CONTINUUM AND NON-CONTINUUM MODELLING OF NANOFLUIDICS
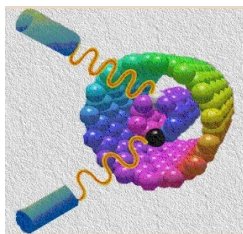
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1. Introduction

  Recent development in nano- and biotechnology has opened a new field of micro- and nanofluidics. Many MEMS (micro-electro-mechanical-systems) and NEMS (nano-electro-mechanical-systems) are based on the fluid motion. Additionally, the analysis of biological samples, drug design and nanomedicine are connected to nanoliter fluid flow. The challenge for understanding such small systems lies in the difficulty to perform experiments as well as in developing theory and simulations methods. Modeling of nanoscale fluid flow is especially complicated, because in contrary to macroscale, general equation are not well defined. Hence, even if the numerical method is well suited for solution of considered problem, the theory needs always be extensively validated with experiments. In this brief summary, the focus will be paid to the numerical models suitable for such systems.
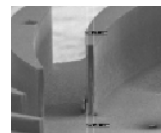
Th micro- and nanofluidics flows are characterized by confinement of the fluid environment. Additionally, the reduction of scale implies that surface effects start to dominate over volume related phenomena (see Table 1). Hence, all models must involve very accurate surface interaction.

Oak Ride National Laboratory Nanomotor	MIT microturbine	Water turbine
nanoscale	**microscale**	**macroscale**

Figure 1. Multiscale engineering design. Devices can resemble some similarities (though rarely), but the physical principles are generally very different. In nanoscale, atomistic and molecular interaction needs to be considered. Microscale resemble continuum is some aspects, but few have to take to account granularity of the matter. Macroscale engineering is based on the continuum, developed through centuries and much more easy to comprehend by everyday life experience.

This overview at first tries to answer the question about the validity of the continuum model at specific scale, provides short description, how it breaks and what models should be used in such circumstances. Second part presents a description of different models which can be applied in micro- and nanoscale environment.

Breakup of the continuum model

The continuum models of fluidic systems are very well developed. Computational methods applied to such configurations give relatively fast, accurate and predictable results. The engineers designing devices in aeronautics and aerospace, turbomachinery, power and heat transfer, are extensively using continuum based simulation tools. The same way does not apply for micro- and nanotechnology. The theoretical models are still under significant development and numerical tools are rather expensive and time consuming. Hence, the engineering design is largely done experimentally. The motivation of the work in micro- and nanofluidics modeling is to change this fact and to develop fast and uniform methods, which can provide visible assistance for engineers. One of the obstacles in this goal lies in the complex physics behind MEMS design. Another limitation is provided by the design of efficient and accurate computational methods. Hence, to understand methodology of micro- and nanofluidics simulations some details of complex physics behind are necessary.

surface to volume ratio for $1\mu m^3$ cube	10^{-6} m
the distance that two water molecules will separate by diffusion in 1s	$30\mu m$
time for a DNA chain to diffuse distance of it own length	10^8 s
gravitational constant	9.81 N/kg
surface tension (water)	0.728 N/m
ion size (Cl$^-$)	covalent radii (neutral) 0.099nm; ionic radii 0.181nm
ion size (Na$^+$)	covalent radii (neutral) 0.157nm; ionic radii 0.095nm
mean free path (air 1atm)	70 nm
average distance between water molecules	3.3 nm
size of water molecule	0.2nm
λ_B (Bjerrum length) water	0.7vm
λ_D (Debye length) water solution	0.7nm-$1\mu m$
λ-DNA size	diameter 2nm; length up to few μm
cell-size	$0.5\mu m$-$2\mu m$
human hair diameter	$17\mu m$
relaxation time for polymers	1ps - 5ns
number of molecules in $1\mu m^3$	25 million (water)
number of molecules in $1\mu m^3$	34 billion (air)

Table 1. Characteristic space and time dimensions for processes in micro- and nanoscale.

Continuum model have several important assumptions about the fluid, and the fluid–solid interaction. The first simplification states that the existence of the *internal structure in the fluid is neglected*.

The assumption of the continuous nature of the media *allows to derive average bulk*

properties, which are defined in every point of the fluid domain. Examples of such physical properties are: velocity, density, temperature, viscosity, thermal conductivity, electric conductivity, ionic solution strength etc. Internal fluid properties, are generally assumed to be constant or change accordingly to well defined theoretical or empirical relations. In real gases, liquids and solids such assumption is not always valid, especially in small and confined environment. Knudsen number is a non-dimensional parameter describing validity of that approximation. It relates the average mean free path to the characteristic length scale (example to the channel diameter)

$$Kn = \frac{\lambda}{L} \quad ; \qquad \lambda = \frac{k_B T}{\sqrt{2} \pi d^2 p} \quad .$$
(1)

Large Knudsen number implies that the characteristics scale is comparable to the mean free path (collision distance between molecules). Such situation occurs if there are fewer atoms in the volume (rarefied medium) or in the confine environment. If the molecules are closed in very small volume, than they can collide with wall more frequent than between themselves. Hence, for microdevices the Knudsen number is large even for dense gases. Knudsen number is mostly defined for gases, but adequate parameter can be applied to liquids. In such a case the intermolecular distance replaces mean free path.

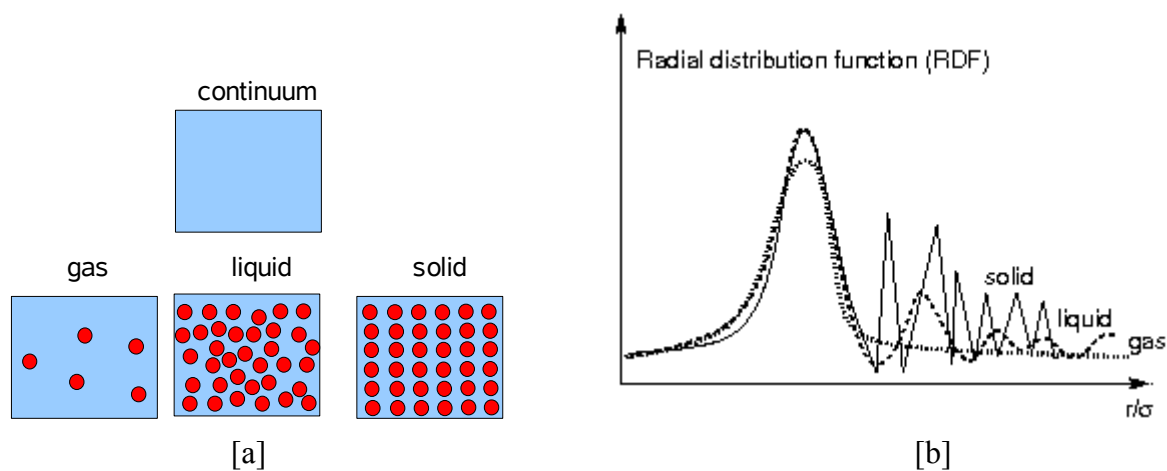[a]   [b]

Figure 2. Conceptual representation of the continuum and real molecular media. [a] Difference in the molecule packing and organization between gases, liquids and solids. [b] Example of radial distribution function for gas, liquid and solid. The number of peaks corresponds to the visibility of the local neighbor structure. In the interaction range for a gas molecules are no distinguishable neighbors. On contrary, solid molecules are influenced by the wide range of neighboring particles.

Taking the Knudsen number definition very strictly, only for Kn = 0 the medium is considered to be continuum. However, the experiments show that continuum regime is still a good assumption for Kn < 0.001. For larger Knudsen numbers the continuum approximation breaks. For gases it is an extensive study [1,2,3] started by Maxwell (1879) [4]. For liquids the work is still not as clear, as the scale is of the order of nanometers and experimental techniques still are a bit limited for extensive investigation of such phenomena. Hence, mostly theoretical work was done using molecular dynamics simulations [5,6].

For the large Knudsen number the fluid bulk properties cannot be considered or defined

continuously. Therefore, bulk properties are being replaced by averages over a number of particles. Fewer particles in the volume will lead to the larger fluctuations in the estimation of mesoscale properties.

Second important approximation imposed in the continuum model is *infinitesimally short time of solid-fluid interaction,* which implies *no-slip boundary condition*. This is not the case in real systems. However, the approximation is fulfilled for a wide range of dimensional scales. In gaseous micro-devices it can break in about 0.1 mm regime and for liquid for $0.1\mu m$ system. For such circumstances, the fluid-solid interaction time starts to be comparable with the average flow time. The molecules have not enough time to obtain equilibrium for momentum and energy transport between fluid and the solid. This, in macroscale world, leads to velocity slip and temperature jump on the solid wall [4,7]

There are another two effects related to the granular properties of matter. The fact that the solid is not a continuum, but has a layer of particles leads to non-uniform interaction field distribution. Hence, the interaction will be stronger and weaker at some points depending on the crystalline or amorphous structure of solid. The solid structure is locally imposed into the fluid domain (especially liquid). The molecular dynamics simulations and also experiments shows such c*ohesive layers in liquids near solid boundaries* [8,9].

Granular property of the matter manifest itself also in the case of particles immersed in the fluid. In principle the particles could be gas, liquid or solid. The microscopic nature of the fluid with immersed particles is represented by *Brownian motion* (1827). This phenomenon relates thermal fluctuations with the viscosity of the solvent and implies that assumption of *flow irreversibly in time breaks*. The importance of Brownian motion can be measured by non-dimensional quantity - Peclet number. It defines the ratio between convection and diffusion forces acting on the particles in the solvent. For large Peclet number convective effects are dominant and Brownian motion influence can be neglected.

$$Pe = \frac{L\,u}{D} \tag{2}$$

If the Peclet number is small than the diffusive effects need to be taken to account. The flow will be time dependent and irreversible. Additionally, in the low Peclet regime the mass and heat transport can be different resulting in double-diffusive convection. Brownian motion is already an approximation, obtained with assumption that solvent molecules are much smaller than the immersed particles. However, validity of that statement was confirmed experimentally for very small scales (example experiments on rod-like particles of anthracene [10]). If the sizes of particles are comparable with the solvent molecules, than the diffusive motion become more of the ballistic type [11].

The another important issue in microfluidics is related to the two fluid interface. The behavior of such surface will be distinguishably different than the one between fluid and the solid. Fluid particles can move freely. Hence, there are two types of possible interactions: miscible and immiscible fluids. The first one will mixed together by means of molecular diffusion. This is the case for all gases and some liquids. More complex behavior takes place for immiscible fluids. The interface between them tries to optimized surface energy and forms droplets or bubbles. The continuum model assume that the interface is a discontinuity with the boundary condition for pressure gradient. The pressure gradient will depend on the surface tension and interface curvature. Two non-dimensional numbers describe magnitude of interfacial effects: capillary number (ratio of viscous to surface tension effects) and Weber number (ratio of inertia to surface tension forces).

$$Ca = \frac{\mu\,u}{\gamma} \qquad\qquad We = \frac{\rho\,u^2 L}{\gamma} \tag{3}$$

The most micro- and nanoscale flows have rather small inertial forces. Hence capillary number is generally more important parameter to follow than Weber number. However, both criteria do not represent a parameter for a continuum breakup. The surface tension will be continuous up to the molecular scale and for the sizes much smaller than the one of fluid-solid interaction (0.9 nm, [12,13]). The another important phenomena related to the two-phase flows in microscale originates from the fact, that gas molecules are not so dense packed as molecules in liquid. Hence, the gases can diffuse in liquids. In macroscale this process is slow to notice. However, in microscale, due to that property, gas bubbles smaller than 50μm diffuse very quickly in water, but water droplets of that size or even a nanometer scale are still very stable. Therefore, practically *micro-bubbles do not exist, but micro- and nano-droples are very common* [14].

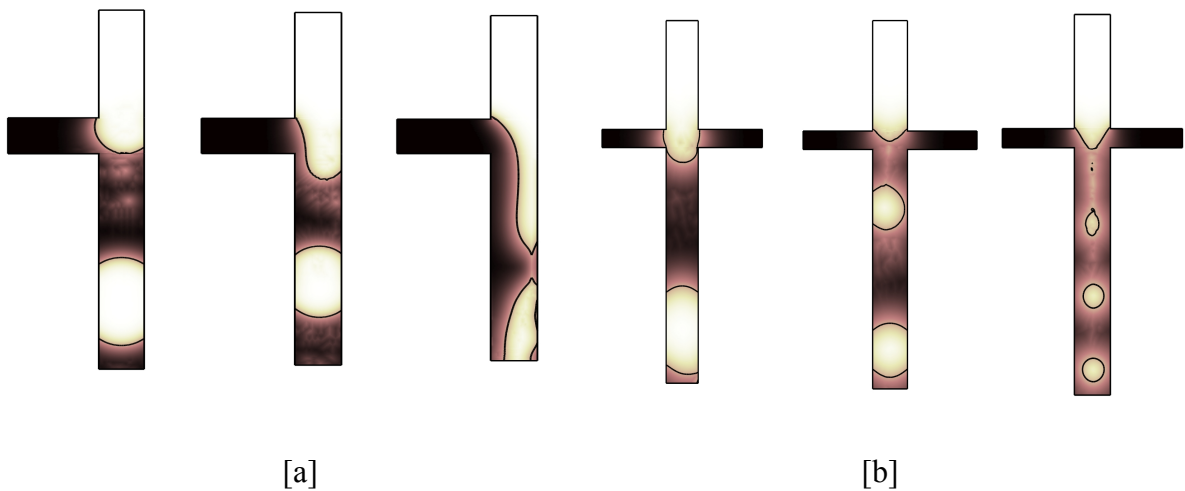[a]   [b]

Figure 3. Microfluidics mono-dispersed droplet formation in T-junction [a] and flow focusing device [b] as a function of mass flow rate [15]. For each device left side represents slower flow than the right figure.

The interface between two fluids can also interact with solid surfaces. In such a case, there are three possibilities. The surface can be completely, partially or non-wettable. The contact angle, between fluid-fluid and the solid, can be altered by: changes in the surface properties such as material type or roughness; or by adding surfactants to modify surface tension.

Finally it needs to be noted, that surface tension is one of the most important forces in microscale. It is a result of the fact, that *surface forces are dominant over the volume one* (example gravity force). Micro-droplets are a fundamental part of many micro-devices (digital microfluidics [16,17]). Moreover, the phase transitions in micro-systems is currently extensively investigated. At present, however, there are no general and simple models to give guidelines, when the continuum approximation breakup occurs.

Additional length and time scales are introduced by immersing elastic bodies, such as polymers, in the micro-system environment. The measure of elastic effects can be estimated by three non-dimensional numbers: Weissenberg number - Wi (relates polymer relaxation time to shear rate time), Deborah number - De   (relates polymer relaxation time to characteristic flow time) and elasticity number - El (relates elastic to inertial effects)

$$Wi = \tau \dot{y} \quad ; \quad De = \frac{\tau}{t} \quad ; \quad El = \frac{\tau \mu}{\rho L^2} \quad . \tag{4}$$

Similarly as with the rigid particles, the elastic object experience Brownian fluctuations,

which is an additional time scale to the scales mentioned above. In macroscale the small *elastic objects* in the flow are modeled as an *altered fluid properties with internal memory*. In microscale, each elastic particles needs to be considered separately. Some elastic particles such as DNA can have length of the order of millimeters and diameter of the order of nanometers. Hence, the continuum approximation for complex fluidics environment breaks for relatively large scale and depends mostly on the properties of elastic objects. [18,19]

Atoms and molecules are generally charged or polarized objects. Reduction of the device size leads to the amplification of the influence of the electromagnetic effects. The most common liquid – water is a polar liquid. The ions will interact with the surface, creating charged molecular layers mainly electric double layer (EDL). On the larger scale, this effect is represented as electro-osmotic slip. In nanoscale flow, distribution of the separate charges needs to be taken to account. Similarly, as in electrically neutral media, in charged media ions experience layering due to the solid structure [20].
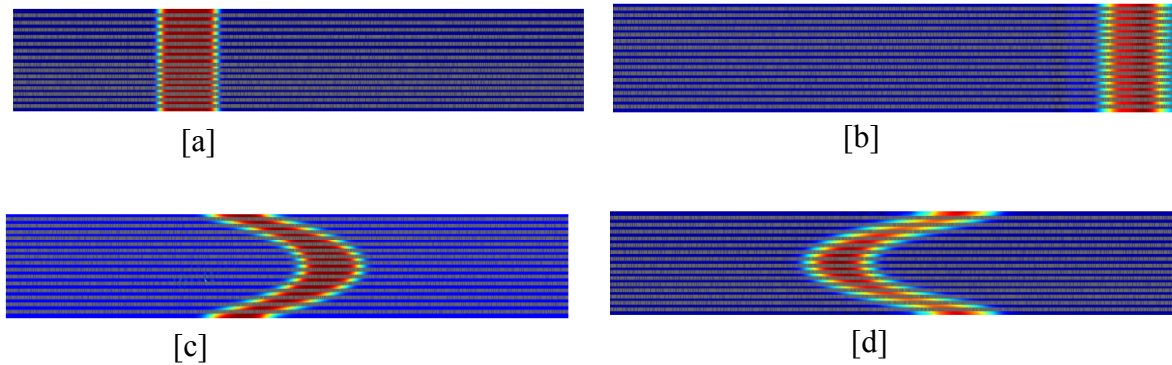

Figure 4. Concentration of dye. The lines indicate electric field. Sample is transported from left to right. [a] Initial configuration. [b] Electro-osmotic transport, when induced slip equilibrates with pressure driven flow. [c] Electro-osmotic slip is too small to compensate viscous effects. [d] Electro-osmotic slip dominates over pressure driven motion.

The parameter representing the electromagnetic granularity effects is a Debye length

$$\lambda_D = \frac{1}{\sqrt{8\pi\lambda_B N_A I}} \quad . \tag{5}$$

The definition resemble mean free path definition and has similar implication. N_A is Avogadro number, I – ionic solution strength and l_B - Bjerrum length. The non dimensional number characterized these type flows is called Debye ratio

$$De = \frac{L}{\lambda_D} \quad , \tag{6}$$

where L represents characteristic diameter. Similarly, as for Knudsen number, there are several regime of distinguishable ions and solution behavior. For small De separate ions need to be modeled. Depending on ionic strength and ion size, charged molecules layers can be visible even in the millimeter-scale. Hence, electro-osmotic and electro-kinetic effects are a driven force for many microfluidics devices. Additionally, high electric fields are easily obtained on that scale, much easier than pressure drop or magnetic interaction [21].

The non-dimensional number, which is widely used in macroscale is Reynolds number. It is representing the ration of inertia to viscous forces

$$Re = \frac{\rho u L}{\mu} \qquad (7)$$

For the majority of micro- and nanodevices Re << 1. Hence, in microscale inertia forces do not play as important role as in the macroscale.

The micro- and nanoflows have a wide application especially in bio-chemical industry [22, 23,24]. However, application generally have combination of most of the effects mentioned earlier. Hence, the modeling is very complex as it requires of the reduction in physics as well as adequate computational techniques choices. Some of the example of devices can be found at micro-pumps [25], micro-mixers[26], micro-reactors [27]. The most common and know one is the acceleration sensor in airbag of the car. The advantage of miniaturization lies in fact that smaller device has much shorter reaction time than the lager one, is more sensitive to small changes (example molecule detectors) and it needs much smaller sample for analysis (DNA analyzers). Some comprehensive reviews considering the physics of micro- and nanoflows are presented in [28,29] .

Computational models

As it was shown in previous section modeling of micro- and nanofluidics is challenging task due to the complex physics. However, there are also several complicated numerical issues which need to be taken to account. Knowing the basic physics of the considered problem and if and when the continuum approximation breaks, correct numerical approach can be taken to account:

- Purely continuum approach; complex fluid phenomena; continuum equations;
- Relatively small continuum breakage:
  - fluid-surface interaction – slip model required;
  - immersed particles, small Peclet number- Langevin equations;
- Invalidity of the continuum approximation
  - molecular models;
  - mesoscale models for computational efficiency
    - coarse grained models (LBM, RSD, DPD, DSMC)
    - hybrid approximation (continuum and molecular model superposition; continuum and mesoscale models; mesoscale models and molecular models combination).

There are two important properties, which should be satisfied by any micro- and nanofluidic numerical model. Firstly, surface effects are dominant at that scale. Hence, correct models for boundaries are necessity. Ideally the values at the boundary would be a result of the simulation itself. Secondly, any meso- and molecular approach needs to predict parameters of motion and properties of media at the same time. This is a challenge, hence, the properties will be an average over molecular parameters and will change with time, while the flow progresses.

Basic Continuum Equations

Continuum approximation is widely used for modeling many micro-devices – especially droplet based micro-reactors (see figure 3), micro-mixers or electro-kinetic reactors (see figure 4). As it was shown in previous section Navier-Stokes relation holds very well for

liquids up to the nanoscale and for gases up to microscale

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \quad ; \tag{8}$$

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = \nabla p + \eta \Delta \boldsymbol{u} + \boldsymbol{f} \quad . \tag{9}$$

Due to the fact, that generally inertia forces are small, Navier-Stokes equations are often reduced to the Stokes approximation for creeping flow. The complexity of simulations does not lie in the solution of the Navier-Stokes equations, as it is a case for macroscale flow simulations. Generally additional equations need to be added to accommodate complex physics. And this is the reason, why microfluidics simulations at the continuum level are also difficult and computationally costly.

As it was shown, many micro devices are driven by electric field. Hence, for simulations additionally the Poisson-Boltzmann equation need to be taken to account

$$\nabla^2 \phi = \frac{-4\pi e}{\epsilon} \sum_{k=1}^{N} n_k^{\infty} z_k \exp \left(-\frac{z_k e \phi}{k_B T} \right) \quad . \tag{10}$$

Addition of that equation significantly complicates simulations. However, in many cases linearization of Poisson-Boltzmann equation can be sufficient (Debye-Hückel theory).

For two phase flow, Laplace equation for the interface curvature needs to be included

$$\Delta p = \gamma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad . \tag{11}$$

Additionally to include elastic effects Oldroyd-B equations can be considered:

$$\nabla \cdot \boldsymbol{u} = 0 \quad ;$$

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} \right) = \nabla \cdot \sigma \quad ; \tag{12}$$

$$\boldsymbol{\sigma} = -p \boldsymbol{I} + \eta (\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T) + G \boldsymbol{A} \quad ;$$

$$\frac{\partial \boldsymbol{A}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{A} - \boldsymbol{A} \cdot \nabla \boldsymbol{u} - (\nabla \boldsymbol{u})^T \cdot \boldsymbol{A} = -\frac{1}{\tau} (\boldsymbol{A} - \boldsymbol{I}) \quad .$$

Continuum model first breaks near the wall and later in the bulk fluid. Hence, it can be still applicable for more cases, if the special treatment of walls is implemented [30]. Slip equation for gas flow are introduced by Maxwell and Smoluchowski and in general form are as present:

$$u_{gas} - u_{wall} = \frac{2 - \sigma_v}{\sigma_v} \lambda \frac{\partial u}{\partial y} + \frac{3}{4} \frac{\mu}{\rho T} \frac{\partial T}{\partial x} \quad ;$$

$$T_{gas} - T_{wall} = \frac{2 - \sigma_T}{\sigma_T} \frac{2\gamma}{\gamma + 1} \frac{\lambda}{Pr} \frac{\partial T}{\partial y} \quad . \tag{13}$$

In figure is given an computational example of the complex flow structures induced only by slip related effects.
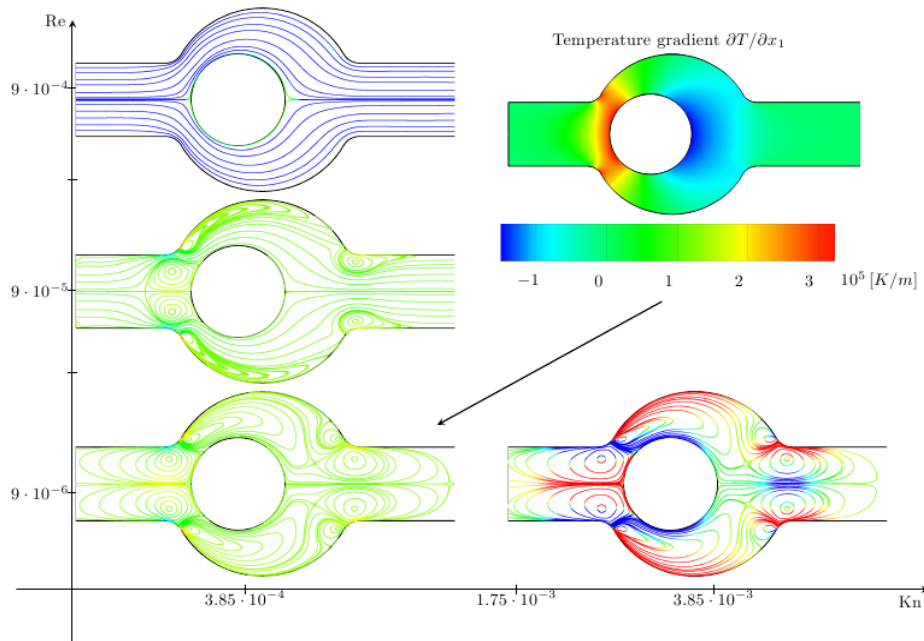
Figure 6. Secondary slip induced structures in gas flow in micro-channel. The plot shows Reynolds and Knudsen number dependency [31].

For electro-osmotic and electro-kinetic flow ionic induced slip is as follow

$$\boldsymbol{u}_{fluid} - \boldsymbol{u}_{solid} = -\frac{\epsilon \, \zeta \, \boldsymbol{E}}{4 \, \pi \, \mu} \quad .$$
(14)

Example of electro-kinetic flow behavior was presented in figure 5.

In the case of the flow, which has many moving surfaces (particle immersed in the fluid), Langevin (1908) equations can be applied. It takes to account fluid molecular structures. The thermal motion of molecules induces random fluctuations, which act on particle in the solvent. Langevin equation is applicable under the condition that immersed particles are much larger than the fluid molecules. For such circumstances intermolecular interaction averages into the stochastic Markovian forces. This implies that the particle does not have a memory about the past. The equation has a form:

$$m \frac{d^2 x}{dt^2} = -\frac{1}{B} \frac{dx}{dt} + F(t) \quad ,$$
(15)

where F(t) represent random force. The choice of the force value is, however, restricted by Einstein-Smoluchowski fluctuation-dissipation theorem

$$\overline{x^2} = \frac{k_B T \, t}{3 \, \pi \eta \, r} \quad ,$$
(16)

which connects magnitude of the random fluctuations with the macroscale viscosity of the fluidic solution.
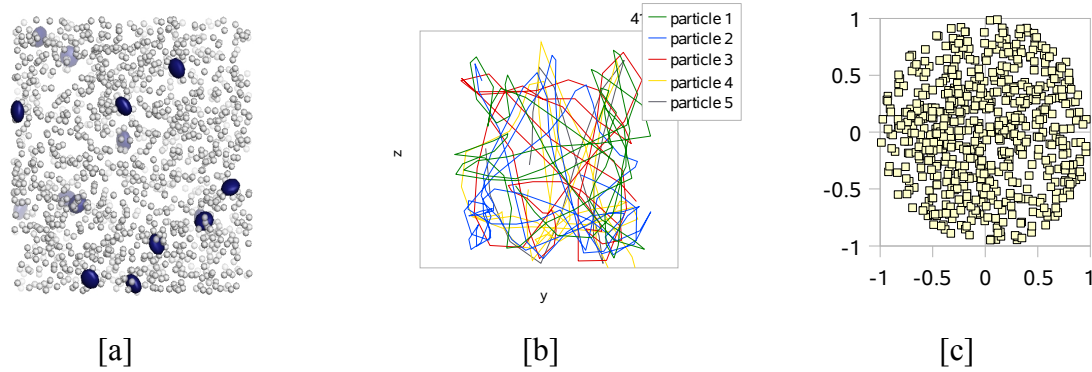
[a]   [b]   [c]

Figure 7. Example of Brownian motion of ellipsoidal particles. [a] molecular simulation instantaneous snapshot; [b] random path over the time of few particles in the confined box – represent translational diffusion coefficient; [c] position of the axis of the particles over time – represent rotational diffusion. Translational and rotational diffusions act independently on the immersed particles.

Numerical methods for the continuum approximation are the same as in the physics of large systems. The only part which need special treatment are stochastic differential equation. The methodology to find solution of such equations is a bit more complicated than for deterministic systems. The stochastic solution can converge to the specific solution path (strong convergence) or to the estimated value (weak solution). Hence, there is a whole set of numerical schemes to accommodate different ways of converging. Details can be found in [32].

The simulation techniques for the continuum approach are relatively well established and widely used in development of various microfluidics devices. However, nanoscale fluidic systems requires much more sophisticated models. Over years physicists has developed tools to study numerically molecular systems. Part of that knowledge can be applied for nanofluidics. Brief description of molecular modeling will be shown in next section.

Molecular models

Molecular approximation is a particle based model. Molecules are Hamiltonian systems. The particle is define by its position and velocity in three-dimensional space. The particles can interact between themselves. Hence, each particle has kinetic energy and potential energy of two, three, four etc. bodies interaction. The latter, in practical application, is generally restricted to two-particle interaction potential. The important difference between continuum and molecular approach is that the model has to give bulk properties as well as the motion at the same time. The continuum model assumes properties from other theories or experiments and only the motion is simulated.

Mesoscale properties

On the molecular scale particles will interact the same regardless if the considered material is in a solid, liquid or gaseous phase. Only the molecular packing factor will change. Hence, the important step, in molecular simulation, is to determine if considered results correspond to the solid, liquid or gas. This can be done, for example, by studying radial distribution function (RDF).

$$g(r) = \rho^{-2} \left\langle \sum_i \sum_{j \neq i} \delta(\boldsymbol{r}_i) \delta(\boldsymbol{r}_j - \boldsymbol{r}) \right\rangle = \frac{V}{N^2} \left\langle \sum_i \sum_{j \neq i} \delta(\boldsymbol{r} - \boldsymbol{r}_{ij}) \right\rangle \qquad (17)$$

RDF is a measure of the distance from the molecules to the neighboring particles. The function can be also compared with the one for the ideal gas

$$n^{id}(b) = \frac{4\pi\rho}{3}[(r+\delta r)^3 - r^3] \quad ;$$

(18)

$$g(r + \tfrac{1}{2}\delta r) = n(b)/n^{id}(b) \quad .$$

This allows to determine the thermodynamical state of the simulation media. The example of RDF are presented schematically in figure 2.
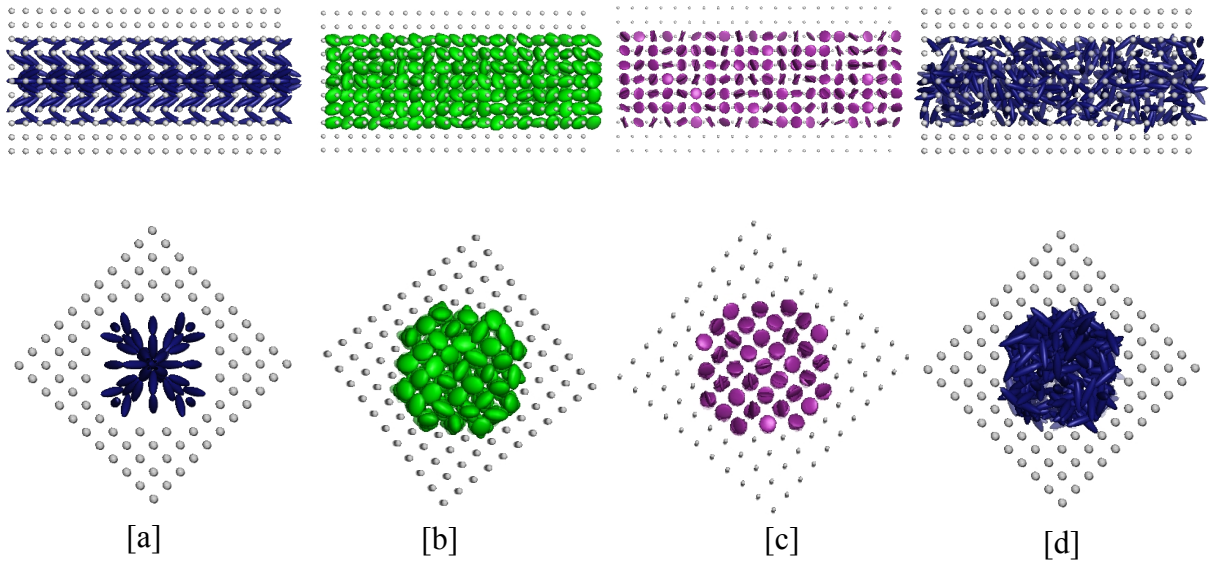

[a]   [b]   [c]   [d]

Figure 8. Simulation of the non-spherical particles in nanotube. Depending on the thermodynamic properties the flow can behave as a self-organized structure [a],[b],[c] or an entirely random [d]. In each of the simulations, the average properties after extraction give parabolic velocity profile.

Estimation of RDF also allows to define macroscopic parameters such as energy

$$E = \frac{3}{2}Nk_BT + 2\pi N\rho \int_0^\infty r^2 v(r)g(r)dr \quad ;$$

(19)

pressure

$$PV = Nk_BT - \frac{2}{3}\pi N\rho \int_0^\infty r^2 w(r)g(r)dr \quad ;$$

(20)

or viscosity

$$\mu = k_BT\ln(\rho\Lambda^3) + 4\pi\rho\int_0^1 d\xi \int_0^\infty r^2 v(r)g(r;\xi)dr \quad ; \quad \Lambda = (\frac{h^2}{2\pi m k_B T})^{(1/2)} \quad .$$

(21)

However, for that purpose, more accurate and efficient are several other algorithms.

Macroscale properties of fluids, such as viscosity or thermal conductivity, are defined as a response to the applied stress. The viscosity is defined from stress-strain relation

$$u_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right), \alpha, \beta = x, y, z \quad ;$$

$$\sigma_{\alpha\beta} = B\,\delta_{\alpha\beta}u_{\zeta\zeta} + 2G\left(u_{\alpha\beta} - \frac{1}{3}\delta_{\alpha\beta}u_{\zeta\zeta}\right) \quad ; \tag{22}$$

$$\sigma_{x,y} = 2G\,u_{x,y} \quad .$$

Similarly the response to applied stress can be defined in elastic solids:

$$\gamma_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial v_\alpha}{\partial v_\beta} + \frac{\partial v_\beta}{\partial v_\alpha}\right) \quad ;$$

$$\sigma_{x,y} = 2\eta\,\gamma_{x,y} \quad . \tag{23}$$

Molecular approach is very similar. The properties are defined as a response to the applied force. However, the response on the molecular level manifest itself in the random fluctuations. Hence, the properties are a correlation functions of initial (with applied force) and current state of the system (undergoing relaxation). The equations providing mesoscale fluid properties are called Green-Kubo relation and were proposed in 1950

$$\Theta = \frac{V}{k_B T}\int_0^\infty ds\langle J(0)|J(t)\rangle \quad . \tag{24}$$

There are several algorithms which allow to obtain in efficient manner average properties of fluid [33].
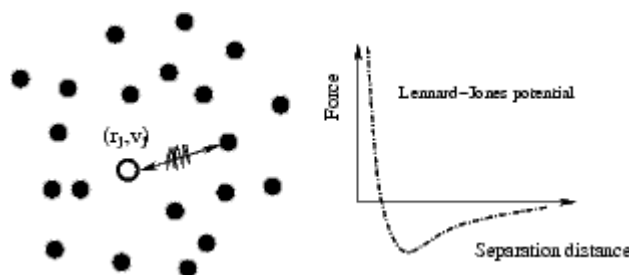

Figure 9. Schematic representation of Molecular Dynamics fluid and the particle bilateral interaction potential.

Molecular simulations: Monte Carlo and Molecular Dynamics Methods

There are two basic approaches to molecular modeling: purely stochastic and purely deterministic. Both assume the media as a set of discrete particles, which can interact between themselves. The stochastic model – Monte Carlo simulations describe the configuration only by random choice of the states of the system and additionally the acceptance-rejection criterion is imposed. It allows to determine if the state can be taken to account for average properties. More detailed description of Monte Carlo technique can be found in [34]. Monte Carlo method works well for obtaining macroscale properties of media. However, is

inefficient for simulation of coherent, global motion of fluid. Much more efficient for fluid motion is a deterministic approach – Molecular Dynamics. Hence, the focus here will be mostly on the definition of that simulation technique. However, it needs to be underline, that despite inefficiency for molecular simulations, some aspects of the Monte Carlo method will be present in the construction of the mesoscale models .These will be shown in more detains in the following sections.

Molecular Dynamics (MD) simulations are based on the Newton's second law applied to Hamiltonian system:

$$m\frac{d^2\boldsymbol{r}_i}{dt^2}=\boldsymbol{F}_i=-\nabla_i V_N(\boldsymbol{r}_i)\quad;\qquad\qquad(24)$$

where interaction potential can be adjusted accordingly. Most commonly used is Lennard-Jones potential:

$$V(r)=\left[4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right)\right]\quad.\qquad\qquad(25)$$

However, there are several other potential such as DLVO (for colloidal suspensions), Morse (for dissociation energy), Gay-Berne (for non-symmetric particles), Born (ionic potential), Tersoff (for 3 atoms, mostly metals) etc. Additionally quantum mechanical computations supply wide variety of more complex potentials [35].

The second order ordinary differential equations are relatively easy to integrate. Example Verlet integration algorithm:

$$\boldsymbol{r}_i(t+\delta t)=-\boldsymbol{r}_i(t-\delta t)+2\boldsymbol{r}_i(t)+\frac{\delta t^2}{2}\boldsymbol{F_i}(t)+\mathcal{O}(\delta t^4)\quad.\qquad\qquad(26)$$

There are several other algorithms developed, example Gear predictor-corrector method. The extensive details considering algorithms can be found in [36,37].

Molecular Dynamics is a very efficient and well established techniques, which allows to simulate wide variety of the systems. Lennard-Jones fluid properties are extensively summarized in [38,39]. Hydrodynamics in confined environment is presented in [40]. Water properties are studied in [41]. Non- equilibrium and equilibrium simulation properties are shown in [42]. Finally flow simulations are presented in binary-mixtures [43] and Rayleigh-Bernard flow [44].

The limitation of the method lies, at present, mainly in the computer power. The number of molecules, which can be handled is still not sufficient or will not be in the nearest future to enhance engineering design (see table 1 for number of molecules in μm cube). Hence, at present, there is an extensive effort to develop mesoscale models, which will be able efficiently simulate physical phenomena in micro- and nano devices. Some of such approaches will be presented in the next sections.

Mesoscale models

As we have seen in previous sections, the real micro- and nanofluidics systems cannot be computed by continuum approximation, because in a lot of cases it is not applicable for such cases. Molecular approach, on the other hand, is still too expensive to be able to proved interesting results in the reasonable time. Hence, an extensive interest in mesoscale models.

Stochastic Rotational Dynamics

- Fluid particles: velocities v_j and positions r_j.
- Rotation of particle velocity relative to mean velocity **u** by angle $\pm\alpha$

Dissipative Particle Dynamics

- Newton equation of motion
- Three types of forces; conservative, dissipative and random
- No artificial lattice

Lattice Boltzmann Method

- Particle interact and move on the fixed lattice
- Kinetic gas theory equations satisfied

Direct Simulation Monte Carlo

- Translation of particle position
- Calculation of collision rate; select collision pairs; adjust trajectories in the imposed mesh;
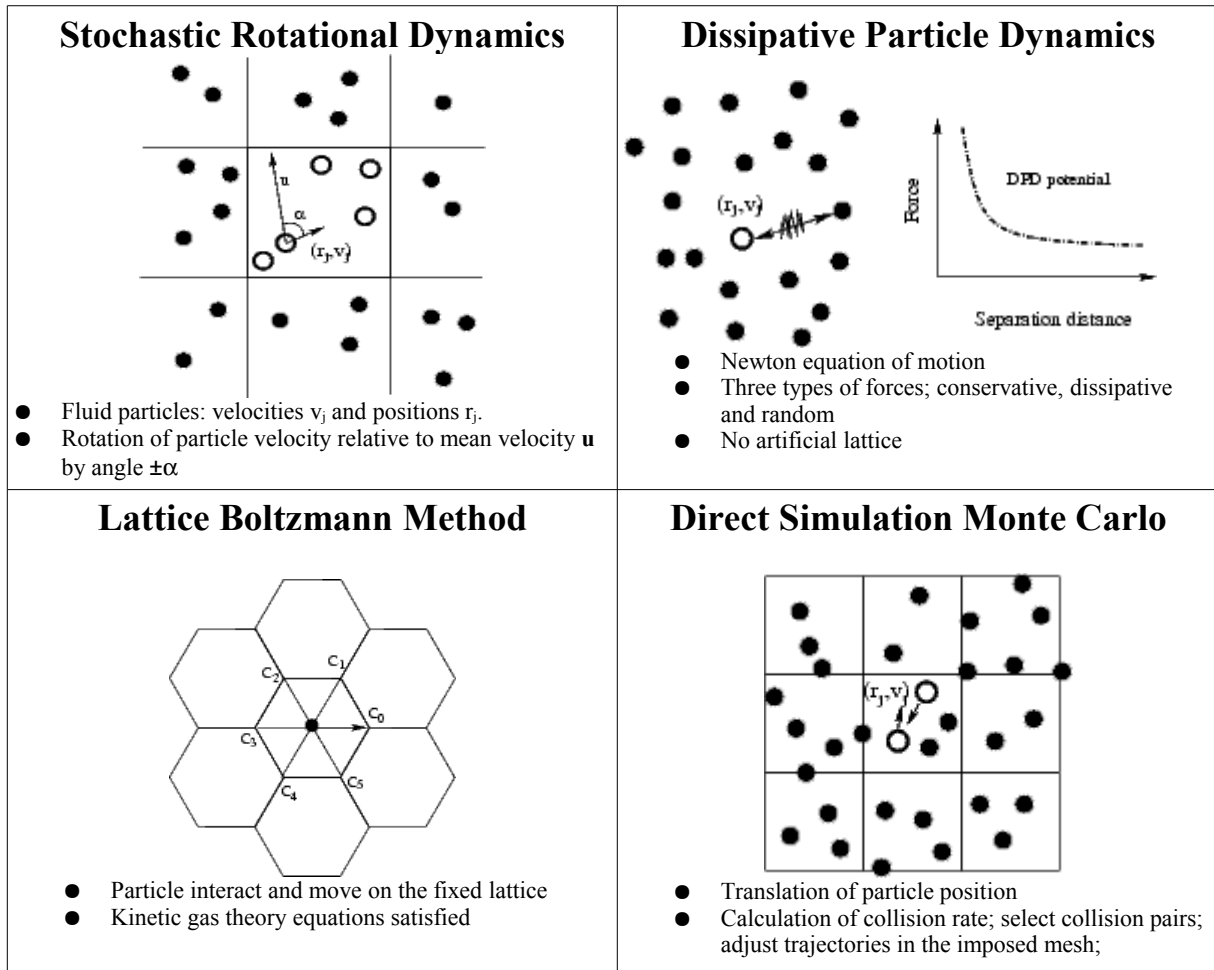
Figure 10. Schematic representation of basic mesoscale models: Stochastic Rotational Dynamics, Dissipative Particle Dynamics, Lattice Boltzmann Method, Direct Simulation Monte Carlo.

There are two distinguishable ways for obtaining mesoscale modeling. One based on the combining molecular and continuum approach, called a hybrid approach. Second way is to derive the mesoscale model from the molecular one, by considering some simplification. The hybrid approach is easy to apply due to the existence of continuum and molecular model. Generally, molecular model is applied near the surfaces and interfaces and in the continuum approach in the bulk region. However, the overlap domain is difficult to define and the proper boundary conditions between molecular and continuum region are hard to impose. Hence, the inner-boundary introduces an error to the model, which is difficult to estimate. Additionally the time scale for continuum and molecular approach do not match and that requires attention. General procedure is to take few mesoscale parameters from the molecular approach and add them the the continuum simulation. This implies that simulations run independently and communicate data between themselves, occasionally. Another large drawback relates to fact, that hybrid methods become inefficient, when there is a need for many interfaces – example colloidal suspension. In such a case multiple surfaces would have to be modeled and than cost of the communication between domain is often larger than purely molecular approach. Hence, here the focus will be placed on the mesoscale models, which are more promising for micro- and nanofluidics computations. The example of some successful applications of hybrid approach can be found in [45,46,47].

Mesoscale models, similarly as molecular one need to provide mesoscale bulk properties of fluid and at the same time also a correct fluid motion. However, the simplification leads also to several drawbacks and in general it is very difficult to obtain both bulk properties and the correct movement. There are two ways of performing the coarse graining procedure. One is to make a discreet lattice, hence to restrict system degrees of freedom. The second is to simplify interaction for the unrestricted particles. For each case every coarse grained particle represent a set real molecules.

Four most common methods will be presented in next few sections.

Lattice Boltzmann Method (LBM)

The Lattice Boltzmann Method was developed from simpler Lattice Gas and is based on the idea of Broadwell (1964) of the simplification of the kinetic equation for particle interaction. The full model for studying time dependent 3-D gas was proposed by Hardy et al (1976) [48]. The method assumes that the molecules move on the fixed latticed and have only specific paths which can follow. Based on that lattice the equation of motion and fluid properties can be derived [49].

Velocity of the particle is given by the characteristic lattice spacing and the characteristic time interval

$$v_i = \frac{\lambda}{\tau} C_i ; i = 0...5 \tag{27}$$

Based on this assumption the properties such as density and fluid velocity can be derived

$$\rho(r,t) = \sum_{i=0}^{5} f_i(r,t) \quad ; \tag{28}$$

$$u(r,t) = \frac{\sum_{i=0}^{5} v_i f_i(r,t)}{\sum_{i=0}^{5} f_i(r,t)} \quad .$$

Additionally, particles will collide with each other and in such a case the rules guiding collision parameters need to be given:

$$f_i(r + \lambda C_i, t+\tau) = f_i(r,t) + \Theta(f(r,t)) \quad . \tag{29}$$

Based on this assumption

$$\sum_{i=0}^{5} \Theta_i(f(r,t)) = 0 \quad ;$$

$$\sum_{i=0}^{5} v_i \Theta_i(f(r,t)) = 0 \quad . \tag{30}$$

The fixed mesh shaped is forced by the need of fulfillment of Galilean invariant (properties should not depend on the direction). Figure shows example lattice for 2D; for 3D cases the lattice has even more complex structure. This is the major drawback of the method, which is difficult to apply for complex geometries and also for moving or immersed objects. There are however, several interesting computations performed using LBM [50,51].

Direct Simulations Monte Carlo (DSMC)

Direct Simulation Monte Carlo is a method highly based on the stochastic properties of fluid. Hence, it is very efficient for gas. It was proposed by Bird (1956) [52]. The idea is based on uncoupling molecular motion from the collisional step and both are performed separately. Molecular motion is model deterministically following. Advection step is characterized by ballistic motion of each particle

$$\boldsymbol{r}_j = \boldsymbol{r}_j + \boldsymbol{v}_j \Delta t \qquad (33)$$

In next step the lattice is imposed and each particle is allocated in cell. In each cell the number of pair undergoing stochastic exchange of momentum and energy are chosen.

$$\partial_t f + v_\alpha \partial_\alpha f + F_\alpha \partial_{v_\alpha} f = \Omega(f); \qquad (34)$$

Collisions are performed in a way to satisfy kinetic theory of gases. Hence the velocities satisfy Maxwell velocity distribution function

$$f(v_j) = \left(\frac{m}{k_B T}\right)^{\frac{3}{2}} v_j\, e^{-m v_j^2/2 k_B T} \quad ; \qquad (35)$$

which is also imposed on the solid boundaries.
The method works especially well for rarefied gases. However, can be used in other application too. The method is sensitive to the random number generation errors and ratio of the lattice size to the mean free path. Some simulation example can be found in [53,54]

Stochastic Rotational Dynamics (SRD)

Stochastic Rotational Dynamics was proposed by Malevanets and Kapral in 1999 and has many commonalities with DSMC. The particle move in two distinguished steps. First is the ballistic motion

$$\boldsymbol{r}_j = \boldsymbol{r}_j + \boldsymbol{v}_j \Delta t \quad . \qquad (36)$$

Second the particles velocities direction are shifted randomly by specific value

$$\boldsymbol{v}_j = \boldsymbol{u}_j + \Omega(\boldsymbol{v}_j - \boldsymbol{u}) \quad ;$$

$$\Omega = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \quad ; \qquad (37)$$

$$\boldsymbol{u} = \frac{1}{N}\sum_{j=1}^{N} \boldsymbol{v}_j \quad .$$

The step of shift assures that Galilean invariants are preserved. However, in contrary to DSMC there are no imposed rules on the properties of stochastic step. All particles are adjusted, not only the chosen one. Hence, this model fits better for simulation of liquids, where the intermolecular interaction is much stronger. The adequate relations for mesoscale properties, such as Green-Kubo formula can be derived [55,56,57].
Currently, however, there are not many microfulidcs simulations using SRD. Some can be found in [58,59,60].

Dissipative Particle Dynamics (DPD)

Dissipative Particle Dynamics is a coarse grained model having its origin in Molecular Dynamics. The DPD was introduced by Koelman and Hoogerbrugge (1992) [61] to model colloidal suspension behavior. The particles can move freely and have interaction potential, which is simplification of Lennard-Jones Potential (see Figure). The potential is generally of the form

$$\omega(\boldsymbol{r}_{jk}) = f\left(1 - \frac{\boldsymbol{r}_{jk}^n}{\boldsymbol{r}_c}\right) \tag{38}$$

.
Equations of motion are as follow:

$$\frac{d\boldsymbol{r}_j}{dt} = \boldsymbol{v}_j(t) \quad ;$$

$$m\frac{d\boldsymbol{v}_j}{dt} = \sum_{j \neq k} \left[\boldsymbol{F}_{jk}^C(\boldsymbol{r}_{jk}) + \boldsymbol{F}_{jk}^D(\boldsymbol{r}_{jk}, \boldsymbol{v}_{jk}) + \boldsymbol{F}_{jk}^R(\boldsymbol{r}_{jk}) \right] \quad . \tag{39}$$

The corresponding forces assure correct fluid behavior. Conservative force is a purely repulsive force and represents pressure.

$$\boldsymbol{F}_{jk}^C = \pi \,\omega(\boldsymbol{r}_{jk}) \boldsymbol{e}_{jk} \quad . \tag{40}$$

Dissipative force reduces velocities between particles. Therefore, it represents friction

$$\boldsymbol{F}_{jk}^D = \gamma \, m \omega(\boldsymbol{r}_{jk})(\boldsymbol{e}_{jk} \cdot \boldsymbol{v}_{jk}) \boldsymbol{e}_{jk} \quad . \tag{41}$$

The random force ensures fulfillment of thermodynamic properties of fluid

$$\boldsymbol{F}_{jk}^R = \frac{\delta \theta_{jk}}{\sqrt{\Delta t}} \omega(\boldsymbol{r}_{jk}) \boldsymbol{e}_{jk} \tag{42}$$

Random force ensures that fluctuation-dissipation theorem is satisfied

$$d\theta \, d\theta^T = 2 k_B \Xi(x) dt \tag{43}$$

Dissipative Particle Dynamics suits well for complex geometries. The drawback, however lies in the modeling the correct Schmidt number(ratio of dissipation to viscous forces). The special thermostats are required [62], hence thermal effects are not modeled. Additionally, imposing correct boundary conditions is a challenge. There are however some microfluidics simulations utilizing DPD properties [63,64,65].

Conclusion

Modeling of micro- and nanofluidics is a challenge. the physical phenomena are generally complex and simplification very rarely can be obtained. Additionally, due to the complexity of the numerical procedure, computations are expensive. Hence, the engineering design of MEMS and NEMS, at present, is not as extensively supported by computer simulations as it is on the macroscale.

Over many years several techniques were developed to obtain fast and accurate mesoscale models. However, such approaches require simultaneously to obtain mesoscale properties and the motion. The coarse graining procedure reduces several interaction from the molecular scale to make it more efficient. For micro- and nanofluidics mesoscale methods still are inefficient and not accurate enough, because they were mostly developed for bulk flow. The crucial physics of fluid-wall interactions is not properly capture. Hence, the micro- and nanofluidics simulation research is still very new and fast growing research field.

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