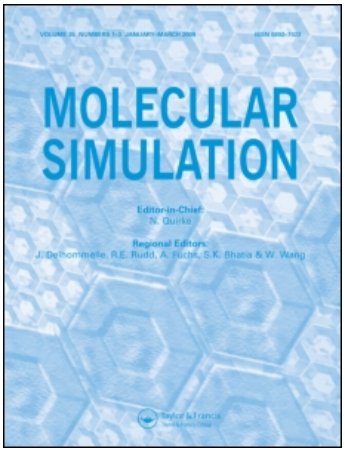

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CROSS-SCALE NUMERICAL SIMULATIONS USING DISCRETE PARTICLE MODELS

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We propose a concept for a homogenous computational model in carrying out cross-scale numerical experiments on liquids. The model employs the particle paradigm and comprises three types of simulation techniques: molecular dynamics (MD), dissipative particle dynamics (DPD) and smoothed particle hydrodynamics (SPH). With respect to the definition of the collision operator, this model may work in different hierarchical spatial and time scales as: MD in the atomistic scale, DPD in the mesoscale and SPH in the macroscale. The optimal computational efficiency of the three types of cross-scale experiments are estimated in dependence on: the system size N – where N is the number of particles – and the number of processors P employed for computer simulation. For the three-hierarchical-stage, as embodied in the MD-DPD-SPH model, the efficiency is proportional to $N^{8/7}$ but its dependence on P is different for each of the three types of cross-scale experiments. The problem of matching the different scales is discussed.

Keywords: Cross-scale simulations; parallel implementation; molecular dynamics; dissipative particle dynamics; smoothed particle dynamics

1. INTRODUCTION

All physical phenomena observed in the macroscale not only modify the macro-scopic parameters of an underlying physical system, but also can influence their atomistic and subatomistic properties as well. When the

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changes in the microscale:

1. can be reflected by respective changes of global parameters of the macroscale models,
2. follow the assumed constitutive relations,
3. do not violate the assumptions of mass, momenta and energy continuity,

then the continuum model describing macroscopic processes can adequately illustrate the system. For less well-defined situations, when the influence of cumulated microscopic effects on the system behavior cannot be explained by the continuum model, the cross-scale computer simulation is essential, (apart from actual physical experiments) for predicting the temporal evolution of the system. The cross-scale endeavor should be regarded as a complex computer simulation, which couples the macroscale and microscale properties of the system. Because of the computational difficulty of this approach, only efficient parallel models and their implementations on the most powerful massively parallel computers can provide a bridge between the microscopic and macroscopic worlds.

The first attempt to cross-scale computations was carried out by Clementi [3] in the 80's. The so-called "global simulation", had to cover a computer model of liquid water ranging from a single molecule to the ocean scale. The computer system dedicated for realization of the idea, consisted of loosely coupled scalar computers, array processors and vector supercomputers. Much more modest but more successful contributions to cross-scale simulations were made a decade later by Abraham [8]; Holian [13] and Vashishta [22]. The problems of the nanoscale to mesoscale interfacial phenomena simulation have been discussed recently at the conferences organized in the Pacific Northwest National Laboratory (PNNL) [23] and at University of Oxford [24]. In spite of the distinct leap in computer power in the last decade, crossing-scale computations are until now at a stage of infancy. The problem lies not in the lack of adequate computer power but rather in the lack of viable ideas on, how to couple the different models operating on diverse time and spatial scales into a single homogenous system.

2. THE MODELS OF CROSS-SCALE SIMULATIONS

Neglecting the scales below the atomic level, we can employ two principal physical paradigms and respective computational models for fluid simulation: the particle paradigm and the continuum approach (see Fig. 1).

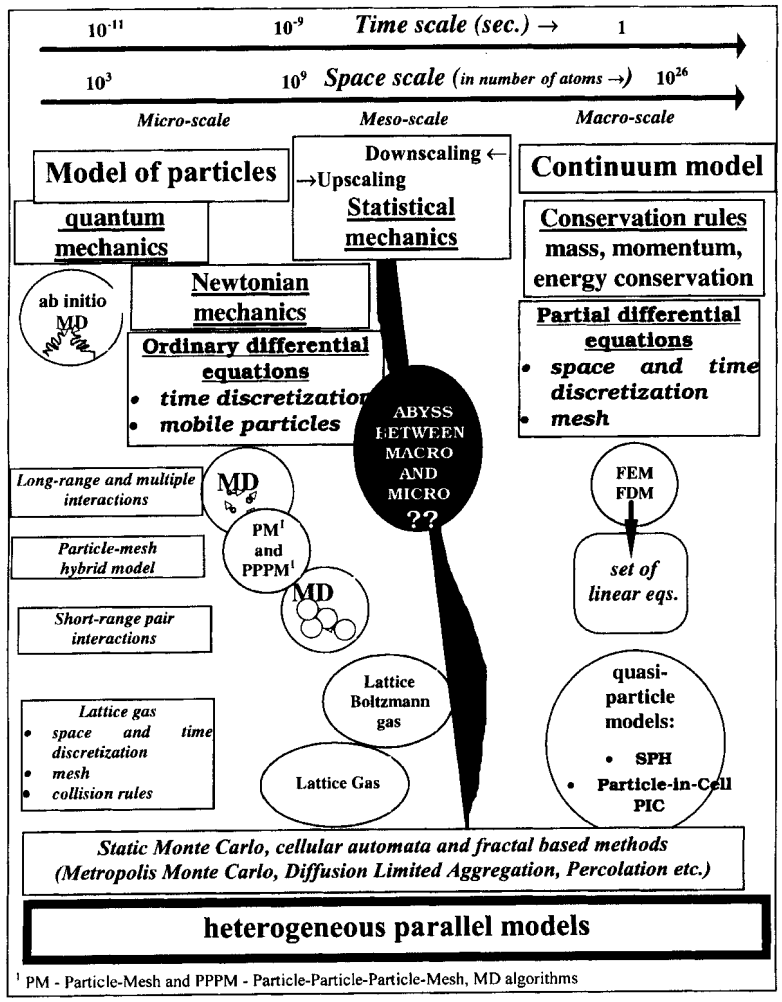

FIGURE 1 Particle and continuum models used in computer simulations.

The paradigm based on interacting atoms, whose temporal evolution obeys the Newtonian laws of motion, and operates in the microscale. Molecular dynamics (MD) technique is the most prominent computational realization of this model. The method consists in the solution of the set of ordinary differential equations in time for each particle, using numerical schemes. As a result, the positions and velocities of particles are updated during the simulation. The global physical parameters of the particle ensemble are computed by temporal and spatial averaging of the statistical

functions of particles positions and velocities, as well as by computing the correlation functions and higher moments.

The paradigms constructed on the basis of mass, momenta and energy streams continuity are used to quantify the macroscopic properties of fluids. Their mathematical models are represented by a set of nonlinear partial differential equations. Computer implementation of these models is based on the space and time discretization on a fixed or reconfigurable mesh. This can be accomplished using finite elements (FEM) or finite differences techniques (FDM). The resulting set of linear equations is solved at each timestep and temporary values of density, momenta and energy in the mesh nodes are computed. For more complex and non-linear mathematical models, the set of nonlinear equations have to be solved at each timestep, which is difficult for continuum methods, especially for problems with steep gradients in physical properties.

As shown in Figure 1, the wide gap opens up between the particle and continuum paradigms. This gap cannot be spanned using only statistical mechanical methods. The existing theoretical models to be applied in the mesoscale, are based on heuristics obtained *via* downscaling of macroscopic models and/or upscaling particle approach. Simplified theoretical models of complex fluid flows *e.g.*, flows in porous media, non-Newtonian fluid dynamics, thin film behavior, flows in presence of chemical reactions and hydrodynamic instabilities formation, involve not only validation but should be supported by more accurate computational models as well. However, until now, there has not existed any precisely defined computational model, which operate in the mesoscale, in the range from 10 Å to tens of microns.

The simplest way to conduct the simulations of mesoscale phenomena possible, consists in downscaling of the continuum approach or upscaling the particle model. The limitation of the first approach is determined by the granular properties of matter, which are revealed for very small system. The behavior of granular fluid is different from that in the bulk. For example, very small systems may exhibit solid–liquid coexistence over a range of temperature different than that for large systems [14].

The upscaling of the particle model can be realized by increasing the grid size, *i.e.*, increasing the number of particles. It is the natural approach to the cross-scale computations. Despite very efficient parallel implementations of MD method, only about 10^9 molecules (the sample 0.5 microns of size) in the time of nanoseconds can be currently simulated using the most powerful massively parallel systems [2, 16]. The nanoscale MD simulations [1, 4, 6, 8, 13, 18, 22] reveal very interesting collective and complex behavior of the particle systems and their importance cannot be underestimated. Especially,

when they are applied for investigations of new materials, mixing phenomena, chemical reactions, interfacial phenomena *etc.* Such atomistic simulations are an valuable tool for obtaining constitutive relations, which can be used in the macroscale models. Some of subcontinuum fluid problems, which can be solved by using large scale MD computations as: rupture in solids or coalescence of liquid drops that occur on interfacial scales, unphysical singularities resulting from such continuum approaches, spreading of wetting films on solid surfaces and behavior of non-Newtonian fluid are discussed in [14].

Fundamental simplifications of particle–particle collision operator and particle motion rules, result in the cellular automata models of fluid dynamics: *i.e.*, lattice gas (LG) and lattice Boltzmann gas (LBG) schemes. Due to the simplifications, the number of calculations needed to change a temporal state of a single LG particle is much smaller than for MD one. Therefore, more LG particles can be simulated and larger physical systems can be explored [21]. This advantage, however, is somewhat misleading. As a matter of fact, the results of application of the lattice gas methods are not more efficient than MD. This concerns the cases, when the simplifications in the physical model cannot be compensated by the number of simulated "particles". A drawback of the lattice approaches is that the dynamics are constrained by the configuration of the lattice. This precipitates many problems, *e.g.*, with 3-D models, averaging, boundary conditions on shaped bodies, simulation of shock phenomena *etc.* Moreover, the lattice-gas techniques fit poorly to the cross-scale computations. It is difficult to conceive that such qualitative models can be suitably combined with other particle or continuum approaches. Unlike LG techniques, the particle approaches operate for strictly defined length and time scale. The matching problem discussed in the following paragraph would be here even more acute than for the MD-FEM heterogeneous cross-scale computations [10, 11, 22].

Cross-scale simulations are usually performed by using a combined heterogeneous micro–macro model [10, 11, 22]. For example, simulations of cracks formation can be performed using MD for tips of the crack but continuum approach for rest of the system. MD (*i.e.*, high resolution model) can be used for the regions of unphysical singularities that result from an application of continuum approaches, *e.g.*, corner-flow singularities, or the interfacial phenomena, for example the Stokes drag on an object falling in a fluid upon impacting a solid surface [14]. The most difficult problem for the MD-FEM heterogeneous cross-scale computations is the problem of matching. How to match two regions that are to be treated at different scales of resolution? The difficulty lies in the fact that the variables of the calculation

in these two regions are very different. This inconsistency comes from the principal differences between continuum and particle approaches as reflected in their physical, mathematical and computational models. This problem can be overcome by using the Schwarz coupling approach [10, 11], which consists in defining an overlap between the regions of different model operation, and performing alternate iterative procedure in the overlap to the convergence. Such an approach, however, results in an inefficient parallel realization of the cross-scale computations. For fitting the boundary conditions between the regions of two heterogeneous models operation and fulfill different requirements of two incompatible parallel algorithms, we sacrifice computational efficiency.

The matching problem could be partially solved by using a homogenous computational model for simulating in the microscale, mesoscale and macroscale phenomena. The particle paradigm is the best candidate to act as the backbone of such the model.

3. MODEL OF PARTICLES

Upscaling of the particle model can be carried out also in a different way than by increasing the number of molecules. As shown in [1, 4, 7], this can be accomplished by:

1. assuming that a particle represents a cluster of matter rather than a single molecule,
2. changing the character of interparticle interactions.

The particle ensemble can be interpreted in terms of the mesoscopic or macroscopic system. The simulation of granular materials [20], where the particles are, in fact, rigid granules, represent a good example of the particle model being applied in the macroscale simulations. This model can also be employed for portraying macroscopic dynamicss according to physical laws [5].

In the same light, for simulation of liquids, a fluid particle has been defined by Español [7] and a special form of a dissipative potential was introduced. Thus the fluid particles can be interpreted as "clusters of molecules". Dissipative particle dynamics method (DPD) [12, 19], a particular case of a fluid particle model, allows one to simulate larger fluid samples and to use smaller particle ensembles than the typical MD simulations. Including DPD as an intermediate particle mode, allows one to reduce the number of MD particles in the cross-scale simulations and thus make them more efficient.

In Figure 2 the snapshots of 2-D MD and DPD simulations of bubbles are shown. Using the DPD approach, we have obtained results of simulation which are more smooth. Some details obtained by MD simulation are lost. They are not relevant at time scales in which rheological processes in complex fluid take place. Additionally, the state presented in Figure 2a was obtained after about 5 hours of simulation on 16 Cray T3E processors. On the contrary, the DPD code needed on 10^5 particles and an hour of CPU time on a workstation with 200 MHz clock.

To resolve the matching problem, the continuum model should be replaced by the particle approach. As shown in Figure 1, quasi-particle methods as: particle in cell (PIC) and especially smoothed particle hydrodynamics (SPH), are interesting alternatives for the continuum models. They were successfully used for simulations in the macroscale [15, 17]. Meshless SPH technique based on interpolation principle, represents

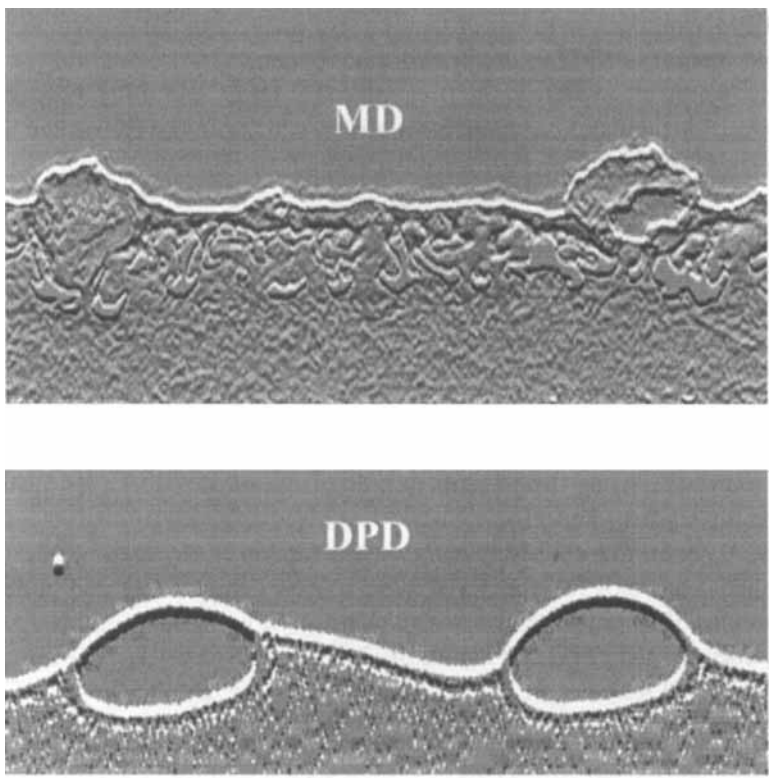

FIGURE 2 The bubble-creation process simulated using MD and DPD codes.

particle formulation of conservation equations of continuum mechanics. In result, the partial differential equations of continuum model are transformed into ordinary differential equations. These equations can be interpreted as the equations of motion of "particles". The SPH "particles" represent the nodes of a "free" grid made of interpolation points. They stand for the "lumps of fluid" undergoing the Newtonian laws of motion. Thus this technique allows one to solve partial differential equations using MD codes. However, the SPH technique by itself, cannot be applied for complex flows simulation, because it is not easy to implement Lagrangian fluctuating hydrodynamics with SPH.

The fluid particle model (FPM) introduced by Español [7], may be viewed as a Lagrangian discretization of the equations of isothermal fluctuating hydrodynamics. This represents the generalization of the smoothed particle dynamics (SPH) approach and is based on the DPD idea. Unlike the former method, FPM conserves the total angular momentum of the system. As is shown in [7], at zero temperature and with no angular variables, the form of the FPM equations is identical to the form of the equations obtained in a simple version of SPH as applied to fluid system.

The temporal evolution in time of MD, DPD and SPH particles is described by the same Newtonian equations, which can be represented in the following discrete form:

$$\begin{aligned} \Delta\vec{\mathbf{p}}_i &= \sum_{i\neq j} \vec{\Omega}_{ij} \cdot \Delta t \\ \Delta\vec{\mathbf{r}}_i &= \frac{\Delta t}{m_i}(\vec{\mathbf{p}}_i + \Delta\vec{\mathbf{p}}_i) \\ r_{ij} &= |\vec{\mathbf{r}}_i - \vec{\mathbf{r}}_j| \end{aligned} \tag{1}$$

where: $\Delta\mathbf{r}_i$, $\Delta\mathbf{p}_i$ – are the changes of position and momentum, respectively, for particle i of mass m_i after single timestep equal to 1, Δt – timestep, Ω_{ij} – collision operator, $\mathbf{e}_{ij}$ – unit vector pointing from particle j to i, r_{ij} – distance between particles i and j.

The type of the collision operator Ω_{ij} (and particle mass m_i) can be classified according to the three types of particle models and different hierarchies of length-time scales. The microscale, mesoscale and macroscale are associated with MD, DPD and SPH models, respectively. The formulae for the MD, DPD and SPH collision operators are as follows:

MD :

$$\vec{\Omega}_{ij}^{\,n}(r_{ij}^n) = \frac{24\varepsilon}{r_{ij}^n}\left[\left(\frac{\sigma}{r_{ij}^n}\right)^6 - 2\left(\frac{\sigma}{r_{ij}^n}\right)^{12}\right] \cdot \vec{\mathbf{e}}_{ij}^{\,n} \tag{2}$$

DPD :

$$\vec{\Omega}_{ij}^{n}(r_{ij}^{n}, \vec{\mathbf{p}}_{ij}^{n}) = \left(1 - \frac{r_{ij}^{n}}{R_{\text{cut}}}\right)\left[\alpha_{ij} - \gamma\left(1 - \frac{r_{ij}^{n}}{R_{\text{cut}}}\right)(\vec{\mathbf{e}}_{ij}^{n} \bullet \vec{\mathbf{p}}_{ij}^{n}) + \frac{\text{Sig}\theta_{ij}}{\sqrt{\Delta t}}\right] \cdot \vec{\mathbf{e}}_{ij}^{n}$$

SPH

$$\vec{\Omega}_{ij}^{n}(r_{ij}^{n}, \vec{\mathbf{p}}_{ij}^{n}, \rho_{i}^{n}, \vec{\mathbf{S}}_{i}^{n}, E_{i}^{n}) - \text{implicit function}$$

where σ, ε – the Lennard-Jones potential parameters, R_{cut} – cut off radius; θ_{ij}, α_{ij}, γ_{ij} – DPD potential parameters, Sig – a random number from $[-1, 1]$ interval; $\mathbf{p}_{ij}$ – difference between momenta of particle i and j, ρ_i – density, $\mathbf{S}_i$ – stress function, E_i – internal energy, n-timestep number, i-particle index. The collision operator for the three types of particle models is short ranged, *i.e.*, for $r_{ij} > R_{\text{cut}}$ (for the SPH model $r_{ij} > 2h$, where h defines a length scale and is interpolation kernel parameter) $\Omega_{ij} = 0$. Due to non-central character of the SPH operator for viscous problems [7], the total angular momentum is not conserved. The FPM model conserves total angular momentum due to the inclusion of a spin variable. Hence, the additional equation of angular momentum conservation in the Newtonian laws of motion should be considered. For macroscale system, with a large number of SPH particles, violation of the angular momentum does not pose a serious problem [7]. Fluid particle method can be used for matching the boundary between the SPH and DPD operating regions.

The homogeneous particle paradigm proposed for the cross-scale computations is presented schematically in Figure 3. The difference between various scales reflects the form of the collision operator. The cross-scale particle system composes of SPH, DPD and MD particle subsystems (see Fig. 4). This physical system can be split into regions with different submodels. MD molecules and intermolecular forces can be used where the microscale simulations are performed. In the mesoscale, DPD molecular clusters interacting *via* dissipative forces are defined, while SPH "lumps of fluids" are used for the regions where the macroscale model is employed. The particles of these subsystems have their own individual characteristic sizes, masses and interparticle potentials. Thus DPD particles are larger and heavier than MD molecules and SPH clusters are the largest and the heaviest. One can assume that the interparticle potential between the particles of different types (*e.g.*, MD-DPD or DPD-SPH) on the boundary between regions of different models operation is defined by the particle model, which is lower in scale. For example, for DPD-SPH particles interactions, the DPD potential can be used. The mass ratios among the SPH, DPD and MD particles determine the inertia of individual particle system and thus define the relaxation time for each model. Such a model can

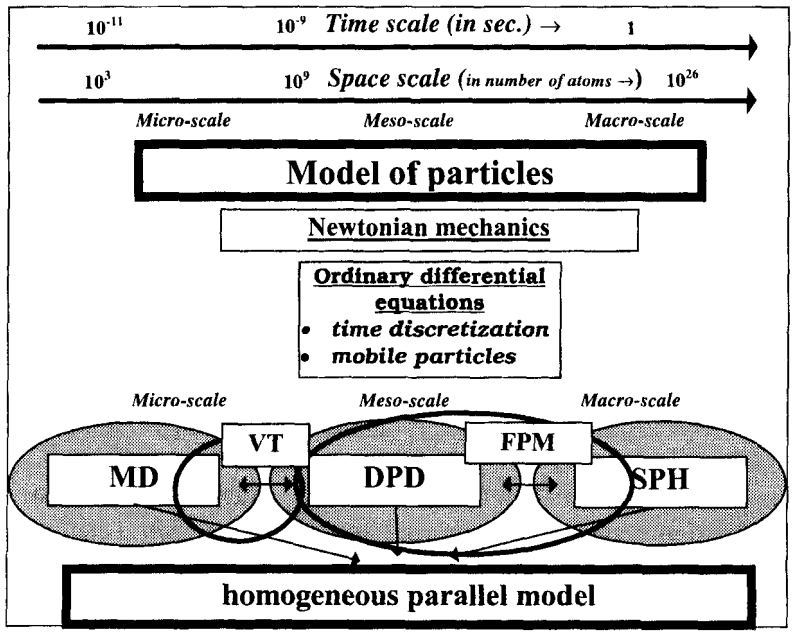

FIGURE 3 Schematic of the particle based cross-scale computational model.

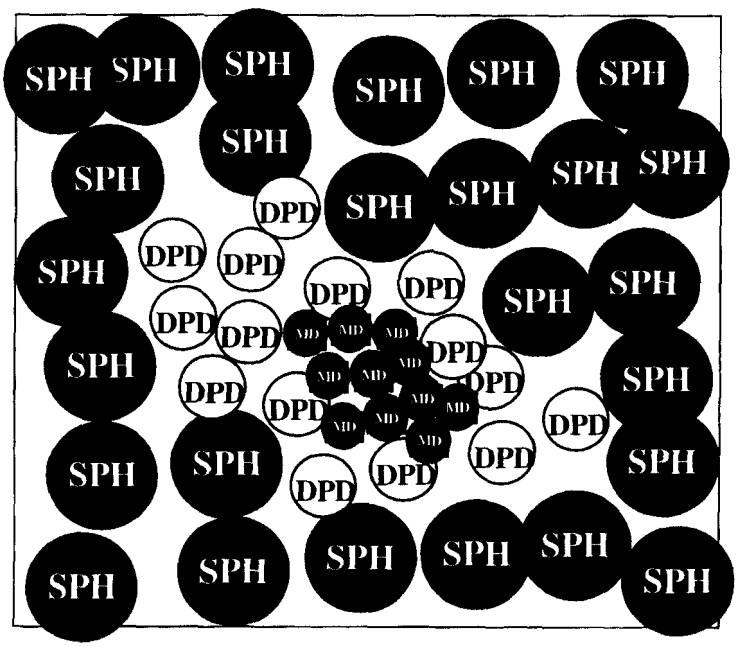

FIGURE 4 SPH, DPD and MD particles within the framework of the cross-scale particle model.

be employed only, when regions of an operation of different particle models are static, for example when MD and DPD are used only at the corners, where flow singularities appear. In the dynamic case, *i.e.*, when region of interest is moving, these three separate particle systems can be used. The smaller-scale scale particle model should have the possibility to be coarsegrained to the higher scale particles using, for example, the Voronoi tessellation (VT) scheme [7]. The computational scheme of dynamic cross-scale computations is displayed in Figure 3.

For implementing this model in a parallel environment, some questions concerned its efficient realization should be addressed. The most fundamental issue concerns the optimal balance between the particle ensembles to minimize the computation time and relations between the time and size of the system and the number of processors used.

4. EFFICIENCY IN THE PARALLEL REALIZATION OF THE MODEL

The idea of parallel algorithm realization of the particle models does not depend on the type of the collision operator used. Because there exist many efficient parallel algorithms and implementations of MD codes, which can be run for large particle ensembles on different platforms (about 10^9 MD particles were simulated by using the code presented in [2, 16]), it is easy to convert them automatically for DPD and SPH methods by creating a single, homogeneous parallel system. As shown in [2, 16], the efficiency of MD parallel codes is higher than 90% for massively parallel computing system for well load-balanced computations. This results in a better outcome for DPD and SPH codes for fewer particles, due to the longer CPU time involved for calculating the forces for these models and better load balancing. For coupled, cross-scale mode, we encounter the problem of an optimal balance between the particle ensembles operating over the different scales of resolution.

Let us assume that a particle ensemble, which consists of l SPH particles, describes a macroscopic system. Each SPH particle consists of m_1 DPD particles, each of which consists of n_1 MD atoms. The scale of the system is represented by the total number of MD atoms N. Let us assume moreover that:

- the computations will be performed using P processors,
- the speed-up of MD, DPD, SPH models parallel implementation is linear with the number of processors,

- domain decomposition algorithm, which divides the computational box on P cells (or strips), is considered.

The number of MD atoms, which fit in the single cell is equal to:

$$l_1 \cdot m_1 \cdot n_1 = N/P \tag{3}$$

where l_1 – is the number of SPH particles in a single cell.

Three computational models are considered. The first one (Fig. 6.1) is based on the scheme of computations shown in Figure 5. It represents the cross-scale computations in which the microscopic region under interest is "zoomed-in" by using the particle models with smaller scales. The temporal evolution of the bulk system is described by the SPH model. The microscopic region consists of DPD and MD subregions. For example [8, 13], in simulations of crack propagation, MD particles are placed at the tip of the crack, the secondary particles represent the tip's close environment, while the continuum computational model is used for the wave propagation in the bulk. Let us assume also that the DPD region (together with MD one) can be covered by $a \cdot P$ SPH particles ($a \geq 1$) thus it consists of $m = aP \cdot m_1$ DPD particles. Similarly, the MD region is covered by $b \cdot P(b \geq 1)$DPD particles and consists of $n = bP \cdot n_1$ MD particles. In this way, the respective region sizes are coupled with the number of processors used.

For the second model (Fig. 6.2), the MD particle ensembles stand for bP separate DPD particles, each consisting of n_1 MD particles. Because, the number of DPD particles $m = aP \cdot m_1 \gg P$, MD clusters can represent bP chosen in random DPD particles or the particles chosen in the critical places of the DPD region. The model exemplifies the situation, when MD simulations are used for realizing DPD particle attributes (such as masses, collision operator coefficients and cut-off radius).

In the third model (Fig. 6.3), the value a of SPH particles for each processor cell are simulated independently by using m_1 DPD particles. Likewise, for each DPD particle ensemble, separate b DPD particles are simulated by n_1 MD particles. For this cross-scale computational model, the particle model with smaller scales serves for the realization or correction of SPH particle characteristics in the different computational regions.

Let us estimate the efficiency of the parallel implementation of the three cross-scale computational models in Figure 6. The CPU time needed for completing particle positions and velocities at one timestep on a single processor is αn_1, βm_1 and γl_1 for the respective particle models. Let us assume that the number of timesteps to perform MD, DPD and SPH computer experiments in the cross-scale simulations is I, M and L,

```
for t=1 to L {Simulate 1 SPH particles for a given t interval on P processors};
   ChooseMesoscaleRegionUnderInterest (covered by aP SPH particles);
   TransformParticles ( aP SPH particles transform into m DPD particles);
   for t=1 to M   {Simulate m DPD particles for a given t interval};
      ChooseMicroscaleRegionUnderInterest (covered by bP DPD particles);
      TransformParticles ( bP DPD particles transform into n MD particles);
         for t=1 to N  { Simulate n MD particles for N timesteps};
         endfor
         TransformParticles( n MD particles transform into P<m DPD particles);
   endfor
   TransformParticles(m DPD particles transform into P SPH particles);
endfor
```

FIGURE 5 Algorithmic scheme of the dynamic cross-scale computation model.

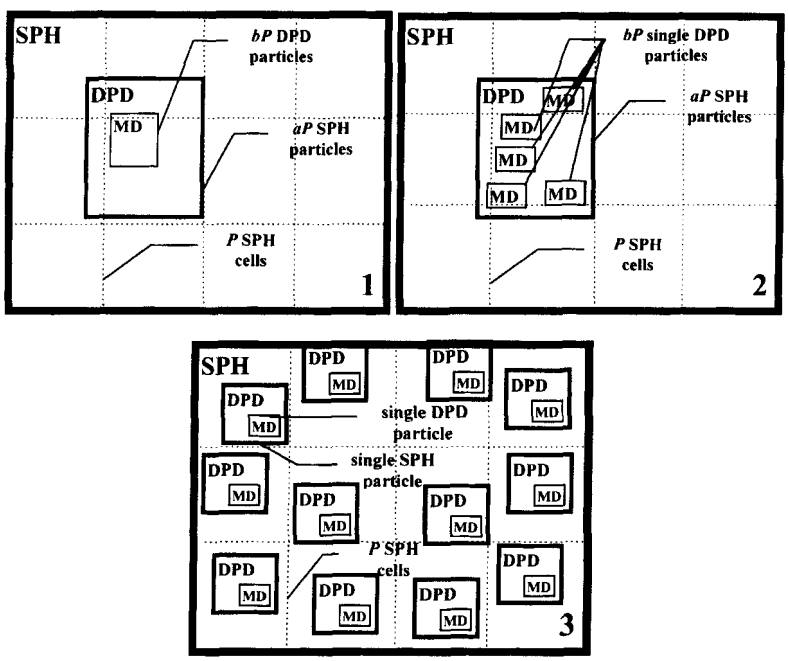

FIGURE 6 Three cross-scale computer models. The SPH region is divided onto P cells. In Figure 6.1 the DPD region can be covered by aP SPH particles and the MD region by bP DPD particles.

respectively. Then the total time for simulation is:

$$\tau = L \cdot M \cdot I \cdot \alpha \cdot n_1 + L \cdot M \cdot \beta \cdot m_1 + L \cdot \gamma \cdot l_1 \tag{4}$$

Moreover, the number of timesteps performed for the particle method is proportional to the number of particles simulated, *i.e.*, $I = \alpha_1 n$, $M = \beta_1 m$, $L = \gamma_1 l$ we obtain that:

$$\tau = \gamma_1 \cdot \beta_1 \cdot \alpha_1 \cdot \alpha \cdot l \cdot m \cdot n \cdot n_1 + \gamma_1 \cdot \beta_1 \cdot \beta \cdot l \cdot m \cdot m_1 + \gamma_1 \cdot \gamma \cdot l \cdot l_1 \tag{5}$$

where:

$$\begin{aligned} &l = P \cdot l_1, \ m = aP \cdot m_1, \ n = bP \cdot n_1 \text{ for the first model (Fig. 6.1),} \\ &l = P \cdot l_1, \ m = aP \cdot m_1, \ n = bn_1 \text{ for the second model (Fig. 6.2),} \\ &l = P \cdot l_1, \ m = am_1, \ n = bn_1 \text{ for the third model (Fig. 6.3).} \end{aligned} \tag{6}$$

From Eq. (5) we can see that the size of MD submodel will determine mainly about the total simulation time. By minimizing the total computational time (5) under condition (3), we obtain:

$$l_1 \propto P^{1/7} \cdot N^{4/7}, \ m_1 \propto P^{-3/7} \cdot N^{2/7}, \ n_1 \propto P^{-5/7} \cdot N^{1/7}, \ \tau_{\min} \propto P^{9/7} N^{8/7} \tag{7}$$

for the first model,

$$l_1 \propto P^{-1/7} \cdot N^{4/7}, \ m_1 \propto P^{-4/7} \cdot N^{2/7}, \ n_1 \propto P^{-2/7} \cdot N^{1/7}, \ \tau_{\min} \propto P^{5/7} N^{8/7} \tag{8}$$

for the second, and

$$l_1 \propto P^{-4/7} \cdot N^{4/7}, \ m_1 \propto P^{-2/7} \cdot N^{2/7}, \ n_1 \propto P^{-1/7} \cdot N^{1/7}, \ \tau_{\min} \propto P^{-1/7} N^{8/7} \tag{9}$$

for the third one.

From Eqs. (7–9), the minimal simulation time for the cross scale models depends on the system size and this increases with N as $N^{8/7}$. The generalization of Eqs. (7–9) for multi-hierarchical-stage system, where the numbers of stages is i, gives $\tau_{\min} \propto N^{2^i(2^i-1)}$. Therefore, by using only MD model ($i = 1$) $\tau_{\min}$ is proportional to N^2 and for two-hierarchical-stage FPM-MD model $\tau_{\min}$ likewise as $N^{4/3}$. The increase of $\tau_{\min}$ with P is based on the assumption that the number of DPD particles used for simulation of mesoscopic region and the number of MD atoms, which cover the microscopic region, are proportional to the number of processors P used.

Thus the increase of P results in increase of the system resolution. This assumption was stated for parallel computations, which could exploit the full power of the computer system for each of the particle model regimes. We also assume that the speed-up time is linear for each system.

As shown in Eqs. (7, 8), the assumption about the increase of the system resolution with the number of processors, causes $\tau_{\min}$ also to increase with P. The only exception lies in the third model for which $\tau_{\min} \propto P^{-1/7}$ (see Eq. (9)). For the first model, in spite of increase in P, the volume of the mesoscale region is decreasing due to growing number of SPH particles. To keep it constant, a and b coefficients should be increased. The number of DPD and MD particles, which build a single SPH particle decreases also with P. Therefore, an increase in the system resolution concerns only the macroscopic and mesoscopic regions. The resolution of a single SPH and DPD particles decreases, *i.e.*, they consist of fewer number of MD particles. The decrease of m_1 and n_1 produces also a drop in the efficiency of parallel com-putations in the DPD and MD regimes for an increasing number of processors due to poor load balancing. These put an upper limit for the number of processors used for the fixed system size N. The precise number of particles of each type in the cross-scale simulations strongly depends also on α, α_1, β, β_1, γ_1, γ coefficients.

5. MATCHING THE DIFFERENT REGIMES

The matching problems involving the different regimes represent the most difficult aspect of the cross-scale computational model and can substantially deteriorate the efficiency of the parallel computer model. The matching problem concerns two critical issues:

1. How to match the type of the cross-scale model to the scale of the physical system considered? How many particles of each type should be taken for simulation?
2. How to match the physical parameters of the different particle models?

Apart from the three-hierarchical-stage SPH-DPD-MD approach, for smaller systems one can apply only two-hierarchical-stage particle model, *i.e.*, DPD-MD, FPM-MD or SPH-FPM types of simulations. In Figure 7 two snapshots from the Rayleigh-Taylor instability simulation obtained using SPH code are presented. There were 3.8×10^4 SPH particles simulated. According to the relations (7–9), such a particle ensemble can represent the "optimal" system consisting of $N \propto 10^8$ atoms. In Figure 8 the

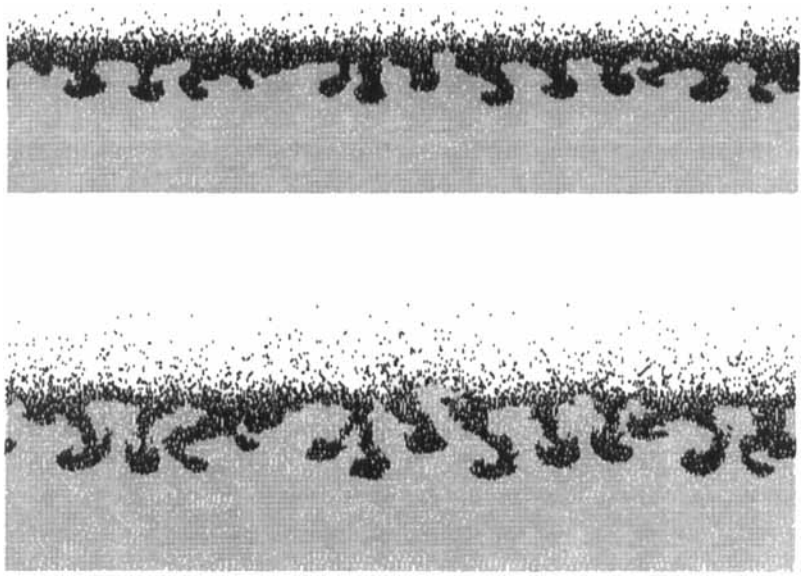

FIGURE 7 The snapshots of the R-T instability simulation using SPH code. The dark gray fluid is heavier than the light gray one. Gravity is directed from the heavier to the lighter fluid. The number of particles simulated is 3.8×10^4.

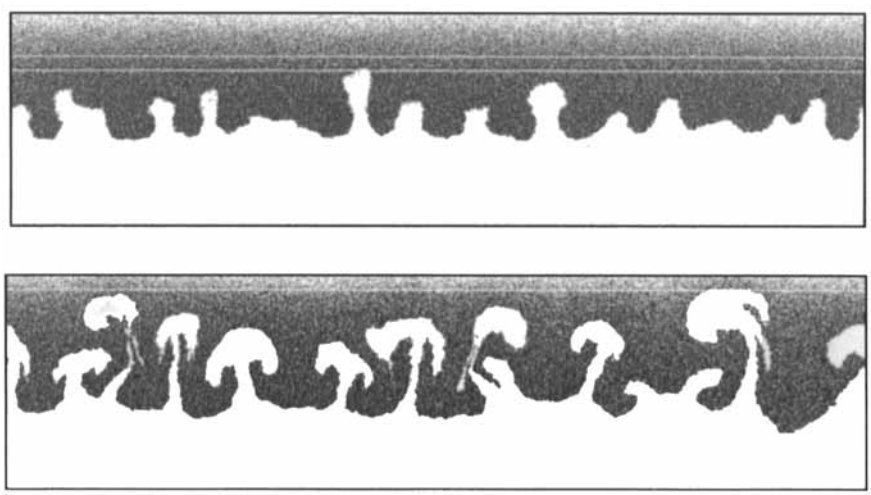

FIGURE 8 The snapshots of the R-T instability simulation in the microscale. MD code was used. The number of particles simulated is 1×10^6.

snapshots of MD simulation of the same phenomena performed for 10^6 MD atoms are shown. In spite of the different parameters of SPH and MD simulations their results are qualitatively similar. However, due to the coarse granulation of the SPH system, an artificial noise is generated and the system looks more noisy than smaller MD system. If, instead of the SPH model, a three-hierarchical-stage SPH-DPD-MD model (Fig. 6.3) would be used, the situation would not be improved. DPD and MD submodels can be used for correction of the interparticle SPH potential, but the noise produced in the SPH simulation is caused not by the unsuitable form of the potential but rather by the coarse granularity of the system.

In Figure 9 the snapshots from DPD simulation of the Rayleigh-Taylor instability are displayed. The number of DPD particles is 2×10^5. Using similar relations as (7–9) but for two-hierarchical-stage particle model, one can calculate that the "optimal" DPD particle system can also represent a physical system consisting of $N \propto 10^8$ MD atoms. Contrary to the SPH simulation, DPD particle system generates much less noise. Therefore, for such a small system size ($N \propto 10^8$) a two-hierarchical-stage MD-DPD (or

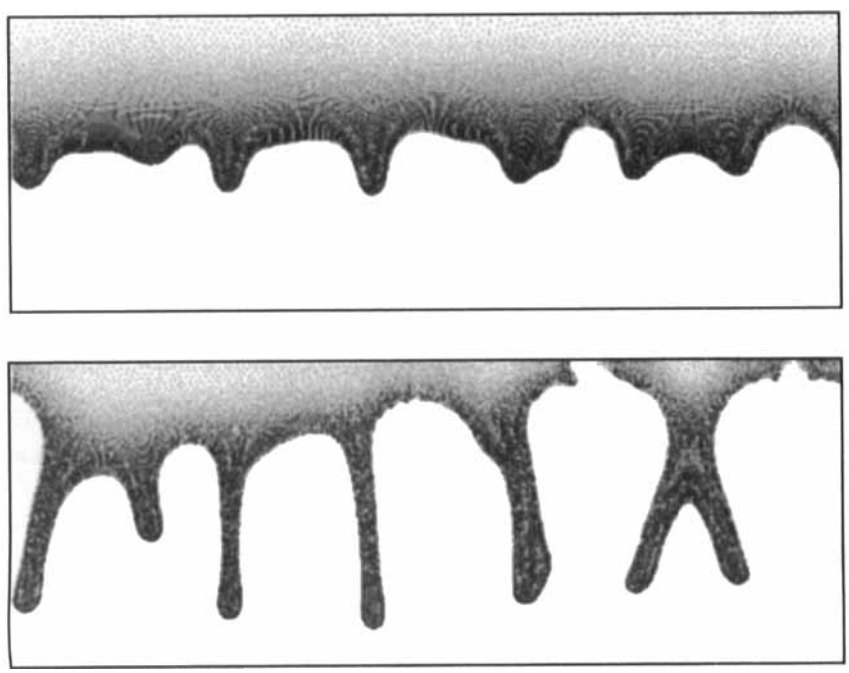

FIGURE 9 The snapshots of the R-T instability simulation in the mesoscale. DPD code was used. The number of DPD particles simulated is 2×10^5.

MD-FPM) is recommended rather than a three-hierarchical-stage model. The parameters of simulations presented in Figs. (7–9) are not matched and represent, in fact, different types of fluids.

To match the type of the cross-scale model to the scale of physical system under interest, one should take into account the available computer power applied. Let us assume, that the power can be expressed in the number of available processors P and the particle model implementation scales linearly with increasing P. The simulation time for pure MD approach scales as $\tau_{\min} \propto N^2/P$. Comparing this relation to the $\tau_{\min}$ given in (7–9) one can estimate the minimal number of processors $P_{\min}$, for which pure MD model is more efficient that the three-hierarchical-stage SPH-DPD-MD cross-scale approach. The $P_{\min}$ values for the respective three models presented in Figure 6 are as follows;

$$P_{\min} \propto N^{3/8}, \quad P_{\min} \propto N^{1/2}, \quad P_{\min} \propto N \tag{10}$$

For the system size $N \sim 10^8$, $P_{\min}$ for the respective models are $10^3, 10^4$ and 10^8. It means that for the first type of the cross-scale simulation model (see Fig. 6.1), assuming that the system is made of about a hundred millions of atoms, pure MD computational model is preferred to be used on the state-of-art computer systems. This agree well with current cross-scale simulation trends [2, 8, 13, 16, 22]. For larger systems, however, combinations of two-or three-hierarchical stage models is recommended.

The second problem concerns the matching of the physical parameters of different particle models used in the cross-scale simulations. This matching problem has a different character from a similar approach used for the heterogeneous models (*i.e.*, MD-FEM) [10, 11, 22]. For the latter case, the variables of the calculations in two regions of different resolution are qualitatively different, *e.g.*, stress tensor for continuum approach and particles positions and velocities for MD calculations. For the particle model, the variables are the same both for MD, DPD and SPH submodels (particle positions and velocities) but the collision operators are entirely different.

For example, the MD the DPD experiments, whose snapshots are shown in Figure 2 represent, in fact, two different physical systems. The MD and DPD simulations refer to a sample with about one micrometer of size. To investigate the influence of different models application on the simulation results or to match MD and DPD models, the DPD potential should be fit to the Lennard-Jones fluid simulated by MD. Because, the properties of substances are expressed in terms of macroscopic quantities (surface

tension, vicosity, stress tensor *etc.*), not in coefficients of the collission operator, the matching is usually done by a fit of the macroscopic parameters. These parameters can be calculated for particles models by averaging statistical functions of particles positions and velocities. By multiple iterations one can obtain the collision operator. The Schwarz coupling approach [10, 11] used for heterogeneous cross-scale models, consists of such iterations in the overlap region along the border between continuum and particle regimes. This process is not efficient. Moreover, a crude matching can produce incompatible simulation results for the two models. An example of the lack of match between different particle models is also presented in Figures 7–9.

Fluid particle model [7] seems to be ideal for matching SPH and DPD models, because it represents the generalization of SPH, including DPD as a special case. Although this generalization concerns only isothermal, thus small systems, one can assume that the larger systems can be simulated by using SPH with adequate resolution. FPM can serve as an intermediate model between SPH and DPD or this can be considered instead of DPD (see Fig. 3). For dynamic cross-scale models, when the microscopic region of interest moves, the particles lower in scale should be transformed into a smaller number of larger particles, which take part in simulations described by the particle model with the larger scale. The larger (for example DPD) should be reduced in size (for example into MD particles). An optimal starting point for construction of such the transformation schemes is the idea of the Voronoi tessellation (VT) applied in the fluid particle definition [7]. This same idea can be applied for MD-DPD matching, which is the most difficult, due to the large "distance" between the macroscale and microscale physical parameters of models. There exist few liquids for which there are experimentally confirmed potentials of molecules interaction. However, as shown in [7, 14], it is too risky to use them for computing kinetic parameters of the respective mesoscopic fluid. Therefore, the iteration schemes similar to Schwarz's one should be applied. However, unlike in the heterogeneous models, the iterations can be done only for the first simulation. Computed parameters of the collisions operators can be applied for other simulations without iterations.

The problems of matching the physical parameters between different stages of cross-scale models truly require more theoretical investigations and numerical modelling. It is also a challenge for experimental physics. We must address the issues of how to measure not only macroscopic properties of fluid but also its microscopic parameters expressed by the coefficients in the fluid particle collision operators.

6. DISCUSSION

In this paper we present out ideas on a cross-scale computer model. This is based on the particle methods. In macroscopic fluid-dynamical turbulance one also employ similar ideas concerning direct numerical simulation (DNS) and large eddy simulation (LES) [9].

Unlike the heterogeneous approaches to the cross-scale computations, which couple particle and continuum models, the homogeneous model is presented. This main assumption is that the molecular dynamics dissipative particle dynamics (or fluid particle model) and smoothed particle hydrodynamics methods coupled together can simulate the physical system from the microscale through the mesoscale and then to the macroscale of tens of microns. The coupling factors for MD, DPD, FPM, SPH models are the notion of particle, particles interactions and the Newtonian laws of momentum conservation. The sole difference among them lies in the different forms of the collision operator. Thus, due to a physical paradigm used for different space and time scales, this model is homogeneous from the physical point of view.

This idea is also homogeneous from both computational and parallel implementation points of view. Very efficient MD parallel algorithms and systems, can be applied directly for coupled hierarchical MD-DPD-SPH approach. This homogeneous approach is different from the heterogeneous atomistic-continuum representation [10, 11, 22].

We have here attempted to estimate the optimal conditions of parallel realization of three models of the cross-scale computations. The minimal computational time, which is needed for simulation of systems consisting of N atoms, for these three models increases with N as $N^{8/7}$, while for pure MD simulation the time will grow as N^2 assuming that $O(N)$ forces calculation algorithm is used. Using relations derived in the paper, one can easily estimate the number of MD, DPD and SPH particles needed for efficient computer realization of the cross-scale computations. The relations obtained can be useful for matching the system scale to the suitable cross-scale model and to the computational power.

The problem of matching represents a challenge also for the particle based cross-scale model. The fluid particle model and Voronoi tessellation, proposed by Espanol in [7] are exciting new ideas for further study. Iteration schemes, which use macroscopic variables for fitting the collision operator coefficients of different particle models in the cross-scale computations, should be replaced by theoretical predictions and experimental constraints.

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References

[1] Alda, W., Dzwinel, W., Kitowski, J., Mościński, J., Pogoda, M. and Yuen, D. A. (1998). "Complex Fluid-Dynamical Phenomena modeled by Large-Scale Molecular Dynamics Simulation", *Computers in Physics*, **12**(6), will appear in Nov./Dec. issue.

[2] Beazley, D. M., Lomdahl, P. S., Gronbech-Jansen, N., Giles, R. and Tomayo, P. (1996). "Parallel Algorithms for Short Range Molecular Dynamics", In: *World Scientific's Annual Reviews of Computational Physics III*, World Scientific, pp. 119–175.

[3] Clementi, E., Chin, S., Corongiu, G., Detrich, J., Dupuis, M., Folsom, D., Lie, G. C., Logan, D., Meck, D. and Sonnad, V. (1986). "Large Scale Computations on Scalar, Vector and Parallel "Supercomputer" and Global ab initio Simulations with a Study on Liquid Water as an Example", IBM Technical Report, KGN 86 (Kingston, New York).

[4] Dzwinel, W., Alda, W., Kitowski, J., Moscinski, J., Wcislo, R. and Yuen, D. A. (1995). "Applications of Molecular Dynamics Method for Simulations in Macroscale", *Molecular Simulation*, **15**, 343–360.

[5] Dzwinel, W. (1997). "Virtual Particles and search for global minimum", *Future Generation Computer Systems*, **12**, 371–389.

[6] Dzwinel, W., Alda, W., Pogoda, M. and Yuen, D. A., "Turbulent Mixing in the Microscale", Physica D, submitted for publication (also in Minnesota Supercomputing Institute Research Report, UMSI 98/167, September 1998).

[7] Español, P. (1998). "Fluid Particle Model", *Physical Review E*, **57**(3), 2930–2948.

[8] Finn, R. (1996). "Exploring Materials in a Simulated World", *IBM Research*, **1**, 16–19.

[9] Galperin, B. and Orszag, S. A. (Eds.) (1993). Large Eddy Simulation of Complex Engineering and Geophysical Flows, Cambridge Univ. Press.

[10] Hadjiconstantinou, N. G. and Patera, A. T. (1997). "Heterogeneous atomistic-continuum representation for dense fluid systems", *Int. Journal of Modern Physics C*, **8**(4), 967–976.

[11] Hadjiconstantinou, N., Hybrid Atomistic-Continuum Formulations and the Moving Contact Line Problem, *Ph.D. Thesis*, Department of Mechanical Engineering, MIT, September 1998.

[12] Hoogerbrugge, P. J. and Koelman, J. M. V. A. (1992). "Simulating Micrscopic Hydrodynamic Phenomena with Dissipative particle Dynamics", *Europhysics Letters*, **19**(3), 155–160.

[13] Holian, B. L. and Ravelo, R. (1995). "Fracture Simulation Using Large-Scale Molecular Dynamics, *Phys. Rev. B.*, **51**(17), 11275–11285.

[14] Koplik, J. and Banavar, J. R. (1998). "Physics of Fluids at Low Reynolds Numbers–A Molecular Approach", *Computers in Physics*, **12**(5), 424–431.

[15] Libersky, L. D., Petschek, A. G., Carney, T. C., Hipp, J. R. and Allahdadi, F. A. (1993). "High Strain Lagrangian Hydrodynamic", *Journal of Computational Physics*, **109**(1), 67–73.

[16] Lomdahl, P. S. and Beazley, D. M. (1994). "State of the Art. Parallel Computing", *Los Alamos Science*, **22**, 44–57.

[17] Monaghan, J. J. (1992). "Smoothed Particle Hydrodynamics", *Annu. Rev. Astron. Astrophys.*, **30**(30), 543.

[18] Mościński, J., Alda, W., Bubak, M., Dzwinel, W., Kitowski, J., Pogoda, M. and Yuen, D. A. (1997). "Molecular Dynamics Simulation of Rayleigh-Taylor Instability", *Annual Reviews of Computational Physics V*, World Scientific, pp. 97–136.

[19] Novik, K. E. and Coveney, P. V. (1997). "Using Dissipative Particle Dynamics to Model Binary Immiscible Fluids", *International Journal of Modern Physics C*, **8**, 909–915.

[20] Ristow, G. H. (1994). "Granular dynamics: a review about recent molecular dynamics simulations of granular materials", *Annual Reviews of Computational Physics I*, World Scientific.

[21] Rothman, D. H. and Zaleski, S. (1994). "Lattice gas models of phase separation: interfaces, phase transitions, and multiphase flow", *Rev. of Mod. Phys.*, **66**(4), 1417–1479.

[22] Vashishta, P., "Multimilion Atom Molecular Dynamics Simulations of High Temperature Ceramics on Parallel Computers", Concurrent Computing Laboratory for Materials Simulations, Louisiana State University, http://www.cclms.lsu.edu.

[23] Yuen, D. A. and Rustad, J., Workshop on Computational Studies of Interfacial Phenomena: Nanoscale to Mesoscale, Pacific Northwest National Lab (PNNL), September 24–25, 1998 Richland, Washington, http://banzai. msi.umn.edu/mel/workshop.html

[24] *7th International Conference on the Discrete Simulation of Fluids*, University of Oxford, 14th–18th July 1998. http://www-thphys.physics.ox.ac.uk/users/Julia Yeomans/conf/prong 1. html