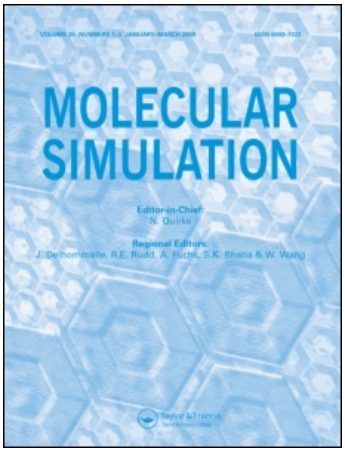

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Macro-Scale Simulations Using Molecular Dynamics Method

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MACRO-SCALE SIMULATIONS USING MOLECULAR DYNAMICS METHOD

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In this paper a new approach to the simulation of shock phenomena is presented. The discrete model of matter description is applied. The system representing a physical object consists of a large number of mutually interacting "particles" ($N \sim 10^5 +$). The model can be used as an alternative to the model of continuous medium described by the sets of partial differential equations solved numerically, using for example the finite elements method. For the presented method, the time evolution of the particle system is described by the Newtonian laws of motion. Application of this approach for simulation of stress and shock phenomena is discussed. The results of selected simulations of the penetration mechanics, explosion and squashing are presented.

KEY WORDS: Particles method, macroscale simulation, classical hydrodynamics, large scale computations.

1 INTRODUCTION

Rapid increase of computational power of modern computers results in development of computational methods for solving problems previously too complex for studying. Investigations of deterministic chaos and the dilemma of order and disorder in nature, being the effect of nonlinearity and instability of the real world [1], can be the interesting examples. Techniques based on fractals [2] and cellular automata (lattice gas, LG) concepts [3] are illustrations of two different approaches to the simulation of such phenomena. The first one is used for simulation of events suffering from lack of classical mathematical models. They are for example: crystal growth, aggregation of adsorption layers, electrical discharge and growth of the biological forms like flowers and trees (L-systems [4]). The second method expresses the tendency of maximal simplification and compression of the classical

mathematical models (described usually by the partial differential equations, PDE) to several rules applied to the particles in the system evolving in pseudo-time on the mesh. Interesting results of this method applied for fluid flow simulations have been obtained [3].

Applications of the classical model of continuous medium, described by the Navier-Stokes equations, are inherently difficult in some cases, for example when used for description of turbulent flows of compressible medium in the case of breaking the assumption of quasi-stationarity of physical processes in the differential volume.

Using the lattice gas model and simplification of the assumptions referring to the simulated system, let us overcome some limitations of the classical approach [3]. However, the fluid simulation by the lattice gas model produces other problems:

- numerical problems concerning computations on the mesh (anisotropy of solutions, difficulties in definition of boundaries of complicated shapes, filtering of short wave solutions components, etc.),
- problems concerning 3D simulation,
- unitary mass, time and velocity units limit considerably the scope and importance of LG applications and causes that the results obtained are difficult for interpretation.

Another method is needed, which in spite of simplification of the classical approach will preserve it's physical meaning for the phenomena well specified by the previous model and will constitute its extrapolation for domains where it fails.

Molecular Dynamics (MD) method which is used for wide range of particle models from molecules to galaxies [5,6], due to increase of the computational power enhances it's area on continuous and non equilibrium systems. In papers [7–11] results of standard hydrodynamic problems solved using MD simulation for large number of particles (10^5–10^6) have been presented. The qualitative agreement with the Navier-Stokes solutions is achieved and a few quantitative results concerning Reynolds numbers values for micro flows versus obstacles are reported. These results obtained for micro-world, some earlier experiences with the PIC method application for macro-scale compressible fluid flows and the results of plastic deformation simulations using particles model published by the authors in [12–14], suggest that the MD method could be used for simulations of macro scale systems by simple rescaling the Newtonian equations of motion and redefinition of the basic notions of this method: particle (atom or molecule) properties and potential. Using the discrete model, the assumptions of quasi-stationarity in differential volumes, continuity of all parameters in the domain described by the model and linearity of equations are not valid any longer. There are no problems with discretization of the space using the regular mesh or finite elements since the MD method does not use any mesh. The grid size determines the minimum wave length acceptable by the solution, cutting off those being below this limit or producing artifacts like superfluous numerical diffusion. The ability of unlimited concentration of the particles in the areas of excessive compression, in the case of the particles approach, can reduce this

effect. These advantages recommend the usage of the MD method for stress and shock phenomena simulation as supersonic flows, shock waves, collisions, squashing [12], perforation [13], tearing off [14], etc. It constitutes an interesting alternative to the investigations of material properties when the assumption of system continuity is broken.

In some sense the smoothed particle hydrodynamics (SPH) [15, 16], originally almost exclusively used for astrophysical applications is similar to MD approach. It does not also apply any mesh and can be treated as a kind of interpretation of the continuous approach.

In this paper we present adaptation of the MD method for macro scale phenomena simulation with the assumptions concerning interpretation of the quasi-particle and quasi-potential ideas. Similarity of the MD model with the Navier-Stokes equations is shown. Discussion of the results obtained with different number of particles in the system is presented. Selected instances of the simulation of penetration mechanism, squashing the plastic object, explosion and tearing off the flat object are shown and discussed.

2 PARTICLES METHOD – BRIEF DESCRIPTION

2.1 Simulation of shock phenomena with continuous and discrete models

The Hard Spheres model and Particle in Cell (PIC) model with collisions were amongst the first computational methods which use particles approach for solving problems in hydrodynamics. Because the particles in typical fluid yield collisions with the neighbouring particles in very short time scale ($\sim 10^{-14}$ sec.) in comparison with the macro events, they do not conserve their energies and momenta during simulation, dissipating them between other particles in the vicinity. Thermal quasi-equilibrium is achieved in the same short time scale.

The PIC technique uses the algorithm of particle motion based on the Newtonian laws with the time dependent equations of the continuous fluid. The crucial point of this technique is that the new momenta and energies of particles obtained in the following time steps are computed from the mesh variables but not from the previous values for the particles. Disadvantage of this method is non-central finite differences approach, which produces considerable large numerical diffusion and numerical problems with computation on the mesh. Nevertheless, this model was used successfully for supersonic flows simulation, *e.g.* bullet-target collisions [17].

The smoothed particle hydrodynamics (SPH) represents another method for solution of Navier-Stokes equations. Like the PIC method, it is the pure Lagrangian particles method. Unlike the former one, however, the SPH technique uses no underlying grid. Absence of the mesh substituted by the interacting particles separated by the distances means that large deformations can be computed without difficulty. The foundation of SPH is the interpolation theory. Computationally, information is known only at discrete points – particles. The functions are evaluated using their values at the discrete points and an interpolation kernel. The SPH

method has been succesfully used for astrophysical applications. In recent publications [15, 16] the simulation results of the problems requiring the entire stress tensor as the Noh's implosion, the cylinder impact test and the penetration mechanics were presented. However, this technique constitutes a realization of the classical Navier-Stokes model. In this sense SPH does not propose any new physical model which could let one to simulate the phenomena out of scope of the Navier-Stokes approach. The numerical problems similar to those for the PIC method, *e.g.* large unphysical oscillations near shocks and non-coherency of the computational model are still present (the problems are partly caused by the ambiguous definition of density, *i.e.*, the particles density is represented by the variable which value is computed by the separate equation, though it is determined by the particles actual positions in space computed using the equation of motion). The way to overcome them is the same both for SPH and for PIC techniques. For example, the numerical oscillations are damped using the artificial viscosity factor. On the other hand the SPH approach is very valuable for MD technique principles foundation. It may constitute the link between pure particles oriented method presented in this paper and the classical hydrodynamic approach. The convergence of these two methods are under investigations and the paper presented constitutes the authors contribution to this discussion.

2.2 *Assumptions of the particle-particle model*

Unlike the PIC and SPH methods, the particle-particle MD model is defined entirely by the properties of particles and the way they interact. The particles are responsible for energy and momentum transport according to the rules of conservation. The basic features of the model are as follows:

- The system consists of N particles.
- Each particle is characterized by the mass, momentum and energy computed during the simulation.
- The way the particles interact is defined by the model of potential. In the case presented, two body, pair potential $\phi(r_{ij})$ is used, for particles i and j.
- Gradient of the total interaction potential for all particles in the vicinity of a single particle i, $-\nabla\Phi_i$, represents the force acting on the particle i.
- Particles motion is described by the Newtonian equations.

The MD simulation was applied previously for computations of different parameters of gases, fluids and solids (diffusion coefficient, specific heat and resistivity etc.) and for investigations of materials microscopic features during phase transition or composition changes. However, the simulations of large ensembles of particles ($N \sim 10^5$–10^6) using MD for micro-flows [7–9] and the Benard convection [10, 11] extend the application area of this method. The obtained results confirm that the same phenomena as: turbulence, convection and advection patterns can be observed in macro- and micro- scales. The application of the MD method as the microscope for observation of eddy formation in macro scale fluid flows simulations are also under consideration [7–9].

For the mesh methods, decrease of the grid size Δ is limited by technical reasons implied by the computational power and memory. However, for small Δ its further decrease is unprofitable and does not give any additional improvement of the results. We expect that this concerns the particle approach as well. As the increasing number of simulated particles corresponds to decrease of the grid size for the mesh techniques, we expect that for large systems further increase of number of particles does not considerably influence the system behaviour.

Main problems concerning both approaches are:

- Do Δ decrease for the mesh methods and particle ensemble size increase for MD approach converge to the same results in the hypothetic common area of applicability of these two models, i.e., for example fluid flows simulation?
- What differences and similarities characterise micro and macro fluids?
- Is it possible to simulate the macro world phenomena using relatively small particles ensembles?
- What additional benefits can we derive using the particle approach on the borders or out of the scope of applicability domain of the traditional mesh techniques?

Although we are not able at present to give ultimate answers for these questions we point out some interesting results already obtained and join discussion about the advantages and disadvantages of the presented method.

3 COMPARISON OF MATHEMATICAL MODELS OF THE PARTICLE METHOD AND THE CONTINUOUS METHOD

Two mathematical models, for Lagrange and for the particles systems are compared below.

Hydrodynamics equations		MD equations	
$\frac{d\rho}{dt} = -\rho\nabla\cdot\vec{v}$	(1)	$\frac{d\vec{r}_i}{dt} = \vec{v}_i$	(4)
$\rho\frac{d\vec{v}}{dt} = -\nabla p$	(2)	$m\frac{d\vec{v}_i}{dt} = -\nabla\Phi_i$	(5)
$\rho\frac{d\varepsilon}{dt} = -p\nabla\cdot\vec{v}$	(3)	$\Phi_i = \sum_{j\in S}\phi_{ij}, \quad \phi_{ij} = \phi(r_{ij})$	(6)
$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{v}\cdot\nabla$	(7)	$r_{ij} = \sqrt{(\vec{r}_i - \vec{r}_j)\cdot(\vec{r}_i - \vec{r}_j)}$	(9)
$\varepsilon = \frac{p}{\rho(\gamma - 1)}$ specific energy	(8)	$\phi(r_{ij})$ – pair potential for i and j	

In (6) summation is taken for the set of neighbors, S, of the particle i. $\phi(r_{ij}) = 0$ for $r_{ij} < R_{cut}$, where R_{cut} is the potential cutoff radius.

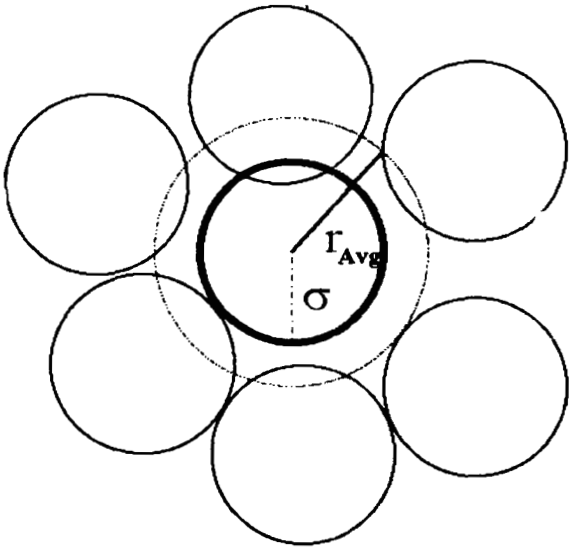

Figure 1 Average distance, r_{Avg}, to the nearest neighbors of chosen particle. σ denotes the distance, for which the repulsive part of the potential dominates.

3.1 Equation of mass continuity

Let us define the average distance $r_{Avg,i}$ to the nearest neighbors of particle i as shown in Figure 1.

Density definition in differential volume δV (for 2-D case) is as follows:

$$V \cdot \rho = m = \text{const} \tag{10}$$

where

$$V = \pi \cdot r_{Avg}^2 \tag{11}$$

m – particle mass and $r_{Avg} = \langle r_{Avg,i} \rangle$ (where $\langle\ \rangle$ is average in δV differential volume).

From equations (4) and (9) we obtain:

$$\frac{dr_{ij}}{dt} = \frac{1}{r_{ij}} (\vec{r_i} - \vec{r_j}) \cdot (\vec{v_i} - \vec{v_j}) \tag{12}$$

$$\frac{dr_{ij}}{dt} = \frac{1}{r_{ij}} \left[(x_i - x_j)^2, (y_i - y_j)^2 \right] \cdot \left[\frac{(v_i - v_j)_x}{(x_i - x_j)}, \frac{(v_i - v_j)_y}{(y_i - y_j)} \right] \tag{13}$$

Assuming that, in the differential volume δV, particles move in the field with the same, constant velocity gradient, $\nabla \vec{v}$ we get:

$$\frac{dr_{Avg}}{dt} = \left\langle \left[\frac{(x_i - x_j)^2}{r_{ij}}, \frac{(y_i - y_j)^2}{r_{ij}} \right] \right\rangle \cdot \tilde{\nabla} \vec{v}, \quad \text{where } \tilde{\nabla} \vec{v} = \left[\frac{\delta v_x}{\delta x}, \frac{\delta v_y}{\delta y} \right] \tag{14}$$

and from density formula:

$$\frac{d\rho}{dt} = -\rho\frac{2}{r_{\text{Avg}}}\left\langle\left[\frac{(x_i-x_j)^2}{r_{ij}}, \frac{(y_i-y_j)^2}{r_{ij}}\right]\right\rangle\cdot\tilde{\nabla}\vec{v} \tag{15}$$

In the case of continuous model, *i.e.* when the isotropic field of particles is assumed in δV the following approximation is considered:

$$\left\langle\left[\frac{(x_i-x_j)^2}{r_{ij}}, \frac{(y_i-y_j)^2}{r_{ij}}\right]\right\rangle \approx \frac{r_{\text{Avg}}}{2}\cdot\vec{e}, \quad \text{where } \vec{e} = [1,1] \tag{16}$$

We finally obtain:

$$\frac{d\rho}{dt} = -\rho\vec{e}\cdot\tilde{\nabla}\vec{v} = \rho\nabla\cdot\vec{v} \tag{17}$$

The particle model is then more sensitive for object anisotropy in micro-scale, especially in dense liquids and solids. The best results in the simulation of hydrodynamic phenomena in micro-scale have been obtained for relative densities of 0.7–0.8 [7–9], when the local structure is typical for *random close packing*. Thus the expression in brackets $\langle\,\rangle$ in Eq.(15) is equal to vector $\vec{e}$.

3.2 *Equation of momentum stream conservation*

The form of equation (5) of the particle momentum is similar to the equation of momentum conservation (2). It is, however, more general. One cannot identify average potential $\Phi = \langle\Phi_i\rangle/2m$ (Φ_i – potential energy of particle i) in volume δV with pressure p in momentum continuity equation although gradients of these quantities are responsible for the change of both particle and fluid element velocities in time. This is because of different interpretation of gradient in both cases. Gradient of Φ_i is actually the sum of gradients of two-particle potentials and differs from gradient calculated as a difference of these values for neighbour particles. According to density definition (10, 11) and equation (5) we receive:

$$\rho\frac{d\vec{v}}{dt} = -\nabla(2\Phi\cdot\rho) - 4\Phi\cdot\rho\nabla\ln(r_{\text{Avg}}) \tag{18}$$

Assuming that the system is isotropic and integrating equation (14) from 0 to the average collision frequency τ (with the constant gradient between collisions) we obtain:

$$\rho\frac{d\vec{v}}{dt} = -\nabla(2\Phi\cdot\rho) - 2\phi\tau\rho\nabla(\nabla\cdot\vec{v}) \tag{19}$$

As one can see, μ coefficient defined as $\mu = 2\Phi\tau\rho$ may be treated as viscosity. This value is dependent (in the macroscopic case) on the collision frequency, density, particle mass and the potential. In Eq. (19) only the part of the Navier-Stokes viscosity tensor $\mathbf{U} = -(\nabla\cdot\vec{v})\mathbf{I}$ (for 2D case) concerning compressibility, is present.

There are no diffusion elements $(\nabla\vec{v}+(\nabla\vec{v})^T)$, however, since for the simulations of shock phenomena in dense liquids momentum diffusion does not follow deformation phenomena and momentum transport via sound wave. In the microscale simulation of shock phenomena, the viscosity element grows automatically in the impact area, because of growth of Φ and $\tau\cdot\rho$. As Φ grows fast with density for dense systems, energy of short waves is changed mainly into the potential energy. In the macroscopic case, due to difficulties in viscosity definition as a function of local parameters (*e.g.*, density, temperature and pressure) artificial viscosity proportional to modulus of velocity gradient is assumed to eliminate oscillations on the grid. This interferes with physical model and creates additional numerical diffusion.

3.3 *Equation of energy conservation*

Let us find changes of Φ_i in time:

$$\frac{d\Phi_i}{dt}=\sum_{j=1}^{S}\frac{d\phi_{ij}}{dr_{ij}}\frac{1}{r_{ij}}[(x_i-x_j)^2,(y_i-y_j)^2]\cdot\left[\frac{(v_i-v_j)_x}{(x_i-x_j)},\frac{(v_i-v_j)_y}{(y_i-y_j)}\right] \tag{21}$$

Assuming that velocity gradient is constant in differential volume δV, the system is equilibrated in δV and $\sum_{i\in\delta V}\Phi_i/2=\Phi_T$ and $\Phi_T/m=\Phi$. With summation of Eq. (20) over particles in δV we obtain:

$$\rho\frac{d\Phi}{dt}=-\left(-\Phi_T+\left(\frac{1}{2}\sum_{i,j<i}f_{ij}r_{ij}+E_K\right)\right)\Big/\delta V\cdot\nabla\cdot\vec{v} \tag{21}$$

The equation is obtained with assumption that the total energy in δV is constant and equal to 0, *i.e.*, $\Phi_T=-E_P=E_K$ where E_P and E_K the potential and kinetic energies in δV. Assuming that $p=(1/2\sum_{i,j<i}f_{ij}r_{ij}+E_K)/\delta V$ in 2-D space (p-pressure) we get:

$$\rho\frac{d\Phi}{dt}=-p\nabla\cdot\vec{v}+\rho\Phi\nabla\cdot\vec{v} \tag{22}$$

Taking in Eq. (18) $p=2\Phi\rho$ as the pressure equivalent in microscale (having in mind, however, a certain incompatibility of these quantities in micro- and macroscale, as described in 3.2), and internal energy $\varepsilon=2\Phi=p/\rho$ for adiabatic process in 2-D, we finally obtain that:

$$\rho\frac{d\varepsilon}{dt}=-p\nabla\cdot\vec{v} \tag{23}$$

what agrees with (3).

Hydrodynamic phenomena simulated in microscale [7–9] have been obtained with relative density 0.7–0.8 or higher and with the flow velocity being a fraction of the Mach number. In these conditions the liquid is weakly compressible and the energy fluctuations do not interfere with the simulated process. Too low Reynold numbers obtained for subsequent phases of eddies formation [7] can result from the difference between density fluctuations in experiment and computer simulation.

4 PARTICLE-PARTICLE METHOD IN MACRO-SCALE PLASTIC DEFORMATION SIMULATIONS

Application of the "particle fluid" and description of the system dynamics directly by the Newton equations enables:

- usage of the well known and well numerically defined simple, homogeneous mathematical model,
- taking into account local anisotropy of the system, thus examining the influence of deformations on material properties of the system (see also section 3.1),
- unconstrained simulation of shock phenomena with no corrections in the model (see section 3.2),
- relation of all material properties to the particles and their interactions.

Relation of all physical properties to the particles, solves a lot of numerical problems.

- easy simulation of discontinuities of the system,
- absence of the grid enables self-adaptation of the system according to its physical nature,
- artificial loss of density on the boundaries can be avoided,
- some numerical difficulties concerning complicated boundary conditions can be eliminated.

By changing definitions of the particles and the potential, as well as by simple rescaling the equations of motion, the particle model may be applied for the description of shock phenomena in dense liquids and solids in macro-scale.

Assumptions concerning the change of interpretation are as follows:

1. Macroscopic object is divided into N elements (quasi-particles).
2. Quasi-particles are large enough to interact only with short range potential (described by quasi potential) and small enough that local fluctuations do not change the object shape.
3. System evolution is represented by the Newtonian equations.

The above assumptions need rescaling of the equations of motion. Using the *leap-frog* scheme [18], Eqs. (4, 5) can be expressed in the discrete form:

$$\vec{v}_i^{\,n+1/2} = \vec{v}_i^{\,n-1/2} - \frac{1}{m_l}\sum_{j\in s} f_{ij}^n \left(\frac{\sigma_{lk}}{r_{ij}^n}\right)\Delta\vec{r}_{ij}^{\,n}\cdot\Delta t \tag{24}$$

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \vec{v}_i^{\,n+1/2}\,\Delta t \tag{25}$$

where n is a timestep number of Δt, l and k represent the kind of particle i and j respectively.

For the short-range 6/12 Lennard–Jones pair potential

$$f_{ij}^n = \begin{cases} \dfrac{24\varepsilon_{ij}}{\sigma_{ij}^2}\left[\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^8 - 2\left(\dfrac{\sigma_{ij}}{r_{ij}}\right)^{14}\right] & \text{for} \quad r_{ij} < R_{\text{cut}} \\ 0 & \text{for} \quad r_{ij} \geqslant R_{\text{cut}} \end{cases} \tag{26}$$

To show the rescaling to macroscale let us assume that the system consists of one kind of particles only and they are distributed according to a statistics:

$$g\left(\frac{mv^2}{k_B T}\right) \tag{27}$$

$g(\cdot)$ can be the Maxwell distribution for the isolated system. Let $g(v_T) = \max$ for

$$v_T = \gamma\sqrt{\frac{k_B T}{m}} \tag{28}$$

where T is average of temperature and k_B – Boltzmann constant.

Rescaling velocities in Eqs. (24, 25) to v_T and coordinates to σ one gets:

$$\vec{V}_i^{\,n+1/2} = \vec{V}_i^{\,n-1/2} - \frac{24\varepsilon}{\gamma^2 \kappa T K}\sum_{j\in S} F_{ij}^n\left(\frac{1}{R_{ij}^n}\right)\Delta\vec{R}_{ij}^n\Delta\tau \tag{29}$$

$$\vec{R}_i^{\,n+1} = \vec{R}_i^{\,n} + \vec{V}_i^{\,n+1/2}\Delta\tau \tag{30}$$

where

$$\vec{V} = \frac{\vec{v}}{v_T}, \quad \vec{R} = \frac{\vec{r}}{\sigma}, \quad \Delta\tau = \frac{\Delta t}{\tau}, \quad \tau = \frac{\sigma}{v_T}, \quad \kappa = \frac{M}{m}$$

$F(\cdot)$ is obtained from $f(\cdot)$, τ – time needed for passing distance σ with velocity v_T, κ – scaling factor: M is the particle mass in the rescaled system and m in micro-scale. Dimensionless timestep $\Delta\tau = \text{const}$ is chosen due to numerical stability of solving of Eqs. (29, 30). The equations do not depend on the number of (quasi-) particles nor system temperature since changes in κ and in T can be compensated by modification of the potential well, ε.

5 PARAMETRIC INVESTIGATIONS FOR THE PARTICLE MODEL

Dependency of the size of the particle model (*i.e.* of the number of particles) on the results of the computer experiment has been investigated for a 2-D object (a slab) hit by a tool. In Figure 2 the systems with 6×10^3, 2.5×10^4 and 1.1×10^5 particles are compared for similar position of the tool. Tool velocity is set proportional to $N^{1/D}$.

The following facts should be mentioned:

- although the physical conditions for the experiments are identical (except the system size) each case in Figure 2 represents a different physical system,
- transients of squeeze are similar in every case.

What does K-times increase of the system mean? It means that each side of the system is increased $K^{1/D}$ times (where D is the system dimensionality) keeping the same "microscopic" characteristics. So the ratio of the potential range to the characteristic system length is decreased in $K^{1/D}$. Using the two body Lennard-Jones potential, the system is unstable for small number of particles. Boundary discontinuity results in fluctuations in the system due to high diffusion coefficient; thus asymmetry in the transients is observed (see Fig. 2 left). System increase effects in fluctuation

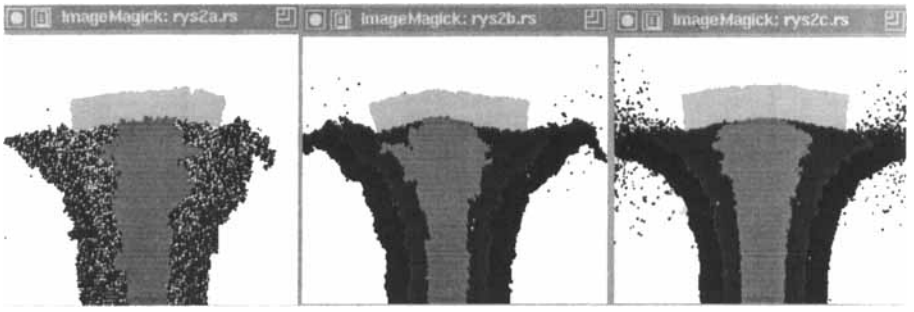

Figure 2 Fast squeeze of the slab consisting of different number of particles (from left): $6 \times 10^3, 2.5 \times 10^4$ and 1.1×10^5.

decrease, more symmetric and smooth transients and in higher brittleness [13]. In Figure 2 the transients are similar in spite of the great difference in number of particles. As it is shown the system increase shows more details too. On the other hand complete elimination of fluctuations is not desirable – results from FEM simulations seem to be "too symmetrical" usually [19]. Influence of the fluctuations can be shown comparing two particle systems run on different machines (see Fig. 3) – the transients are entirely different. The brittleness can be adjusted also by modifying the potential parameters and the system initial temperature. For example, influence of the temperature on the penetration mechanism is shown in Figure 4.

For the small-size systems with spherical (too ideal), pair potential, statistical fluctuations turn out to be the main drawback of the presented method. This is especially valid for simulation of phenomena, for which the group velocity is much smaller than the average velocity in thermal equilibrium. This is shown in Figure 5, where velocity distribution is presented for different velocities of the tool. (Averages in cells are calculated with the PICASSO code.)

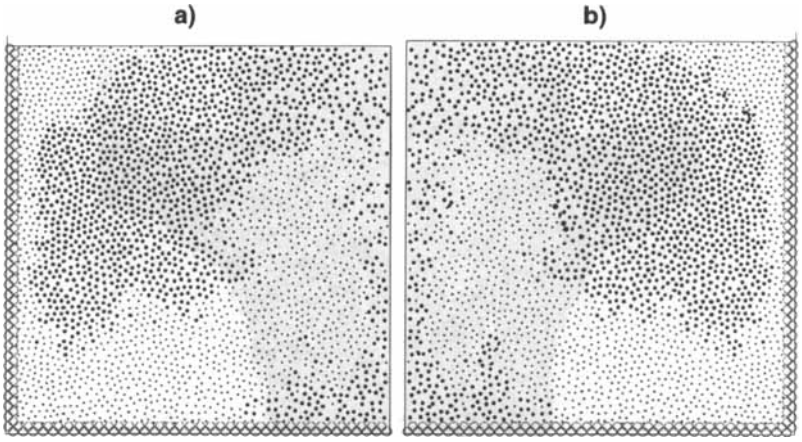

Figure 3 Transients in the same time for identical physical conditions. The heavy particles above and the lighter ones below. The direction of mixing depends on initial fluctuations.

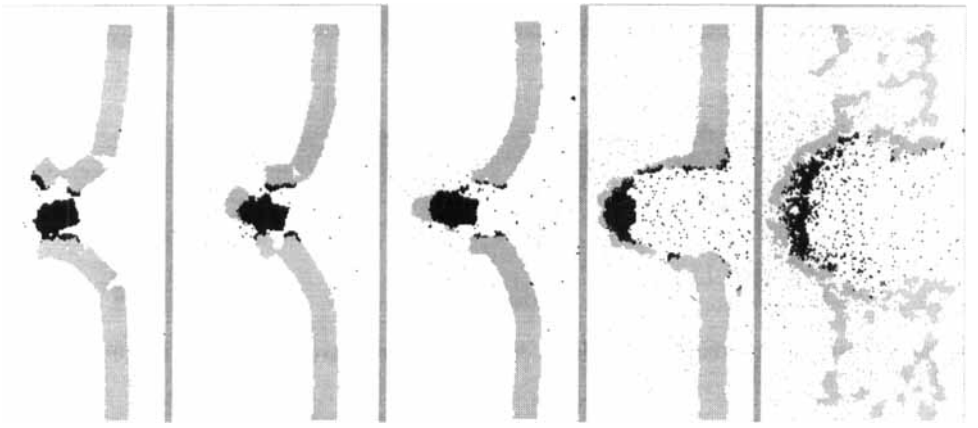

Figure 4 Sample simulation snapshots for the simulation with the particle method concerning object penetration for different temperatures of the system (from left): $T = 0.2, 14, 28, 56, 84$ (arbitrary units).

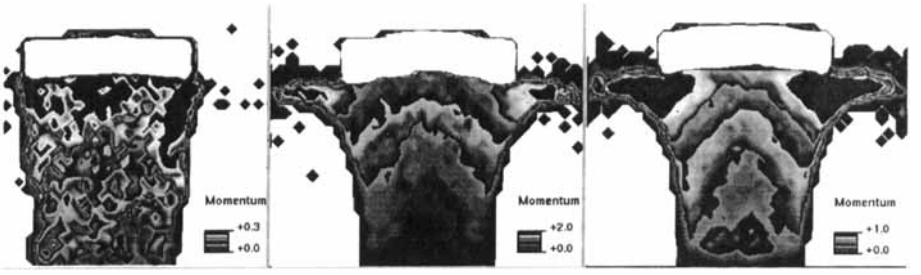

Figure 5 Squeeze of the slab for different tool velocities (from left): $v, 2v, 4v$.

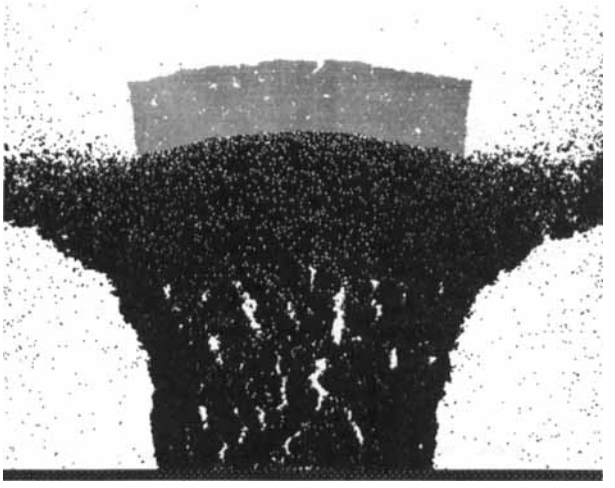

Figure 6 Squeeze of the slab – the crack effect obtained in the central part.

For higher velocities the velocity distributions are much more smooth; this support the assumption on constant velocity gradient in neighbourhood of the particle (Eqs. 13, 18, 20). For the tool optimization distributions of temperature, velocity, density and pressure could be used for tool optimization. For the shock phenomena, high gradient with constant direction of the velocity field causes some additional geometric anisotropy of the velocity divergence operator (see (15) and (17)) and results in longitudinal cracks (cf. Fig. 6). For the mechanical penetration or explosion (see Figs. 7 and 8) mechanical effects are yet more destructive. In the continuous medium model such results are difficult if not impossible to be obtained due to the symmetry of the velocity divergence operator, equal to zero for the incompressible medium.

It should be mentioned that some macroscopic simulations can be performed for the number of particles $N \sim 10^3$. In [20] we presented a case study for the falling sheet in the gravitational field. For 400 particles the system represents the sheet

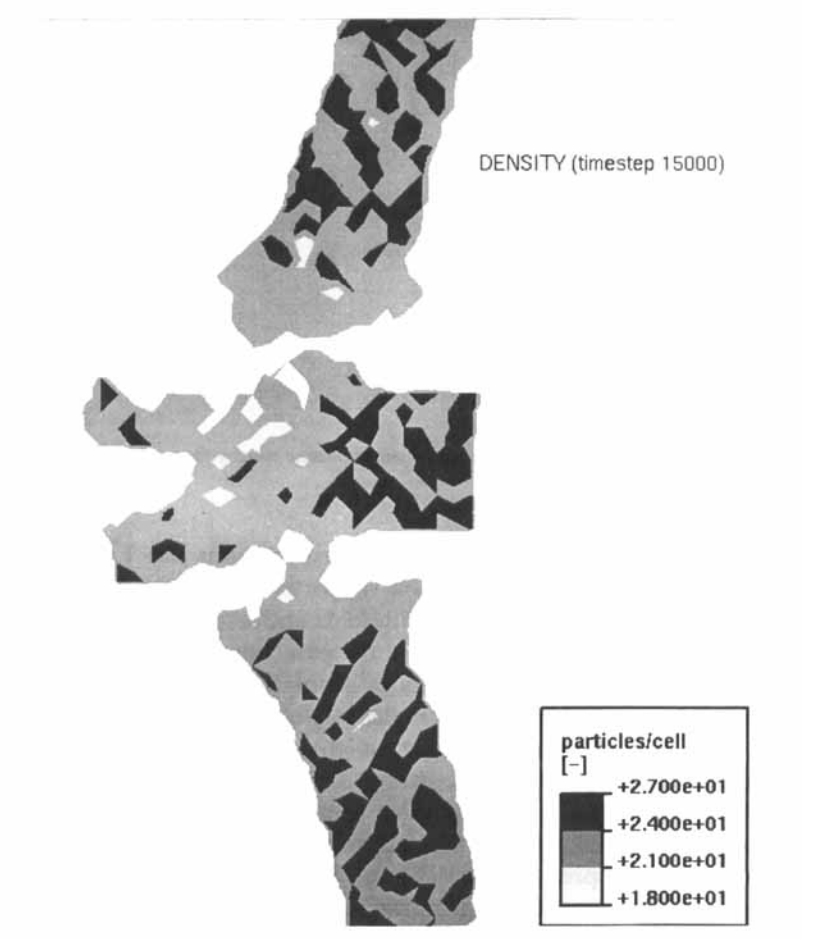

Figure 7 Density distribution in the wall and the object representing shearing forces.

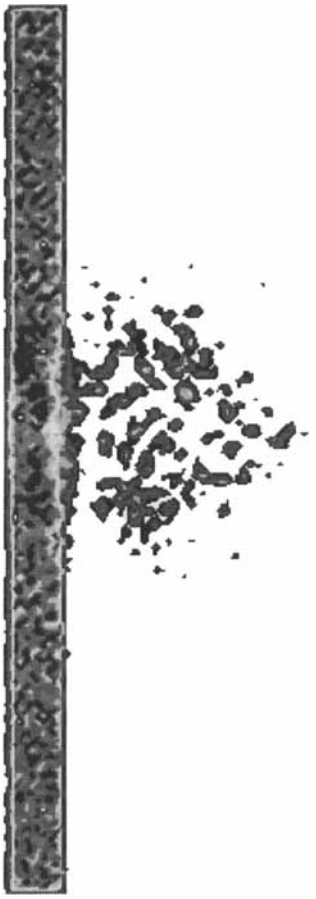

Figure 8 A snapshot for the object explosion nearby the wall.

dynamics in good quality according to human expectations (see Fig. 9). This case links the computer graphics with simulation via particles. Increase of the number of particles makes the sheet more unstable with folds and wrinkles (the sheet becomes more soft). Another example is animation of the parachute movement (rather artificial at the moment – cf. Fig. 10). In the both simulations the only external forces have been adopted (gravitational for example), neglecting the air resistance.

For the sheet and parachute simulation the harmonic potential has been chosen (with the range concerning the nearest neighbours only) with the viscosity proportional to the velocity. For the other simulations the 6/12 Lennard-Jones potential has been adopted, for which ε and σ as well as the cutoff radius R_{cut} are assumed. The first one represents the depth of the potential well, thus the material hardness (for solids) or compressibility (for gases).

Brittleness can be modelled with σ and R_{cut} parameters [19]. For the system with one-kind particles, change in the mass is equivalent in change of the depth of the

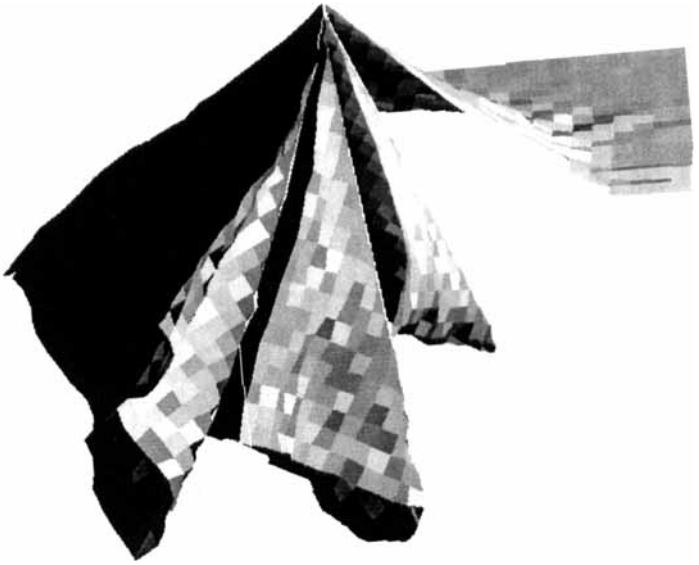

Figure 9 Snapshots for the falling sheet in the gravitational field.

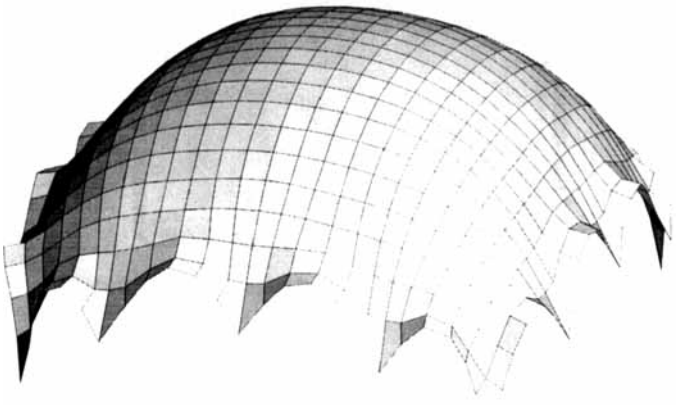

Figure 10 Example of the parachute movement.

potential well (see Eq. 29) for the assumed temperature. For mixtures, combination of the parameters enables one to perform more flexible studies.

Difficulties in determination of local pressure and local temperature seem to be one of the drawback of the method. Using the virial theorem, one gets the high pressure statistical fluctuations. Taking Eq. (23) for determination of the pressure distribution needs still more theoretical work. For temperature distribution one has to eliminate thermal fluctuations. This could be done using arbitrary units for determination of averages in the cells.

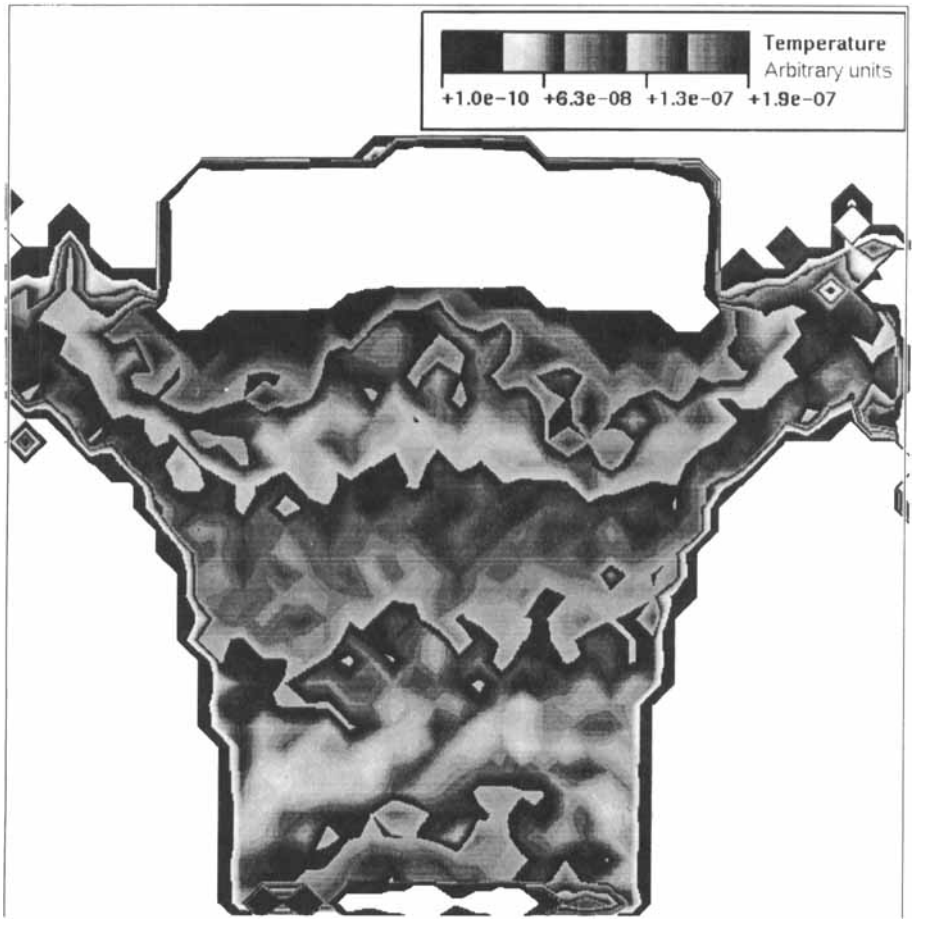

Figure 11 Temperature distribution in the squeezed object. Arbitrary units.

In Figure 11 we present the temperature distribution for the squeeze object with the method proposed. To some extend it could be accepted.

In Figure 12 results from the computer experiments concerning object penetration through the soft and hard walls are presented. The layers differ in ε values. Such experiments are required due to the lack of a direct link between micro- and macro-parameters of the medium.

The calculations were done using simulation programs written in C language [14], [20], [21–24], based on linked list approach [25, 26]. Two graphical interfaces to the programs were applied [27]–[29]. The simulations were run on the workstations (IBM RS/6000-320 and 520H, HP 9000/720 and SUN SPARCstation 2). Parallel and distributed versions of the programs were also used and run on the cluster of workstations.

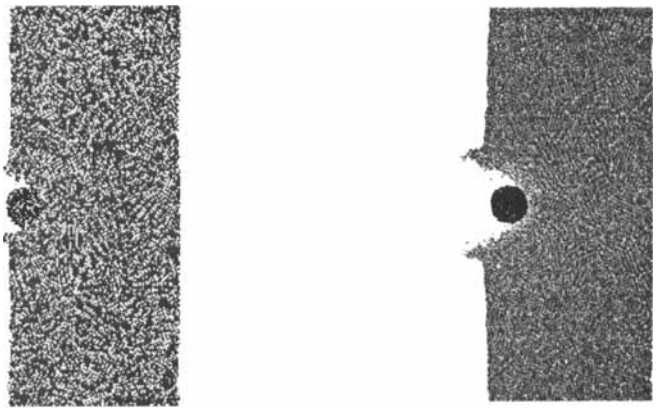

Figure 12 Snapshots for the object penetration through the wall with different hardness defined by different ε. ε – left, 2ε – right.

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