
M. BAKUMENKO,¹ V. BARDIK,¹ D. NERUKH²

¹ Taras Shevchenko National University of Kyiv
(2, Prosp. Academician Glushkov, Kyiv 03022, Ukraine;
e-mail: marynabakumenko@gmail.com, vital@univ.kiev.ua)

² Aston University
(Birmingham, UK; e-mail: D.Nerukh@aston.ac.uk)

**THE MULTISCALE HYBRID
METHOD WITH A LOCALIZED CONSTRAINT.
I. A MODIFIED CONTROL VOLUME
FUNCTION FOR THE HYBRIDIZED MASS
AND MOMENTUM EQUATIONS**

UDC 539

A new hybrid multiscale model has been developed on the basis of the modified control volume function. Following the two-phase analogy of the same substance, the continuum and particle representations are coupled together in the framework of the mass and momentum conservation laws. The new functional form of the control volume function is elaborated by using the continuum discretization principle based on the Delaunay triangulation. The derived mass and momentum equations possess the invariant form for both micro-scale particle and large-scale continuum representations.

Keywords: molecular dynamics, multiscale method, control volume function, hydrodynamic equations.

1. Introduction

Two basic approaches are usually widely applied for the description of processes in liquid systems: the hydrodynamic approach provides information on the continuum level and the molecular dynamics gives a detailed information at the molecular or atomistic level, depending on the time and spatial scales.

Citation: Bakumenko M., Bardik V., Nerukh D. The multi-scale hybrid method with a localized constraint. I. A modified control volume function for the hybridized mass and momentum equations. *Ukr. J. Phys.* **68**, No. 8, 517 (2023). <https://doi.org/10.15407/ujpe68.8.517>.

Цитування: Бакуменко М., Бардік В., Нерух Д. Мультимасштабний гібридний метод з локалізованим обмеженням. I. Модифікована функція контрольного об'єму для гібридизованих рівнянь маси та імпульсу. *Укр. фіз. журн.* **68**, № 8, 519 (2023).

The molecular dynamics (MD) is one of the most accurate methods based on solving the Newtonian equations of motion for each molecule [1], but the atomistic simulation of biological systems is very computationally consuming due to calculations for each particle. Modern specialized computers simulate the molecular systems with hundreds of millions of atoms (tens of nanometers in resolution) based on the classical MD methodology. However, the correct simulation of processes at biologically relevant time scales (microseconds–milliseconds) is infeasible in the framework of the modern MD concept, which describes the dynamics of the system at times from hundreds of picoseconds to a few nanoseconds. Biological systems consist of millions of atoms and most of them are water molecules with sizes and characteristic times much smaller than for biomolecules. Sol-

ving the equation of motions for each water molecule at small characteristic times leads to the fact that the modelling of such systems is computationally expensive, thus simulation of the biomolecule water surrounding consumes approximately 90% of computational resources. Considering the water surrounding molecules is especially important for the protein dynamics, when water molecules guide and correct the biomolecule's conformation motion.

A major opportunity to reduce the computational resources required for the biological system modelling is the procedure, which significantly simplifies the simulation of surrounding water, by considering the macromolecule's environment as a structureless continuum in areas, where the atomistic representation is not necessary (away from the macromolecule's surface) and the possibility to link different scales. Using several different scales simultaneously in a hierarchy of levels provides a complete picture of the biomolecular system. The importance of such a description is accepted, and multiscale approaches are elaborated very actively lately [2, 3, 12, 14, 20, 23].

There are several methods to realize multiscale approaches. The coarse-grained methods reduce the resolution by the formation of the pseudo-spheres from the atom clusters [32]. O'Connell and Thompson [24] applied the method of constraints to derive the equation of motions for the correct description of the link between the MD and hydrodynamic representations, which is a basis for many studies in this field. There are a lot of constraint procedures, and the choice of constraint variables is a very disputed question due to the lack of universal solutions [4, 10, 11, 20]. The majority of the literature data illustrate that Hamilton's principle is widely applied to derived constraint equations and for a further obtaining of the motion equations. However, works [8, 9] demonstrate that Hamilton's principle and the principle of least action, in some cases, fail to reproduce the Newtonian equations of motion and apparently can be applied to holonomic constraints. Besides, it is unclear whether Hamilton's principle is formally true for the semiholonomic constraints. While, as it was shown [7], Gauss's principle of least constraint is a true minimization principle and is valid for any type of constraint.

In this paper, we develop the concept of the hybrid particle proposed in the works [17–19] for deriving the coupled equations of motion within the framework of the least action and least constraint principles. The

development of the hybrid equations of motion on the basis of the proposed model and the application of the variational principles are the subject of the next article. The paper is organized as follows: Sec. 2 explains the necessity of introducing the control volume concept and describes the control volume function and the continuity of control volume equations. In Sec. 3, the uniform distribution of the hydrodynamic mass over the cell is enforced, and the hybrid mass and momentum equations are introduced.

2. Control Volume Function

To build a model, following the works [3, 17–19, 22], we consider a liquid system as the hybrid two-phase analogy model for multiresolution simulations. This approach is based on the large-scale continuum (hydrodynamic phase) and micro scale particle (MD phase) representations of the same chemical substance, which is nominally a two-phase fluid. The concentrations of phases are defined by the hybridization parameter S . The parameter S is a user-defined function that describes which part of the system can be represented by discrete particles or molecules and which by a continuum. It takes values in the interval from 0 to 1, and, at the boundary cases, where $S = 0$, the microscale particle or the MD phase is represented, and $S = 1$ corresponds to the large-scale continuum or hydrodynamic phase (Fig. 1). Simulation of the hydrodynamic phase provides the development of fluid-flow mathematical models and application of simulation techniques for numerical solutions of these models.

For the simulation of the large-scale continuum, there are several widespread methods such as the Finite Difference Method (FDM) [21], the Finite Element Method (FEM) [15], and the Finite Volume Method (FVM) [6]. FDM involves directly approximating pointwise gradients of the flow solution on a numerical grid. FEM solves the equations of motion in a weak form by expanding the solution into a set of analytic finite-support basis functions. The governing PDE is first integrated in space and then manipulated into a linear algebraic system for the expansion coefficients using the chain rule. FVM solves the governing equations of motion in terms of grid-cell-averaged quantities, where the solution gradients are evaluated using the divergence theorem. This makes the conservation fluxes of mass, momentum, and en-

ergy automatically preserved, thereby preserving the conservation laws at the discrete level.

The control volume (CV) concept is widely used in fluid mechanics and thermodynamics for the analysis of flows within a certain volume and streamlines the calculation of forces and energy cumulative effects [16, 29]. Moreover, the CV formulation couples the dynamics equations on various scales: particle, mesoscale, and large-scale continuum. Thus, this concept provides the correct coupling between different scales. It should be noted that Irving and John G. Kirkwood [13] derived basic continuum equations within the framework of the statistical approach using the CV concept.

Within the framework of the CV, the mass continuity equation can be expressed in the form (1)

$$\frac{\partial}{\partial t} \int_V \rho dV = - \oint_S \rho \mathbf{U} d\mathbf{S}, \quad (1)$$

where ρ is the mass density, \mathbf{U} is the fluid velocity, $d\mathbf{S} = \mathbf{n}dS$ is the unit normal \mathbf{n} of the control surface times the area dS .

The rate of change of the momentum is defined by the momentum advection and the balance of forces (2)

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{U} dV = - \oint_S \{\rho \mathbf{U} \mathbf{U} + \Pi\} d\mathbf{S} + F_b, \quad (2)$$

where Π is the stress tensor on the CV surface, F_b is external forces over the control volume.

The similar expression for the rate of change of the energy can be defined as

$$\frac{\partial}{\partial t} \int_V \rho \varepsilon dV = - \oint_S \{\rho \varepsilon \mathbf{U} + \Pi \mathbf{U} + Q\} d\mathbf{S} + F_{\text{body}} \mathbf{U}, \quad (3)$$

where Q is a heat flux. The above system of equations is supplemented with necessary constitutive relations such as the equation of state and stress-stress relations. The assumption of an infinitesimal volume is not necessary for Eqs. (1)–(3), as they have been rewritten to express the conservation laws based on changes that occur within a finite volume and the fluxes that take place across its bounding surfaces. The evolution equations can be also obtained for molecular systems in the CV form. The three-dimensional integral of the Dirac delta functional was

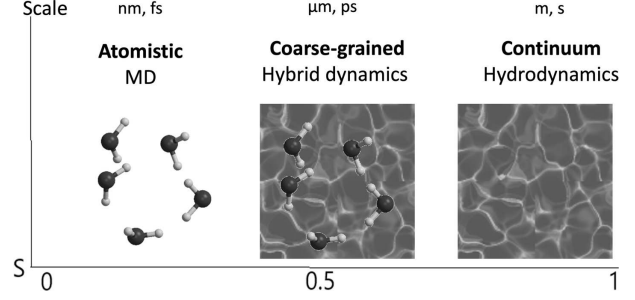


Fig. 1. Schematic representation of the hybrid system for different values of the parameter S

applied to develop the Control Volume form [13]

$$\theta_i \times \equiv \{H(x^+ - x_i) - H(x^- - x_i)\} \times \{H(y^+ - y_i) - H(y^- - y_i)\} \times \{H(z^+ - z_i) - H(z^- - z_i)\}, \quad (4)$$

where H is the Heaviside functional.

Smith [4, 30, 31] used a similar approach to derive a discrete analog of the continuum CV equations. The CV function (4) selects a certain molecule inside the given CV. In Smith's approach, the CV boundaries correspond to cell boundaries used for the computer simulation. The value of the CV function depends on the given cell and particle position relative to this cell. The CV operator derivatives have the form

$$dS_{xi} = \frac{\partial \theta_i}{\partial x} = \{\delta(x^+ - x_i) - \delta(x^- - x_i)\} \times \{H(y^+ - y_i) - H(y^- - y_i)\} \times \{H(z^+ - z_i) - H(z^- - z_i)\}. \quad (5)$$

If $\theta_i = 1$, the particle is in the control volume, with a zero value outside. The derivative of θ_i acquires non-zero values only when crossing the CV boundary.

The discrete analogs of Eqs. (1) and (2) proposed by Smith have the following form including the mass evolution:

$$\frac{d}{dt} \sum_{i=1}^N m_i \theta_i = - \sum_{i=1}^N \mathbf{p}_i d\mathbf{S}_i, \quad (6)$$

where m_i – mass of the molecule, \mathbf{p}_i – momentum. Momentum evolution in the CV is given by

$$\frac{d}{dt} \sum_{i=1}^N \mathbf{p}_i \theta_i = - \sum_{i=1}^N \frac{\mathbf{p}_i \mathbf{p}_i}{m_i} d\mathbf{S}_i + \frac{1}{2} \sum_{i,j}^N \zeta_{ij} d\mathbf{S}_{ij} + \sum_{i=1}^N \mathbf{f}_{i\text{ext}} \theta_i, \quad (7)$$

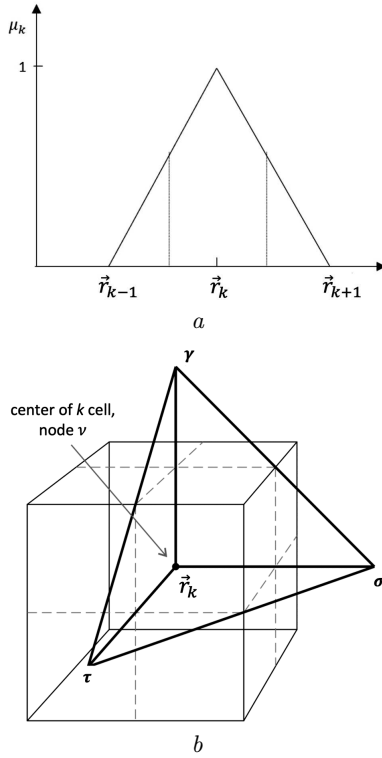


Fig. 2. Shape of the modified control volume function μ_k : for 1-dimensional system (a); for 3-dimensional system (b)

where ς_{ij} – intermolecular stress tensor, and $\mathbf{f}_{i_{\text{ext}}}$ – term defining external forces.

Using the CV representation and Eqs. (6–7), Smith derived the equation of motion for a discrete particle to obtain a discrete momentum of the control volume equal to the hydrodynamic momentum

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i} - \frac{\theta_i}{M_I} \times \left\{ - \int_V \rho \mathbf{U} dV + \sum_{n=1} \mathbf{p}_n \theta_n \right\}, \quad (8)$$

$$\begin{aligned} \ddot{\mathbf{r}}_i = & \frac{\mathbf{F}_i}{m_i} - \frac{\theta_i}{M_I} \times \left\{ - \frac{d}{dt} \int_V \rho \mathbf{U} dV + \right. \\ & \left. + \sum_{n=1} \mathbf{F}_n \theta_n - \sum_n m_n \dot{\mathbf{r}}_n \dot{\mathbf{r}}_n d\mathbf{S}_n \right\}. \quad (9) \end{aligned}$$

Thus, Smith’s main idea was to bring the discrete analogs of Eqs. (1)–(2) closer to the form of these equations and to obtain hybridized equations of motion of discrete particles, the total momentum of which is equal to the hydrodynamic momentum, according to the Gauss principle [31].

At the same time, in Smith’s approach, the discontinuity through the infinitely thin boundary appears in the equations of motion, which is caused by the fact that the derivative of the CV function acquires only two possible values. The obtained equations of motion do not provide a smooth transition from one description to another one. Thus, these equations cannot be used to simulate a multiscale system, when both descriptions should be considered.

To avoid discontinuity, in our study, the CV function has been modified in the way such that the particle should “feel” the boundary at approaching it. Thus, the boundary should be blurred in space, and the linear decreasing function μ_k has been introduced instead of the rectangular function. One can say that μ_k nominally stretches the border by half of the cell k and half of the neighbouring cell. The μ_k takes values from 0 to 1. The schematic illustration of this function is presented in Fig. 2.

The cell k is defined by four elements τ , σ , γ , and ν designate as e_k . The function $\mu_k(r)$ has the form of a pyramid, which is decomposed into sub-pyramids, the characteristic function $\theta_{e_k}(r) = 1$ inside the triangle and zero outside, as it is schematically presented in Fig. 2, b.

To obtain the CV function in the explicit form, the continuum discretization has been performed basing on the Delaunay triangulation [5, 25–28]

$$\sum_k \nu_k \delta_k(r) = 1, \quad (10)$$

where ν_μ – volume element. The relation between the discrete delta function and the CV function is expressed by

$$\delta_{k(r)} = \frac{\mu_k(r)}{\nu_k}. \quad (11)$$

In general, $\mu_k(r)$ is given by

$$\mu_k(r) = \sum_{e_k} t_{e_k} \theta_{e_k}(r), \quad (12)$$

where $\theta_{e_k}(r)$ is the characteristic function, and the parameter t_{e_k} is presented as the sum of vectors

$$t_{e_k} = a_{e_k} + b_{e_k}. \quad (13)$$

Equations (10) and (11) determine the properties of $\mu_k(r)$

$$\sum_k \mu_k(r) = 1, \quad (14)$$

$$\nabla\mu_k(r) = \sum_{e_k} b_{e_k} \theta_{e_k}(r). \quad (15)$$

To obtain expressions for a_{e_k} and b_{e_k} , the sub-volume e_k , which is the pyramid formed by nodes $\nu, \tau, \sigma, \gamma$, as it is expressed in Fig. 2, b , has been considered. In the 3-dimensional case, each face of the pyramid divides the space into two half-spaces, in one of which the opposite vertex is located. The searched function θ_ν can be represented by the product of four θ functions constructed for the half-spaces formed by the corresponding faces.

The edge $\gamma\nu$ is normal to the plane formed by the face (ν, τ, σ) . To determine the position of a point relative to the formed half-space, the scalar product of the normal to the plane ($r_{\gamma\nu}$) and the vector $r_{\gamma\nu}$ has been calculated.

If the product is positive, then the angle α between these vectors $0 < \alpha < 90$ degrees, and this point is in the given half-space.

In the general case, the face $(\mu\sigma\gamma)$ is formed by the vectors $\mathbf{r}_\sigma - \mathbf{r}_\tau$ and $\mathbf{r}_\gamma - \mathbf{r}_\tau$ and passing through the point τ with coordinates (x_τ, y_τ, z_τ) is considered.

The equation of the plane is given by the determinant

$$\begin{vmatrix} x - x_\tau & x_\sigma - x_\tau & x_\gamma - x_\tau \\ y - y_\tau & y_\sigma - y_\tau & y_\gamma - y_\tau \\ z - z_\tau & z_\sigma - z_\tau & z_\gamma - z_\tau \end{vmatrix} =$$

$$= (x - x_\tau) [(y_\sigma - y_\tau)(z_\gamma - z_\tau) - (y_\gamma - y_\tau)(z_\sigma - z_\tau)] -$$

$$- (y - y_\tau) [(x_\sigma - x_\tau)(z_\gamma - z_\tau) - (x_\gamma - x_\tau)(z_\sigma - z_\tau)] +$$

$$+ (z - z_\tau) [(x_\sigma - x_\tau)(y_\gamma - y_\tau) - (x_\gamma - x_\tau)(y_\sigma - y_\tau)] = 0. \quad (16)$$

Accordingly, the normal vector to the plane $\mathbf{n}_{\tau\gamma\sigma} = (n_x, n_y, n_z)$, where

$$n_{x\tau\gamma\sigma} = (y_\sigma - y_\tau)(z_\gamma - z_\tau) - (y_\gamma - y_\tau)(z_\sigma - z_\tau), \quad (17)$$

$$n_{y\tau\gamma\sigma} = (x_\gamma - x_\tau)(z_\sigma - z_\tau) - (x_\sigma - x_\tau)(z_\gamma - z_\tau), \quad (18)$$

$$n_{y\tau\gamma\sigma} = (x_\sigma - x_\tau)(y_\gamma - y_\tau) - (x_\gamma - x_\tau)(y_\sigma - y_\tau). \quad (19)$$

The coordinates of the point on the face through which the normal to the plane passes starting from the point ν can be derived using the expression

$$\mathbf{a}_{\nu\tau\sigma\gamma} = (a_x, a_y, a_z) = (x_\nu, y_\nu, z_\nu) + \lambda_{\nu\tau\sigma\gamma}(n_x, n_y, n_z). \quad (20)$$

The expression for λ is defined as

$$\lambda_{\nu\tau\sigma\gamma} = \frac{n_x(x_\tau - x_\nu) + n_y(y_\tau - y_\nu) + n_z(z_\tau - z_\nu)}{n_x^2 + n_y^2 + n_z^2} \quad (21)$$

and

$$\lambda_{\nu\tau\sigma\gamma} = \frac{\mathbf{n}(\mathbf{r}_\mu - \mathbf{r}_\nu)}{\mathbf{n}^2}. \quad (22)$$

The point on the plane has the following coordinates:

$$\mathbf{a}_{\nu\tau\sigma\gamma} = (a_x, a_y, a_z) = (x_\nu, y_\nu, z_\nu) + \lambda_{\nu\tau\sigma\gamma}(n_x, n_y, n_z). \quad (23)$$

Therefore, the normal vector drawn from ν is

$$\mathbf{c}_{\nu\tau\sigma\gamma} = \mathbf{a}_{\nu\tau\sigma\gamma} - \mathbf{r}_\nu = \lambda_{\nu\tau\sigma\gamma} \mathbf{n}_{\tau\gamma\sigma}. \quad (24)$$

The point whose position needs to be determined has coordinates $r = (x, y, z)$. Then the vector drawn from this point to point a is

$$\mathbf{vec} = \mathbf{r}_\nu + \lambda_{\nu\mu\sigma\gamma} \mathbf{n}_{\tau\gamma\sigma} - \mathbf{r}, \quad (25)$$

and the function θ has the form

$$\theta_{\nu\tau\gamma\sigma}(\mathbf{r}) = \theta((\lambda_{\nu\tau\sigma\gamma} \mathbf{n}_{\tau\gamma\sigma})(\mathbf{r}_\nu + \lambda_{\nu\tau\sigma\gamma} \mathbf{n}_{\tau\gamma\sigma} - \mathbf{r})). \quad (26)$$

In the 3-D case, $t_{\nu\tau\sigma\gamma}$ is the ratio of the volumes of tetrahedrons constructed on the vectors $\mathbf{r}_\sigma - \mathbf{r}_\nu$, $\mathbf{r}_\gamma - \mathbf{r}_\nu$, $\mathbf{r}_\tau - \mathbf{r}_\nu$, and $\mathbf{r}_\sigma - \mathbf{r}$, $\mathbf{r}_\gamma - \mathbf{r}$, $\mathbf{r}_\tau - \mathbf{r}$.

If we consider a tetrahedron constructed on the vectors $\mathbf{r}_\sigma - \mathbf{r}_\nu$, $\mathbf{r}_\gamma - \mathbf{r}_\nu$, $\mathbf{r}_\tau - \mathbf{r}_\nu$, the volume of the tetrahedron is determined as

$$V_{\nu\mu\gamma\sigma} = \frac{1}{6} \begin{vmatrix} x_\sigma - x_\nu & y_\sigma - y_\nu & z_\sigma - z_\nu \\ x_\gamma - x_\nu & y_\gamma - y_\nu & z_\gamma - z_\nu \\ x_\tau - x_\nu & y_\tau - y_\nu & z_\tau - z_\nu \end{vmatrix}. \quad (27)$$

After the simplifications, we have

$$V_{\nu\tau\gamma\sigma} = \frac{a_{\tau\gamma\sigma}}{6} + \frac{1}{6} \mathbf{r}_\nu \mathbf{b}_{\tau\gamma\sigma}, \quad (28)$$

$$a_{\tau\gamma\sigma} = x_\sigma y_\gamma z_\tau - x_\sigma y_\tau z_\gamma + x_\gamma y_\tau z_\sigma -$$

$$- x_\gamma y_\sigma z_\tau + x_\tau y_\sigma z_\gamma - x_\tau y_\gamma z_\sigma, \quad (29)$$

$$\mathbf{b}_{\tau\gamma\sigma} =$$

$$= \begin{pmatrix} [(y_\gamma - y_\tau)(z_\sigma - z_\tau) - (y_\sigma - y_\tau)(z_\gamma - z_\tau)] \\ -[(x_\gamma - x_\tau)(z_\sigma - z_\tau) - (x_\sigma - x_\tau)(z_\gamma - z_\tau)] \\ [(x_\gamma - x_\tau)(y_\sigma - y_\tau) - (x_\sigma - x_\tau)(y_\gamma - y_\tau)] \end{pmatrix}. \quad (30)$$

The next section describes the procedure of developing the hybrid equation of motions using the derived form of the CV function and the contribution of the hydrodynamic mass.

3. Contribution of Hydrodynamic Mass

For the formulation of hybrid equations of mass and momentum for hybrid particles, the contribution from the continuum representation per particle is taken into account. In the hybrid region, the nominally hybrid particle with the mass distributed into molecular dynamics and hydrodynamics contributions has been considered. As was stated above, the hybridization parameter S defines the part of each contribution.

In the continuum representation, the volume of the cell is fixed with a certain density ρ_k . The mass of the cell k is defined as

$$M_k = \rho_k V_k = \int_V \rho_k dV. \quad (31)$$

We assume that the hydrodynamic mass is uniformly distributed over the cell, and its parts vary depending on the scale. Then, on the microscale particle representation, the hydrodynamic mass is the mass of a molecule and, on the large-scale level, is the mass of a fluid in the cell. If we suggest that particles are accounted for the equal parts of the cell, the mass distribution is expressed by

$$m_{\mathbf{r}_i, k} = \frac{1}{N_k} M_k, \quad (32)$$

where N_k – number of particles in the cell k . Then, using the CV function, the mass distribution is presented by the formula

$$m_{\mathbf{r}_i} \sum_{k=1} m_{\mathbf{r}_i, k} \mu_k = \sum_{k=1} \frac{1}{N_k} M_k \mu_k(\mathbf{r}_i). \quad (33)$$

In contrast to the mass, the velocity of the cell is fixed, and each position is associated with a certain velocity of the cell.

Hydrodynamic momentum of the entire cell $\mathbf{P}_k = M_k \mathbf{U}_k$, using Eq. (33), can be expressed as the sum of momenta of the cell parts

$$P_{\mathbf{r}_i} = m_{\mathbf{r}_i} U_k = \sum_{k=1} \frac{1}{N_k} M_k U_k \mu_k(\mathbf{r}_i). \quad (34)$$

Equations (33) and (34) represent the continuum contribution to hybrid particles. The MD contribution is determined by the atomistic mass and velocity of each

particle. Considering the influence of each contribution as the concentration of each phase and introducing the hybridization parameter, the hybrid mass equation is written as

$$m_i = (1 - s)m_i' + s \sum_{k=1} \frac{1}{N_k} M_k \mu_k(\mathbf{r}_i), \quad (35)$$

where m_i' – molecular mass or nominally the MD mass. Thus, in the hybrid region, the particle mass consists of the molecular-dynamic mass and continuum mass contributions.

Similarly, we obtain the momentum equation of the hybrid particle:

$$p_i = (1 - s)m_i' \dot{r}_i' + s \sum_{k=1} \frac{1}{N_k} M_k \mu_k(\mathbf{r}_i) U_k. \quad (36)$$

Equations (35) and (36) give consistency for different values of the hybridization S . So, in the extreme cases where $S = 1$, we have the continuum equations for mass and momentum, and $S = 0$ corresponds to the microparticle scale, we have the equation of mass and momentum for one molecule. One can say that the derived equations retain the invariant form for both phases.

4. Conclusions

A hybrid model is proposed for the multiscale coupling between the microparticle scale dynamics (MD) and the large-scale continuum hydrodynamics of the same liquid system. This model is based on elaborating the new form of the CV function, which does not comprise discontinuity on the cell borders. The new form of the CV function allows one to control the momentum and mass in the localized region of a molecular simulation, and the localization is attained by the continuum discretization based on the Delaunay triangulation.

The concept of the hybrid particle has been used. On the basis of the proposed CV function, we have introduced the mass and momentum equations for the hybrid particle, which contain contributions from both phases, are consistent for different phases and retain the invariant form. In comparison with Smith's studies [4], [31], in our model, the hybridization parameter S has been used for the smooth and controlled coupling between the MD and HD representations, which can be realized in one framework and combined with the pure MD simulation.

The next article will focus on the development of the hybrid equations of motion on the basis of the proposed model with the implementation of variational principles, as it was noted above.

We thank the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Research and Innovation Staff Exchange, MSCA-RISE-2018, Proposal number: 823922, AMR-TB for financial support.

1. M.P. Allen, D.J. Tildesley. *Computer Simulation of Liquids* (Oxford university press, 2017).
2. W.A. Curtin, R.E. Miller. Atomistic/continuum coupling in computational materials science. *Model. Simul. Mat. Sci. Eng.* **11** (3), R33 (2003).
3. D. Davydov, J.P. Pelletier, P. Steinmann. Comparison of several staggered atomistic-to-continuum concurrent coupling strategies. *Comput. Methods Appl. Mech. Eng.* **277**, 260 (2014).
4. E. Smith. *On the Coupling of Molecular Dynamics to Continuum Computational Fluid Dynamics* (School of Mechanical Engineering, 2013).
5. P. Espanol, M. Revenga. Smoothed dissipative particle dynamics. *Phys. Rev. E* **67** (2), 026705 (2003).
6. R. Eymard, T. Gallouët, R. Herbin. Finite volume methods. *Handb. Numer. Anal.* **7**, 713 (2000).
7. M.R. Flannery. D'Alembert-Lagrange analytical dynamics for nonholonomic systems. *J. Math. Phys.* **52** (3), 032705 (2011).
8. M.R. Flannery. The enigma of nonholonomic constraints. *Am. J. Phys.* **73** (3), 265 (2005).
9. I.R. Gatland. Nonholonomic constraints: A test case. *Am. J. Phys.* **72** (7), 941 (2004).
10. H. Goldstein, C. Poole, J. Safko. Classical mechanics. *American J. Phys.* **70**, 782 (2002).
11. N.G. Hadjiconstantinou. Hybrid atomistic-continuum formulations and the moving contact-line problem. *J. Comput. Phys.* **154** (2), 245 (1999).
12. N.G. Hadjiconstantinou, A.T. Patera. Heterogeneous atomistic-continuum representations for dense fluid systems. *Int. J. Mod. Phys. C* **08** (04), 967 (1997).
13. J.H. Irving, J.G. Kirkwood. The statistical mechanical theory of transport processes. IV. The equations of hydrodynamics. *J. Chem. Phys.* **18** (6), 817 (1950).
14. J. Hu, I.A. Korotkin, S.A. Karabasov. A multi-resolution particle/fluctuating hydrodynamics model for hybrid simulations of liquids based on the twophase flow analogy. *J. Chem. Phys.* **149** (8), 084108 (2018).
15. V. Jagota *et al.* Finite element method: An overview. *Walailak J. Sci. Tech.* **10** (1), 1 (2013).
16. N. Nangiaad, H. Johansen, N. Patankar, B. Neelesh ad P. Amneet. A moving control volume approach to computing hydrodynamic forces and torques on immersed bodies. *J. Comput. Phys.* **347**, 437 (2017).
17. S. Karabasov *et al.* Multiscale modelling: Approaches and challenges. *Philos. Trans. R. Soc. A* **372** (2021), 20130390 (2014).
18. I. Korotkin *et al.* A hybrid molecular dynamics/fluctuating hydrodynamics method for modelling liquids at multiple scales in space and tim. *J. Chem. Phys.* **143** (1), 014110 (2015).
19. I.A. Korotkin, S.A. Karabasov. A generalised Landau-Lifshitz fluctuating hydrodynamics model for concurrent simulations of liquids at atomistic and continuum resolution. *J. Chem. Phys.* **149** (24), 244101 (2018).
20. Ju Li, Dongyi Liao, Sidney Yip. Coupling continuum to molecular dynamics simulation: Reflecting particle method and the field estimator. *Phys. Rev. E* **57** (6), 7259 (1998).
21. T. Liszka, J. Orkisz. The finite difference method at arbitrary irregular grids and its application in applied mechanics. *Comput. Struct.* **11** (1-2), 83 (1980).
22. A. Markesteyn *et al.* Concurrent multiscale modelling of atomistic and hydrodynamic processes in liquids. *Philos. Trans. R. Soc. A* **372** (2021), 20130379 (2014).
23. X.B. Nie *et al.* A continuum and molecular dynamics hybrid method for micro-and nano-fluid flow. *J. Fluid Mech.* **500**, 55 (2004).
24. S.T. O'connell, P.A. Thompson. Molecular dynamics-continuum hybrid computations: A tool for studying complex fluid flows. *Phys. Rev. E* **52** (6), R5792 (1995).
25. P. Espanol, J. Anero, I. Zúniga. Microscopic derivation of discrete hydrodynamics. *J. Chem. Phys.* **131** (24), 244117 (2009).
26. P. Espanol, P.B. Warren. Perspective: Dissipative particle dynamics. *J. Chem. Phys.* **146** (15), 150901 (2017).
27. P. Espanol, P.B. Warren. Statistical mechanics of dissipative particle dynamics. *EPL* **30** (4), 191 (1995).
28. P. Espanol, I. Zúniga. On the definition of discrete hydrodynamic variables. *J. Chem. Phys.* **131** (16), 164106 (2009).
29. C.S. Peskin. The immersed boundary method. *Acta Numer.* **11**, 479 (2002).
30. E.R. Smith *et al.* A localized momentum constraint for non-equilibrium molecular dynamics simulations. *J. Chem. Phys.* **142** (7), 074110 (2015).
31. E.R. Smith *et al.* Control-volume representation of molecular dynamics. *Phys. Rev. E* **85** (5), 056705 (2012).
32. G. Voth, S. Izvekov. A multiscale coarse-graining method for biomolecular systems. *J. Phys. Chem. B* **109** (7), 2469 (2005).

Received 31.03.2023

M. Бакуменко, В. Бардік, Д. Нерух

МУЛЬТИМАСШТАБНИЙ ГІБРИДНИЙ
МЕТОД З ЛОКАЛІЗОВАНИМ ОБМЕЖЕННЯМ.
I. МОДИФІКОВАНА ФУНКЦІЯ КОНТРОЛЬНОГО
ОБ'ЄМУ ДЛЯ ГІБРИДИЗОВАНИХ
РІВНЯНЬ МАСИ ТА ІМПУЛЬСУ

Розроблено нову гібридну мультимасштабну модель на основі модифікованої функції контрольного об'єму. Беручи за основу двофазну аналогію, представлення континууму та частинок об'єднані разом у рамках законів збережен-

ня маси та імпульсу. Розроблено нову функціональну форму функції контрольного об'єму з використанням принципу континуальної дискретизації на основі триангуляції Делоне. Отримані рівняння маси та імпульсу мають інваріантну форму як для мікромасштабних частинок, так і для великомасштабних представлень континууму.

Ключові слова: молекулярна динаміка, мультимасштабний метод, функція контрольного об'єму, гідродинамічні рівняння.