Modeling of Heterogeneous Hydrodynamics Processes with Phase Transition

Gennadiy Sandrakov

Faculty of Computer Science and Cybernetics
Taras Shevchenko National University of Kyiv
Kyiv, Ukraine
gsandrako@gmail.com

Abstract— **A new mathematical and numerical method of modeling for heterogeneous hydrodynamics processes with take of phase transitions like graphite-diamond will be presented. The method is based on an approximation 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 modeling method simulation.**

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

I. Introduction

A new mathematical and numerical method of simulations for processes of heterogeneous hydrodynamics with take of phase transitions will be discussed. 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 with small transited drops dynamics are considered. These are hydrodynamics 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 relevant approximation of conservation laws for masses, momentums, and energies in integral and differential forms. The approximation is natural and numerical simulations are realized as direct computer experiments. 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.

The method is a combination of the Harlow's particle-in-cell method and Belotserkovskii's large particles method (see [1] and [2]), where Euler's and Lagrange's approaches are used simultaneously. Let us recall some background of the methods before to give more details on the method combination. .

The time approximation in the particle-in-cell method is natural. Simulations are conducted step by step with small enough time interval starting from an initial configuration. The space approximation in the method is more complicated and dynamics are taking into consideration. Fluid region is divided into cells with small size 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 are specified for every such cell at the moment. Corresponding time step of the simulation is split up to three stages so the discrete conservation laws are faithful. For example, total mass of the particles is saved at every time step of such approximation.

On first stage of the time step, intermediate velocities of particles by pressure forces are calculated. This is the Euler's stage for approximations of transport free momentums equations 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 that is 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-cell method is effective enough for numerical evaluations of homogeneous fluid dynamics by boundary conditions and external forces. Concrete types of fluid are defined here by a form of state equation. 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 approximation in the method is similar to the one in the particles in cells method. The space approximation 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 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 ones. 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. 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. Thus total mass of the fluid under consideration is saved at every time step of such approximation 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 lead to corresponding modifications of conservation laws and on the discrete level also. The momentums and energy transports are modeling in similar manners. The approximations are rationale also. Thus the large particles method is effective for simulations of fluid dynamics and the data is not very massive.

Let us return to presented method. The method is designed to numerical modeling of the main fluid with small transited drops dynamics. The time approximation in the method is as in above methods. The space approximation 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 also. 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. The remaining stages are similar to the stages of above methods.

II. Mathematical modeling

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 also 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. Hydrodynamics equations 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 [3, 6]. Alternative methods and corresponding references for the problem may be found in [7], where smoothed particles are used for simulations of hydrodynamics processes.

References

[1] O. M. Belotserkovskij, Yu. M. Davidov, "The large particles method in gas dynamics," Moscow: Nauka, 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, № 1 (558), pp. 317–324, 2006.

[3] S. B. Boyko, G. V. Sandrako, "Parameter computing of hydrodynamics processes with phase transitions," Bulletin of Taras Shevchenko National University of Kyiv, Series: Physics & Mathematics, Special Issue, pp. 11–16, 2013.

[4] G. V. Sandrako, S. B. Boyko, "Mathematical modeling of complex heterogeneous fluid dynamics," Journal Num. and Appl. Math., № 1 (104), pp. 109–120, 2011. (in Russian).

[5] S. B. Boyko, G. V. Sandrako, "Parameter computing of hydrodynamics processes with phase transitions," Journal Num. and Appl. Math., № 2 (108), pp. 88–109, 2012. (in Russian).

[6] S. B. Boyko, V. V. Mischenko, G. V. Sandrako, "The numerical investigation method for evaporated plasma," Journal Num. and Appl. Math., № 2 (95), pp. 3–12, 2007.

[7] G. R. Liu, M. B. Liu, "Smoothed particle hydrodynamics. A meshfree particle method," New Jersey: World Scientic Publishing, 2003.