Direct Monte Carlo simulation of development of the Richtmyer-Meshkov instability on the Ar/He interface

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Abstract. The Richtmyer-Meshkov instability developing on the interface between helium and argon gases hit by a propagating shock wave is simulated numerically. In contrast with conventional approach based on the Navier-Stokes equations, the simulation in the current paper is performed on the molecular level using the Direct Simulation Monte Carlo method. The data averaging over short time periods is employed to decrease statistical scattering. The instability development is successfully reproduced with relatively moderate computer resources used. The time evolution of the transmitted shock wave and contact surface velocities are retrieved from numerical data as well as the instability growth rates.

1. Introduction

Instability of flows of liquids and gases is a widespread phenomenon, playing an important role in many scientific problems and technical applications. It is usually studied on the basis of the continuum approach [1, 2, 3], since it occurs, as a rule, at large Reynolds numbers and, therefore, small Knudsen numbers. However, in a number of important cases, instability can be observed for conditions when rarefaction effects can play a significant role.

One of the examples of such instabilities is the Richtmyer-Meshkov instability, which emerges under the influence of body force, the role of which in this case is played by the inertia force in non-inertial reference frame associated with a gas accelerating in a shock wave on either side of a contact surface. The shock wave moves through the contact surface from less dense to more dense medium. Natural or artificially imposed disturbances on the contact surface play the role of the initial “seed” which then grows during the instability development.

In this paper, we consider the development of two-dimensional Richtmyer-Meshkov instability at the boundary separating helium and argon for relatively low Reynolds number conditions. Numerical simulation is performed using the Direct Simulation Monte Carlo (DSMC) method. The problem statement is similar to continuum computations: at the initial time moment sinusoidal disturbance of the interface imposed, so that the initial stages of development of instability occur in the single mode regime. The resulting flow evolution reminds the flow patterns observed in experiments and continuum numerical simulations.
2. The DSMC method
The Direct Simulation Monte Carlo (DSMC) method [4] is a stochastic numerical method for solving the Boltzmann equation. In DSMC simulations, the gas flow is modeled on the basis of an ensemble of model particles, each representing a large number of real gas molecules. The simulation process is divided into two stages:

(i) free-molecular transfer of a particle according to its individual velocity
(ii) stochastic intermolecular collisions modeled in a cells of a computational grid [5, 6].

The DSMC is the most widely used technique for the numerical simulation of rarefied gas flows. The degree of rarefaction is usually characterized by the Knudsen number Kn, defined as Kn = λ/L, where λ is the mean free path of gas molecules and L is the characteristic length scale of a flow. As the Knudsen number Kn decreases the number of model particles required for the correct DSMC simulation grows rapidly and can reach hundreds of millions and even billions of particles. However, modern supercomputers allows one to perform the DSMC simulation of the flows with Knudsen numbers as low as Kn ∼ 10^{-4} ÷ 10^{-5}.

3. Richtmyer–Meshkov instability
The Richtmyer-Meshkov instability (RMI) develops when a shock wave passes through an interface between two media with different densities. It is special case of the Rayleigh-Taylor instability when permanently acting body force is replaced by an impulsive action of a shock wave. This instability is widespread in natural phenomena and technical applications including astrophysics and nuclear technology. Usually it is considered on the basis of the continuum description, namely Navier-Stokes equations [7, 8, 9]. Modern computational systems, however, allows one to use kinetic approaches, including the DSMC, to simulate hydrodynamic instabilities. Kinetic approach can provide new insights to the process of an instability development [10, 11] and help in understanding of process of an instability emergence on a molecular level. Besides, many hydrodynamic instabilities can emerge in rarefied flows where the continuum approach is inapplicable.

Recently a DSMC simulation of the RMI [12] was performed using the SPARTA code [13]. However, the study was conducted for the standard atmospheric conditions in 50 µm by 400 µm domain. Approximately 10^{11} model particles and up to 1.57 × 10^{6} cores of Sequoia, an IBM Blue Gene/Q supercomputer at Lawrence Livermore National Laboratory, were used in the computations. Using so much resources makes it difficult to run RMI multiparametric study. One of the goals of the present paper is to investigate the possibility to reproduce RMI numerically using moderate computational resources.

4. Results
A 2D plane channel with a specular solid walls (i.e. symmetry lines) was considered. The geometry of the computational domain is shown in figure 1. The left section of the channel is filled with helium, and the right one is filled with argon. The interface between these gases has a form of a half period of a sine curve with an amplitude equal to 10% of a wavelength. A shock wave with the Mach number M = 2.5 propagates through helium from left to right. The main gasdynamic parameters are presented in table 1. 55 million of model particles and a computational grid consisting of 5000×100 cells were used in the simulation. The time step was constant and equal to Δt = 10^{-7} s and 300,000 steps were made during the computation. Macroparameters were averaged over 1000 steps to reduce statistical fluctuation, inherent in the DSMC method. The numerical simulation was performed using 26 cores of a Intel Xeon E5-2695v4 CPU with a SMILE++ DSMC code [14, 15, 16], which is a successor to the well-known SMILE code [17].
**Figure 1.** Computational domain geometry and initial flowfield configuration.

**Table 1.** Initial flowfield conditions.

|       | He<sup>a</sup> | He<sup>b</sup> | Ar  |
|-------|----------------|----------------|-----|
| ρ, kg/m³ | 2.7 × 10⁻⁵    | 10⁻³           | 10⁻⁴|
| P, Pa  | 47            | 6.2            | 6.2 |
| T, K   | 839           | 300            | 300 |
| V, m/s | 1605          | 0              | 0   |
| Kn    | 6 × 10⁻⁴      | 10⁻³           | 4 × 10⁻⁴|

**Figure 2.** Density flowfields.
Figure 2 shows the density flowfields at different time moments. The computations were performed for the interface with a half-period of a sine disturbance but for better visual representation the flowfield was mirrored twice with respect to the X axis. As can be seen, the shock wave passed through the interface quickly becomes plane, while the interface itself stretches taking a mushroom-like shape. The figure 3 shows the evolution of the shock wave (SW) and contact surface (CS) positions at the Y coordinate values corresponding to the bubble and the spike. As can be seen, SW evolution is identical for both the cases, except for a short period at the beginning of the computation, while the difference in CS positions seems to be growing linearly in time. In figure 4 the difference between CS position of the bubble and the spike is shown. It is evident that instability “stretching” rate decreases and the distance between the spike and the bubble tends to a constant value. Figure 5 demonstrates the velocities of CS and SW for the spike and the bubble. Oscillations appear as a result of differentiation of the data containing stochastic fluctuations. The theoretical values of velocities of the discontinuities are calculated from the solution of the 1D Riemann problem. It can also be seen, that SW speed almost immediately reaches its theoretical value. The speed of CS spike at first is higher than the theoretical value, while the speed of CS bubble is slowly grows up its theoretical value.

Thus, the development of the RMI was simulated numerically using the DSMC method without employment of huge computational resources. It is worth mentioning that in the present computations the number of model particles in a virtual volume with a linear size equal to the local mean free path (so called λ-cell) was close to unity. As was shown in [18], one model particle in λ-cell is sufficient to keep the deterministic DSMC error low enough to ensure reasonably accurate numerical results. It seems that such a large number of particles in [12] was used to reduce statistical fluctuations. In the present work it was shown that averaging over 1000 time steps is sufficient in this kind of simulations.

5. Conclusion
The DSMC method was successfully used for the numerical simulation of the Richtmyer-Meshkov instability developing at the interface between helium and argon. The instability development patterns are in good agreement with the continuum simulations and experimental data. The present work confirms that the DSMC method has reached a high level of maturity and currently allows one to simulate, on molecular level, complicated unsteady flows, previously considered only on the basis of the Navier-Stokes equations.
Acknowledgments
The current study was supported by Russian Science Foundation Grant No. 18-11-00246. This support is gratefully acknowledged. Computational resources were kindly provided by Siberian Supercomputer Center of the Institute of Computational Mathematics and Mathematical Geophysics SB RAS (sscc.ru) and Computational Center of Novosibirsk State University (nusc.nsu.ru)

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