}},$$

$$\bar{v}^n_{i,j,k} = v^n_{i,j,k} - \frac{p^n_{i,j+1,k} - p^n_{i,j-1,k}}{2\Delta y}\frac{\Delta t}{\rho^n_{i,j,k}},$$

$$\bar{w}^n_{i,j,k} = w^n_{i,j,k} - \frac{p^n_{i,j,k+1} - p^n_{i,j,k-1}}{2\Delta z}\frac{\Delta t}{\rho^n_{i,j,k}},$$

$$\bar{E}^n_{i,j,k} = E^n_{i,j,k} - \qquad (3)$$

$$-\frac{p^n_{i+1/2,j,k}u^n_{i+1/2,j.k} - p^n_{i-1/2,j,k}u^n_{i-1/2,j,k}}{\Delta x}\frac{\Delta t}{\rho^n_{i,j,k}} -$$

$$-\frac{p^n_{i,j+1/2,k}u^n_{i,j+1/2.k} - p^n_{i,j-1/2,k}u^n_{i,j-1/2,k}}{\Delta y}\frac{\Delta t}{\rho^n_{i,j,k}} -$$

$$-\frac{p^n_{i,j,k+1/2}u^n_{i,j.k+1/2} - p^n_{i,j,k-1/2}u^n_{i,j,k-1/2}}{\Delta z}\frac{\Delta t}{\rho^n_{i,j,k}},$$

where

$$p^n_{i+1/2,j,k} = \frac{p^n_{i+1,j,k} - p^n_{i,j,k}}{2}, \quad p^n_{i-1/2,j,k} = \frac{p^n_{i,j,k} - p^n_{i-1,j,k}}{2},$$

$$u^n_{i+1/2,j,k} = \frac{u^n_{i+1,j,k} - u^n_{i,j,k}}{2}, \quad u^n_{i-1/2,j,k} = \frac{u^n_{i,j,k} - u^n_{i-1,j,k}}{2},$$

$$v^n_{i,j+1/2,k} = \frac{v^n_{i,j+1,k} - v^n_{i,j,k}}{2}, \quad v^n_{i,j-1/2,k} = \frac{v^n_{i,j,k} - v^n_{i,j-1,k}}{2}$$

and similar formula is used for $p^n_{i,j+1/2,k}, \ldots, w^n_{i,j,k-1/2}$.

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

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

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

In order to avoid the problem it is possibly to use the largeparticles method. The time discretization in the method is similarto the discretization in the particles in cells method. The spacediscretization in the method is following. Fluid region is dividedinto cells with small size and the fluid filling every such cellis considered as a large particle or drop. Every such particlehave own mass, volume and energy that are specified at an initialmoment. In addition the density, velocity, and full energy arespecified for every such cell at the moment. But the volume ofparticle is coincided with the volume of cell now. Therefore themass and energy of particle are defined by the density and fullenergy. Thus the data is not so massive in the method.

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

$$
\begin{aligned}
M^n_{i+1/2,j,k} &= \bar{\rho}^n_{i+1/2,j,k}\,\bar{u}^n_{i+1/2,j,k}\Delta y\Delta z\Delta t,\\
M^n_{i-1/2,j,k} &= \bar{\rho}^n_{i-1/2,j,k}\,\bar{u}^n_{i-1/2,j,k}\Delta y\Delta z\Delta t,\\
M^n_{i,j+1/2,k} &= \bar{\rho}^n_{i,j+1/2,k}\,\bar{v}^n_{i,j+1/2,k}\Delta x\Delta z\Delta t,\\
M^n_{i,j-1/2,k} &= \bar{\rho}^n_{i,j-1/2,k}\,\bar{v}^n_{i,j-1/2,k}\Delta x\Delta z\Delta t,\\
M^n_{i,j,k+1/2} &= \bar{\rho}^n_{i,j,k+1/2}\,\bar{w}^n_{i,j,k+1/2}\Delta x\Delta y\Delta t,\\
M^n_{i,j,k-1/2} &= \bar{\rho}^n_{i,j,k-1/2}\,\bar{w}^n_{i,j,k-1/2}\Delta x\Delta y\Delta t,
\end{aligned}
\qquad (4)
$$

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

$$
\begin{aligned}
\bar{\rho}^n_{i+1/2,j,k} &= \begin{cases} \rho^n_{i,j,k}, & if\ \bar{u}^n_{i+1/2,j,k} \ge 0,\\ \rho^n_{i+1,j,k}, & if\ \bar{u}^n_{i+1/2,j,k} < 0, \end{cases}\\
\bar{\rho}^n_{i-1/2,j,k} &= \begin{cases} \rho^n_{i-1,j,k}, & if\ \bar{u}^n_{i-1/2,j,k} \ge 0,\\ \rho^n_{i,j,k}, & if\ \bar{u}^n_{i-1/2,j,k} < 0, \end{cases}\\
\bar{\rho}^n_{i,j+1/2,k} &= \begin{cases} \rho^n_{i,j,k}, & if\ \bar{v}^n_{i,j+1/2,k} \ge 0,\\ \rho^n_{i,j+1,k}, & if\ \bar{v}^n_{i,j+1/2,k} < 0, \end{cases}\\
\bar{\rho}^n_{i,j-1/2,k} &= \begin{cases} \rho^n_{i,j-1,k}, & if\ \bar{v}^n_{i,j-1/2,k} \ge 0,\\ \rho^n_{i,j,k}, & if\ \bar{v}^n_{i,j-1/2,k} < 0, \end{cases}\\
\bar{\rho}^n_{i,j,k+1/2} &= \begin{cases} \rho^n_{i,j,k}, & if\ \bar{w}^n_{i,j,k+1/2} \ge 0,\\ \rho^n_{i,j,k+1}, & if\ \bar{w}^n_{i,j,k+1/2} < 0, \end{cases}\\
\bar{\rho}^n_{i,j,k-1/2} &= \begin{cases} \rho^n_{i,j,k-1}, & if\ \bar{w}^n_{i,j,k-1/2} \ge 0,\\ \rho^n_{i,j,k}, & if\ \bar{w}^n_{i,j,k-1/2} < 0. \end{cases}
\end{aligned}
\qquad (5)
$$

On the thirdstage, 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

$$
\begin{aligned}
&\rho^{n+1}_{i,j,k} = \rho^n_{i,j,k} -\\
&-\mathrm{O}^{-1}_{xyz}\{M^n_{i+1/2,j,k} - M^n_{i-1/2,j,k} + M^n_{i,j+1/2,k} -\\
&-M^n_{i,j-1/2,k} + M^n_{i,j,k+1/2} - M^n_{i,j,k-1/2}\},\\
&u^{n+1}_{i,j,k} = \frac{\rho^n_{i,j,k}}{\rho^{n+1}_{i,j,k}}u^n_{i,j,k} -\\
&-\mathrm{O}^{-1}_{xyz}\{\bar{u}^n_{i+1/2,j,k}M^n_{i+1/2,j,k} - \bar{u}^n_{i-1/2,j,k}M^n_{i-1/2,j,k} +\\
&+\bar{u}^n_{i,j+1/2,k}M^n_{i,j+1/2,k} - \bar{u}^n_{i,j-1/2,k}M^n_{i,j-1/2,k} +\\
&+\bar{u}^n_{i,j,k+1/2}M^n_{i,j,k+1/2} - \bar{u}^n_{i,j,k-1/2}M^n_{i,j,k-1/2}\},\\
&v^{n+1}_{i,j,k} = \frac{\rho^n_{i,j,k}}{\rho^{n+1}_{i,j,k}}v^n_{i,j,k} -\\
&-\mathrm{O}^{-1}_{xyz}\{\bar{v}^n_{i+1/2,j,k}M^n_{i+1/2,j,k} - \bar{v}^n_{i-1/2,j,k}M^n_{i-1/2,j,k} +\\
&+\bar{v}^n_{i,j+1/2,k}M^n_{i,j+1/2,k} - \bar{v}^n_{i,j-1/2,k}M^n_{i,j-1/2,k} +\\
&+\bar{v}^n_{i,j,k+1/2}M^n_{i,j,k+1/2} - \bar{v}^n_{i,j,k-1/2}M^n_{i,j,k-1/2}\},\\
&w^{n+1}_{i,j,k} = \frac{\rho^n_{i,j,k}}{\rho^{n+1}_{i,j,k}}w^n_{i,j,k} -\\
&-\mathrm{O}^{-1}_{xyz}\{\bar{w}^n_{i+1/2,j,k}M^n_{i+1/2,j,k} - \bar{w}^n_{i-1/2,j,k}M^n_{i-1/2,j,k} +\\
&+\bar{w}^n_{i,j+1/2,k}M^n_{i,j+1/2,k} - \bar{w}^n_{i,j-1/2,k}M^n_{i,j-1/2,k} +\\
&+\bar{w}^n_{i,j,k+1/2}M^n_{i,j,k+1/2} - \bar{w}^n_{i,j,k-1/2}M^n_{i,j,k-1/2}\},\\
&E^{n+1}_{i,j,k} = \frac{\rho^n_{i,j,k}}{\rho^{n+1}_{i,j,k}}E^n_{i,j,k} -\\
&-\mathrm{O}^{-1}_{xyz}\{\bar{E}^n_{i+1/2,j,k}M^n_{i+1/2,j,k} - \bar{E}^n_{i-1/2,j,k}M^n_{i-1/2,j,k} +\\
&+\bar{E}^n_{i,j+1/2,k}M^n_{i,j+1/2,k} - \bar{E}^n_{i,j-1/2,k}M^n_{i,j-1/2,k} +\\
&+\bar{E}^n_{i,j,k+1/2}M^n_{i,j,k+1/2} - \bar{E}^n_{i,j,k-1/2}M^n_{i,j,k-1/2}\},
\end{aligned}
\qquad (6)
$$

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

Thus total mass of the fluid under consideration is saved atevery time step of such discretization if there are no externalmass sources under the simulation of course. For

example, the masssources may be induced by boundary conditions and external forcesthat leads to corresponding modifications of conservation laws in(1) and on the discrete level also. The momentums and energytransports are modeling in similar manners.The approximations are rationale also. Thus largeparticles method is effective enough for numerical evaluationsof homogeneous fluiddynamics alsoand the recalculateddata is not very massive as in particle-in-cell method.

Let us return to presented method. The method is designed tonumerical modeling of the main fluid with small transited dropsdynamics. The time discretization in the method is as in abovemethods.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 largeparticle while the transited drops are considered as thecollection of a few "small" particles in the cell. Every largeparticle have own mass, volume and energy that are specified at aninitial moment. Every small particle have own mass, volume,energy, and coordinates that are specified at the moment. Inaddition the density, velocity, and full energy are specified forevery such cell. This is a combination of above methods atthe initial moment. Corresponding time step of the simulation is split up to threestages with additional preliminary stage.

On the preliminarystage, energies of large particle and small particles in everycell are distributed between the particles so that a pressure inthe cell is uniform. Indeed the large particle induce somepressure by own state equation and the small particles induce somepressure by own state equation and it is natural to distributeenergies of the particles so that the first pressure coincideswith second pressure. Moreover on the stage, it is possible toobserve phase transitions of the small particles by the pressure,for example. The phase transitions are realized if the pressure ismore than critical pressure by the corresponding phase diagram. Inthe case the small particles may change own volume, energy, andstate equation. Thus the heterogeneous fluid may have three ormore phases. Thus, we use formulas (3) on the stage to calculate the intermediate velocities $\overline{u}^n, \overline{v}^n, \overline{w}^n$ and the energy $\overline{E}^n$ ofparticles 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 ofcorresponding share of large particle mass and small particlesmasses from the cell to corresponding surrounding sell by formulas (5), which are used in (6).

Thus totalmass of the heterogeneous fluid under consideration is saved atevery 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 acombination of above methods from step to step during the coursesof corresponding numerical simulations. The method seems to bereasonable 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 cellsmethod 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 incomputer experiments by the method.

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

The presented method was applicable to numerical simulations ofplasma dynamics according to [6]. The plasma may be considered as gas with ionizedparticles. The gas and particles were defined by correspondingstate equations. Equations (2) were coupled with Maxwell'sequations and on the discrete level also. Inducing motions of theheterogeneous plasma in some region it was possible to observeabsorption of the ionized particles on relevant boundaries incomputer experiments by the method coupling with appropriatemethod for Maxwell's equations [3, 6]. Alternative methods and corresponding references for the problem may be found in [7]. Nevertheless, thepresented method seems to be perspective for numerical simulations ofother absorption and diffusion processes in complex fluidand plasma dynamics.

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