4-бөлім **Раздел 4** **Section 4**

Қолданбалы математика **Прикладная математика** **Applied mathematics**

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3D-SIMULATION OF IMMISCIBLE TERNARY FLUIDS BY PHASE-FIELD-BASED FREE ENERGY LBM

This paper discusses the use of the Lattice Boltzmann equations method with free energy based on the phase field approach and implemented in the D3Q27 scheme for modeling the dynamics of a three-component fluid flow in a three-dimensional cavity. Based on this method, a program has been created and it has been verified using a test problem that includes modeling the separation of a ternary liquid mixture. The results demonstrate the dependence of the mixture separation on time, the influence of surface tension and gravity. For example, at a high surface tension, the separation of the components occurs faster. Data on the average kinetic energy of the flow and the rate of energy dissipation under various conditions are also presented. In addition, an analysis of the performance of the developed software is performed, including a comparison of the serial and parallel versions of the program. Particular attention is paid to the physical aspects of the model: the transition regions between the components are described using a phase parameter changing according to the Cahn-Hilliard equation. The method allows one to model complex structures and predict the time it takes for the system to reach a stable state. The results confirm the correctness and efficiency of the proposed approach for studying the dynamics of multicomponent fluids.
Key words: Ternary fluid, fluid mixtures separation, Cahn-Hilliard equation, phase-field based lattice Boltzmann equations method.

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Фазалық өріс негізіндегі бос энергиялы LBM әдісі арқылы араласпайтын үштік сұйықтықтарды 3D-модельдеу

Бұл жұмыс үш өлшемді облыста үш компоненті бар сұйықтық ағынының динамикасын модельдеу үшін фазалық өріс тәсіліне негізделген және D3Q27 схемасында жүзеге асырылған бос энергиясы бар торлы Больцман теңдеулері әдісін (Lattice Boltzmann equations method) қолдануды қарастырады. Осы әдіс негізінде сұйықтықтардың үштік қоспасын бөлуді модельдеуді қамтитын сынақ есебінің көмегімен тексерілген бағдарлама құрылды. Алынған нәтижелер сұйықтық қоспасының бөлінуінің уақытқа тәуелділігін, беттік керілу мен ауырлық күшінің әсеріне тәуелділігін көрсетеді. Мысалы, беттік керілу күшінің жоғары мәндері кезінде компоненттердің бөлінуі едәуір тезірек жүреді. Сондай-ақ ағынның орташа кинетикалық энергиясы және әр түрлі жағдайларда энергияның таралу жылдамдығы туралы мәліметтер берілген. Сонымен қатар, бағдарламаның сериялық және параллельді нұсқаларын салыстыруды қамтитын әзірленген бағдарламалық қамтамасыз етудің өнімділігіне талдау жүргізілді.

Модельдің физикалық аспектілеріне ерекше назар аударылады: компоненттер арасындағы ауысу аймақтары Канн-Хиллиард теңдеуіне сәйкес өзгеретін фазалық параметр арқылы сипатталады. Әдіс күрделі құрылымдарды модельдеуге және жүйенің тұрақты күйге жетуіне кететін уақытты болжауға мүмкіндік береді. Нәтижелер көпкомпонентті сұйықтықтардың динамикасын зерттеу үшін ұсынылған тәсілдің дұрыстығы мен тиімділігін растайды.
Түйін сөздер: Үш компонентті сұйықтық, сұйықтар қоспасын бөлу, Кан-Хиллард теңдеуі, фазалық өріс негізіндегі Больцманның торлы теңдеуі әдісі.

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3D-моделирование не смешивающихся тройных жидкостей методом решеточных уравнений Больцмана со свободной энергией на основе фазового поля

В данной работе рассматривается использование метода решеточных уравнений Больцмана (Lattice Boltzmann equations method) со свободной энергией, основанного на подходе фазового поля и реализованного на схеме D3Q27, для моделирования динамики трехкомпонентного потока жидкости в трехмерной полости. На базе этого метода создана программа, которая верифицирована с помощью тестовой задачи, включающей моделирование разделения тройной смеси жидкостей. Полученные результаты демонстрируют зависимость разделения смеси от времени, влияния поверхностного натяжения и силы тяжести. Например, при высоком значении поверхностного натяжения разделение компонентов происходит быстрее. Также представлены данные о средней кинетической энергии потока и скорости диссипации энергии при различных условиях. Кроме того, проведен анализ производительности разработанного программного обеспечения, включая сравнение последовательной и параллельной версий программы. Особое внимание уделено физическим аспектам модели: переходные области между компонентами описываются с помощью фазового параметра, изменяющегося согласно уравнению Канна-Хиллиарда. Метод позволяет моделировать сложные структуры и прогнозировать время достижения системой стабильного состояния. Результаты подтверждают корректность и эффективность предложенного подхода для изучения динамики многокомпонентных жидкостей.
Ключевые слова: Тройная смесь жидкостей, разделение смеси жидкостей, уравнение Кана-Хилларда, метод решеточных уравнений Больцмана на основе фазового поля.

1 Introduction

The dynamics of interfaces in multicomponent immiscible fluids are commonly observed in various processes and technologies. Examples include petrochemical industry, food processing, pharmaceutical industry, cosmetic industry, environmental technology, nanotechnology, etc.

In scientific research, two numerical approaches are developed to describe the dynamics of a complex interface: the diffuse interface method [1] and the sharp interface method [2]. Our paper uses the diffuse interface method. Compared to sharp interface method, the diffuse interface method uses thin transition regions of nonzero thickness. The key concept involves introducing an order parameter that changes continuously across these layers while remaining mostly uniform within the bulk phases. The change over time of this parameter is determined by the Cahn–Hilliard equation [3].

In recent years, the lattice Boltzmann equations method (LBM) has become a widely used diffuse interface method for modeling complex multiphase and multicomponent flows. In particular, various force modeling of the interfaces between components were built: color-gradient LBM [4], Shan-Chen LBM [5], free-energy LBM [6], and phase-field-based LBM [7].

Among the above-mentioned methods, phase-field-based LBM should be highlighted, which has been used in a number of scientific studies over the past few years due to its application simplicity and efficiency [8].

To date, the authors behind this study have carried out 2D numerical simulations to analyze the devision process of a three-component fluid mixture [9]. This work introduces a three-dimensional mathematical model for incompressible ternary fluids. The proposed numerical model is built upon a phase-field approach using the free energy lattice Boltzmann method with the D3Q27 scheme. The efficiency and accuracy of the method used are tested on the basis of the results presented, include the separation of a three-component fluid mixture as a function of time with and without gravity, the change in average kinetic energy and energy dissipation rate at different surface tension values. The paper describes the parallelization of the algorithm using MPI technology, and also examines the performance analysis of sequential and parallel programs. The findings confirm the accuracy of the utilized 3-D model for a ternary fluid system.

2 Problem statement and numerical method

To study the process, a limited cavity in the shape of a cube with dimensions $[0, L] \times [0, L] \times [0, L]$ (Figure)1) is taken. The cavity is filled with fluid, the components of which have different densities: $\rho_1 > \rho_2 > \rho_3$. Fluid with the lowest density is blue, fluid with the medium density is white, and fluid with the highest density is red.

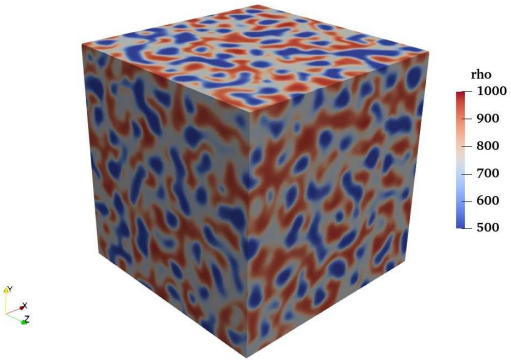


Figure 1: Scheme of the computational domain.

The LBM approach in the Bhatnagar-Gross-Krook approximation of the collision operator with the D3Q27 model is applied to numerical realization of the problem:

$$f_i(\overrightarrow{x} + \overrightarrow{e}_i\Delta t, t + \Delta t) - f_i(\overrightarrow{x}, t) = \Delta t \left[-\frac{f_i(\overrightarrow{x}, t) - f_i^{eq}(\overrightarrow{x}, t)}{\tau_f} + F_i \right],$$
$$g_i^m(\overrightarrow{x} + \overrightarrow{e}_i\Delta t, t + \Delta t) - g_i^m(\overrightarrow{x}, t) = \frac{\Delta t}{\tau_m}[g_i^m(\overrightarrow{x}, t) - g_i^{m,eq}(\overrightarrow{x}, t)] \quad (1)$$

where $m = 1, 2, 3$ – fluid components, f_i, g_i^m – velocity and phase field distribution functions, e_i – discrete lattice velocity, $\tau_f = \frac{1}{2} + c_1\left(\tau_1 - \frac{1}{2}\right) + c_2\left(\tau_2 - \frac{1}{2}\right) + (1 - c_1 - c_2)\left(\tau_3 - \frac{1}{2}\right)$, $\tau_m = 0.8$

– relaxation times, F_i – force component, Δt – lattice time step, f_i^{eq}, $g_i^{m,eq}$ – equilibrium distribution functions for velocity field and phase field, respectively.

The equilibrium distribution functions are determined by the following formulas [11]

$$f_i^{eq} = \begin{cases} \rho - \sum\limits_{i\neq 0} f_i^{eq}, & i = 0 \\ \omega_i \rho \left(1 + \sum\limits_{m=1}^{3} \dfrac{c_m \mu_m}{\rho c_s^2} + \dfrac{e_{i\alpha} u_\alpha}{c_s^2} + \dfrac{u_\alpha u_\beta \left(e_{i\alpha} e_{i\beta} - c_s^2 \sigma_{\alpha\beta}\right)}{2c_s^2}\right), & i \neq 0 \end{cases}$$

$$g_i^{m,eq} = \begin{cases} c_m - \sum\limits_{i\neq 0} g_i^{m,eq}, & i = 0 \\ \omega_i \left(\dfrac{\Gamma_m \mu_m}{c_s^2} + \dfrac{c_m e_{i\alpha} u_\alpha}{c_s^2} + \dfrac{c_m u_\alpha u_\alpha \left(e_{i\alpha} e_{i\beta} - c_s^2 \sigma_{\alpha\beta}\right)}{2c_s^2}\right), & i \neq 0 \end{cases} \tag{2}$$

where $c_s = c/\sqrt{3}$ is the lattice speed of sound, $c = \Delta x/\Delta t$, Δx and Δt are the lattice space and time steps, which are equal to unity, and A_m is the phase field for the fluid components:

$$\sum_{m=1}^{3} c_m = 1. \tag{3}$$

In the D3Q27 scheme (Figure 2) the discrete velocities are defined using the formulas

$$\vec{e}_i = \begin{cases} (0,0,0)c, & i = 0, \\ (\pm 1,0,0)c,\ (0,\pm 1,0)c,\ (0,0,\pm 1)c, & i = 1-6, \\ (\pm 1,\pm 1,0)c,\ (0,\pm 1,\pm 1)c,\ (\pm 1,0,\pm 1)c, & i = 7-18, \\ (\pm 1,\pm 1,\pm 1)c, & i = 19-26, \end{cases}$$

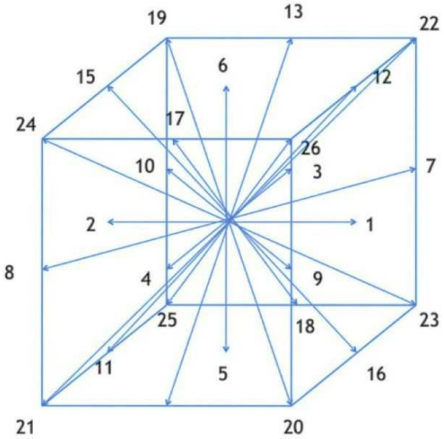


Figure 2: D3Q27 scheme.

The weighting coefficients values are defined by:

$$\omega_i = \begin{cases} 8/27, & i = 0, \\ 2/27, & i = 1-6, \\ 1/54, & i = 7-18, \\ 1/216, & i = 19-26, \end{cases}$$

μ_m in equation [2] is the chemical potential, which is obtained by varying the bulk free energy function with respect to the concentration ratio of the fluids. For a multicomponent fluid flow the free energy functional F can be determined based on the concentrations of the fluid components [10]:

$$F\left(c,\nabla c\right)=\int\left[F_0\left(c\right)+\sum_{i,j=1}^{3}\frac{\lambda_{ij}}{2}\nabla c_i c_j\right]d\Omega$$

where $F_0(c)=\sum_{i,j=1}^{3}\beta_{ij}[g(c_i)-g(c_j)-g(c_i+c_j)]$ is the bulk free energy, $g(c)=c^2(1-c)^2$, $\beta_{ij}=\dfrac{3}{D}\sigma_{ij}$ and $\lambda_{ij}=-\dfrac{3D}{4}\sigma_{ij}$ are the constants, where σ_{ij} is the surface tension between the fluid components and D is the transition layer thickness. Then, the chemical potential μ_m takes the form:

$$\mu_1=12[\lambda_1 c_1(1-c_1)(1-2c_1)-2\lambda_T c_1c_2(1-c_1-c_2)-2\lambda_T c_1c_3(1-c_1-c_3)]/D-(3D/4)\lambda_1\Delta c_1$$

$$\mu_2=12[\lambda_2 c_2(1-c_2)(1-2c_2)-2\lambda_T c_1c_2(1-c_1-c_2)-2\lambda_T c_2c_3(1-c_2-c_3)]/D-(3D/4)\lambda_2\Delta c_2$$

$$\mu_3=12[\lambda_3 c_3(1-c_3)(1-2c_3)-2\lambda_T c_1c_3(1-c_1-c_3)-2\lambda_T c_2c_3(1-c_2-c_3)]/D-(3D/4)\lambda_3\Delta c_3$$

where $\lambda_1=\sigma_{12}+\sigma_{13}+\sigma_{23}$, $\lambda_2=\sigma_{12}+\sigma_{23}+\sigma_{13}$, $\lambda_3=\sigma_{13}+\sigma_{23}+\sigma_{12}$, $\lambda_T=3/(1/\lambda_1+1/\lambda_2+1/\lambda_3)$.

To obtain the correct governing equations, we incorporate the force term F_i in the LB evolution equation by using the scheme proposed by Guo et al. [12]

$$F_i=\omega_i\left(1-\frac{\Delta t}{2\tau_f}\right)\left[\frac{\vec{e}_i-\vec{u}}{c_s^2}+\frac{\vec{e}_i(\vec{e}_i\cdot\vec{u})}{c_s^4}\right]\cdot\vec{F},$$

where $\overrightarrow{F}=F_s+\overrightarrow{F}_b=\sum_{i=1}^{3}\mu_i\nabla c_i+\rho\overrightarrow{g}$ is the total force of surface tension and gravity.

The collision and streaming stages are used to update the distribution functions:

$$f_i{}^*(\overrightarrow{x},t)=f_i(\overrightarrow{x},t)+\Delta t(-\frac{f_i(\overrightarrow{x},t)-f_i{}^{eq}(\overrightarrow{x},t)}{\tau_f}+F_i)$$

$$g_i{}^{m,*}(\overrightarrow{x},t)=g_i{}^m(\overrightarrow{x},t)+\Delta t(-\frac{g_i{}^m(\overrightarrow{x},t)-g_i{}^{m,eq}(\overrightarrow{x},t)}{\tau_c})$$

$$f_i(\overrightarrow{x}+\overrightarrow{e}_i\Delta t,t+\Delta t)=f_i{}^*(\overrightarrow{x},t)$$

$$g_i^m(\overrightarrow{x}+\overrightarrow{e}_i\Delta t,t+\Delta t)=g_i^{m,*}(\overrightarrow{x},t)$$

Then the macro variables (density, velocity, phase field) are found:

$$\rho=\sum_{i=0}^{26}f_i,\quad \rho\overrightarrow{u}=\sum_{i=0}^{26}f_i\overrightarrow{e}_i+\frac{\Delta t}{2}\overrightarrow{F},\quad c_m=\sum_{i=0}^{26}g_i^m,\quad m=1,2.$$

The parameter A_3 can be found from the formula (3).

The second order isotropic differences are used to calculate derivatives of macro variable c_i [10]:

$$\nabla^2 c_m(\overrightarrow{x},t)=\sum_{i=0}^{26}\frac{2\omega_i[c_m(\overrightarrow{x}+\overrightarrow{e}_i\Delta t,t)-c_m(\overrightarrow{x},t)]}{c_s^2\Delta t^2}.$$

3 Simulation results

We consider the dynamics of the ternary fluid mixture in a rectangular computational domain with dimensions: $N_x \times N_y \times N_z$, $N_x = 80$, $N_y = 80$, $N_z = 80$. The physical length is $L = 0.01\ m$. The time and space steps are $\Delta x = \dfrac{L}{N_x} = 0,000125$, $\Delta t = 0.000117188$, $N_t = 80000$ – maximum number of time iterations. The *iter* parameter in the figures denotes the number of iterations. Also dimensionless *time* is used in the figures – $time = iter/Nt$.

Values of physical quantities: the density of fluids – $\rho_1 = 1000\dfrac{kg}{m^3}$, $\rho_2 = 750\dfrac{kg}{m^3}$, $\rho_3 = 500\dfrac{kg}{m^3}$ and the viscosity – $\eta_1 = \eta_2 = \eta_3 = 0.01\ Pa*s$, the acceleration of gravity – $g = 9.8\dfrac{m}{s^2}$.

The initial conditions for the phase field are as follows:

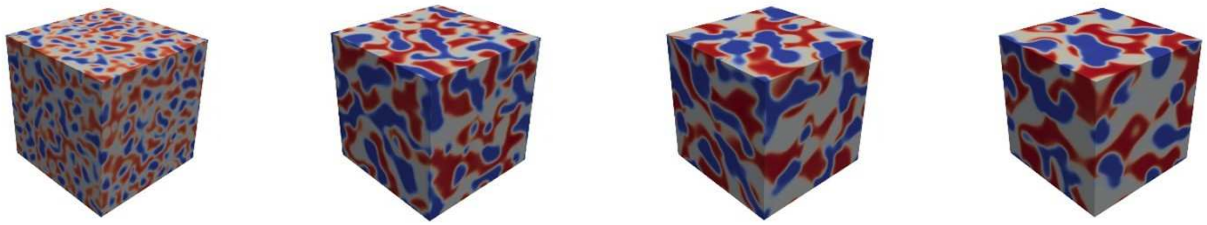
$$c_1(\overrightarrow{x}, 0) = \bar{c}_1 + \alpha \times rand(\overrightarrow{x})$$

$$c_2(\overrightarrow{x}, 0) = \bar{c}_2 + \alpha \times rand(\overrightarrow{x})$$

$$c_3(\overrightarrow{x}, 0) = 1 - c_1(\overrightarrow{x}, 0) - c_2(\overrightarrow{x}, 0)$$

Numerical simulation by the LBM is performed in lattice units. Transformation coefficients $Cu = 1.06667$, $Cg = 9102.22$ are used to obtain the lattice analogues of physical parameters: the density – $\rho_1 = 1.33$, $\rho_2 = 1$, $\rho_3 = 0.67$, relaxation times – $\tau_1 = \tau_2 = \tau_3 = 0.8$, the surface thickness – $D = 2$, the acceleration of gravity – $g = 0.00107666$, and $U_{lbm} = 0.293484$. The values of the concentration fractions are $(\bar{c}_1, \bar{c}_2, \bar{c}_3) = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$.

When gravity is not taken into account, spinodal decomposition of the three-component fluid (Figure 3) occurs due to surface tension forces.

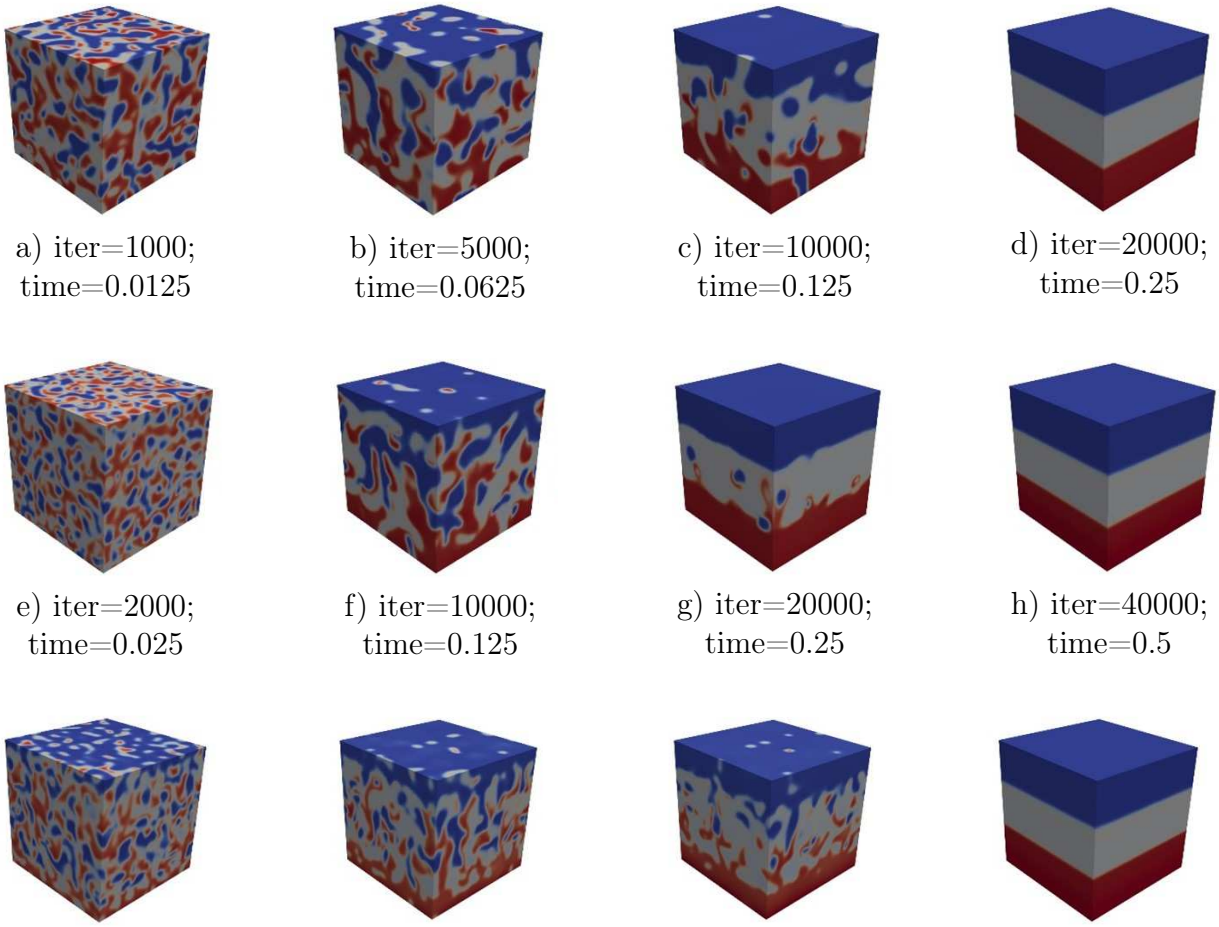


a) iter=2000; time=0.025 | b) iter=10000; time=0.125 | c) iter=20000; time=0.25 | d) iter=40000; time=0.5

Figure 3: Spinodal decomposition of the fluid mixture with concentration fractions $(\bar{c}_1, \bar{c}_2, \bar{c}_3) = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$ depending on time for (a)-(d) $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.01$.

Figure 4 presents the illustrations of the dynamic variation of fluid components, highlighting the separation of immiscible fluids under the influence of gravitational forces. One can see that surface tension affects the rate of fluid separation. With a higher value of surface tension, the separation of fluid components occurs faster.

At an early stage the fluid with the lowest density moves up, while the fluid with the highest density moves down. Due to the acceleration of gravity, three stable layers of fluid components are formed.



a) iter=1000; time=0.0125 | b) iter=5000; time=0.0625 | c) iter=10000; time=0.125 | d) iter=20000; time=0.25

e) iter=2000; time=0.025 | f) iter=10000; time=0.125 | g) iter=20000; time=0.25 | h) iter=40000; time=0.5

i) iter=20000; time=0.25 | j) iter=30000; time=0.375 | k) iter=40000; time=0.5 | l) iter=80000; time=1

Figure 4: Ternary fluid separation with concentration fractions $(\overline{c}_1, \overline{c}_2, \overline{c}_3) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ depending on time for (a)-(d) $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.02$, (e)-(h) $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.01$, (i)-(l) $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.001$.

Figure 5 shows the time evolution of (a) the average kinetic energy and (b) the energy dissipation rate at three values of surface tension. Average kinetic energy computed in physical space:

$$E_k = \frac{u_1^2 + u_2^2 + u_3^2}{2}.$$

The energy dissipation rate is given by:

$$\varepsilon = \frac{1}{2}\vartheta \sum_{i,j} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right), \quad u_i' = u_i - u_j,$$

where u_i – actual velocity, ϑ – kinematic viscosity.

In the Figure 5, the average kinetic energy and dissipation rate for $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.02$ are shown in black, for $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.01$ in red, and for $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.001$ in blue. Among them, the largest value is taken at $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.02$, which corresponds to the

highest level of turbulent activity. The decay process is slower at $\sigma_{12} = \sigma_{13} = \sigma_{23} = 0.001$. One can see that the obtained results demonstrate the suitability of the proposed model for a ternary fluid.

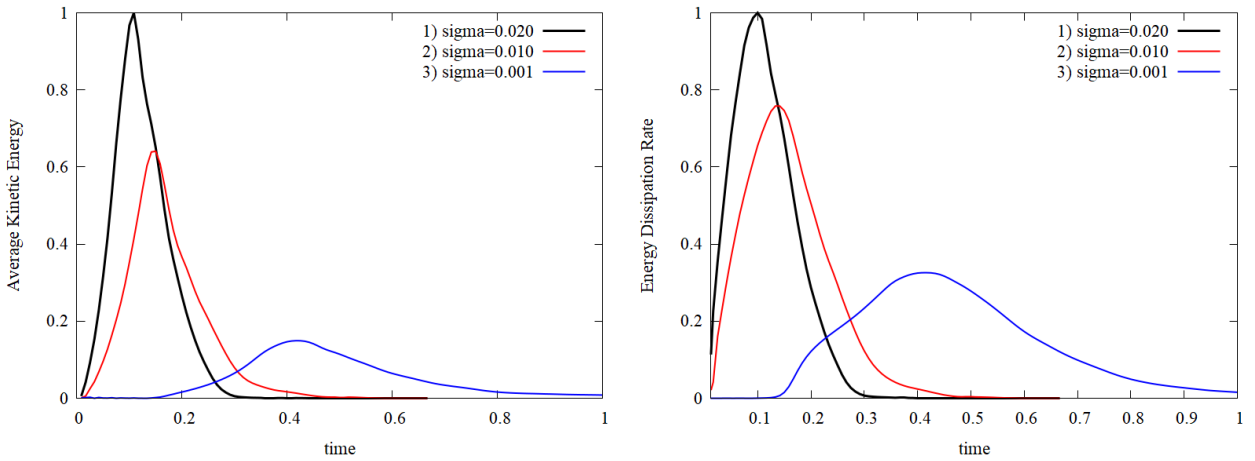


Figure 5: Time evolutions of (a) the average kinetic energy and (b) the energy dissipation rate at different σ.

The implementation of the numerical algorithm for modeling the dynamics of a three-component fluid flow in a three-dimensional cavity taking into account surface tension forces is performed in the Fortran 2008 programming language. Parallelization uses the method of three-dimensional decomposition of the computational domain and is performed using the Cartesian decomposition function of the MPI library [15]. Synchronization between the cores and nodes of the computing platform is performed by introducing an additional layer of intermediate cells (halo layer). The code is compiled by calling the make command, which will generate the executable file main. To call the code in parallel mode, it is necessary to specify the necessary parameters in the config.nml file. Then call the main command using *nohup numactl – membind=1 mpirun - np 256./main &*.

The characteristics and theoretical performance of the computing platform used are shown in Table 1.

Table 1: Characteristics of the computing system

Number of nodes	Number of processors in one node	Total number of cores	Cache memory	Processor frequency	Performance (theoretical)
5	2	280	42 Mb	2.6 GHz	8.9 TFlops

Parallel performance measurements of the numerical implementation were carried out on a computer system with 280 cores. The value of the running time of the numerical algorithm on the grid 80^3, calculations were carried out for 500 iterations:

Table 2: Time taken to perform 500 steps of the LBM algorithm

3D decomposition	Number of CPU cores	Computational time	Speedup
$1 \times 1 \times 1$	1	7574,39	1
$2 \times 1 \times 1$	2	4324,71	1,751421
$2 \times 2 \times 1$	4	1670,77	4,533473
$2 \times 2 \times 2$	8	838,33	9,035094
$4 \times 2 \times 2$	16	400,81	18,89771
$4 \times 4 \times 2$	32	226,91	33,38059
$4 \times 4 \times 4$	64	146,55	51,68468
$8 \times 4 \times 4$	128	99,94	75,78937
$8 \times 8 \times 4$	256	74,02	102,329

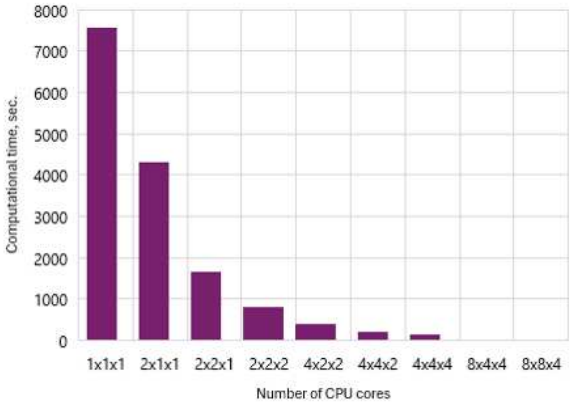


Figure 6: Reduction in program execution time with an increase in the number of involved computing cores based on the 3D decomposition method of the computational domain.

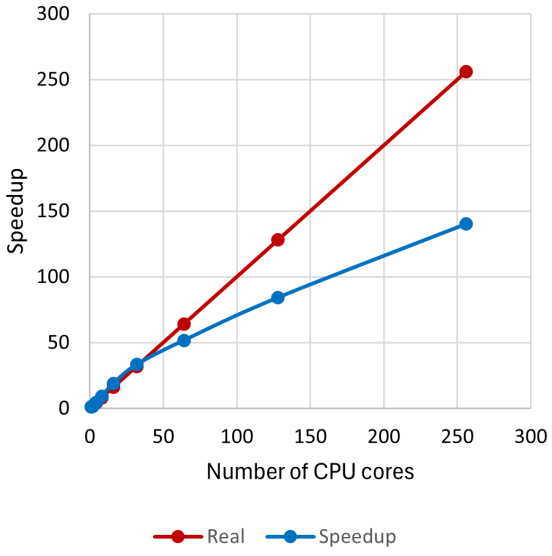


Figure 7: Acceleration of computation with an increase in the number of involved computing cores and a fixed size of the original problem.

Figure 6 shows the trend of decreasing program execution time with increasing number of cores used, the abscissa corresponds to the activated processor topology. Figure 7 presents the acceleration data obtained as a result of this computational experiment. It is evident that the acceleration of the used implementation is less than ideal, however, the calculation time can be reduced when using up to 256 cores.

4 Conclusion

Our paper discusses the development and application of a three-dimensional numerical simulation model to study the dynamics of immiscible ternary fluids. We utilize the phase-field-based free energy LBM with a D3Q27 lattice scheme to simulate the separation process in a cubic cavity. This method demonstrates flexibility in modeling different surface tension values and concentration fractions. This work has potential applications in fields requiring an understanding of fluid mixtures, such as petrochemical processes, pharmaceuticals, and environmental technology. For further insight, the work is supported by references to key studies and validated through prior research on 2D ternary fluid separation. The availability of an adaptable software package ensures its utility in diverse scientific and industrial applications.

It can be concluded that the proposed numerical algorithm is ideal for operation on modern multiprocessor computing systems, allowing to significantly reduce the waiting time for 3D modeling results. The performance analysis of the code used suggests that a further increase in the number of nodes involved will require additional optimization of the MPI library data exchange process, or a transition to reducing the memory load by adapting a discrete speed model with a smaller number of nodes (for example, D3Q19 or D3Q13) will be required.

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