

SIMULATION OF FLUID FLOW WITH INTERACTING PARTICLES

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Abstract: In the paper a method for modeling flows in the presence of interacting particles is briefly presented. The method is based on merging classical, continuous approach of numerical solution of Navier-Stokes equations on the 2D mesh with discrete particles interacting with the fluid and among themselves by means of central and friction forces. Several sample simulations have been described presenting the flow through porous medium and convection flow driven by sedimentation.

Keywords: computational fluid dynamics, particle methods, porous medium, sedimentation

1. Introduction

In many applications of fluid mechanics, geology, biology and chemistry there exist systems consisting of particles suspended in fluid or gas. Let us mention just a few of many examples [1]:

1. Processes of sedimentation and mixing in the presence of sediment which occur in water reservoirs supplied by rivers carrying sand.

2. Geological processes in which motion of liquid magma takes place in the presence of solid suspended matter.
3. Flow in hydraulic and pneumatic pipes with sedimentation of impurities.
4. Flow of blood in capillary vessels.

Immobilization of particles may be used as a model of porous medium. The presence of particles in the fluid, assuming their high density, changes significantly the character of the flow, compared to the pure liquid so the classical approach based on Navier-Stokes equations is no longer valid. Despite the complex nature of the mentioned process there are relatively simple models, which enable to solve the above phenomena, at least for small values of Reynolds number.

The goal of the presented work is the description of two-phase flow model, suitable for computer experiment concerning flow through porous medium and/or sedimentation. One phase is a liquid modeled with Navier-Stokes equations, while the other is represented by moving or non-moving particles. In order to implement the model, *Finite Element Method* (FEM) has been applied for the fluid flow. The second, particle phase has been introduced in the manner similar to those used in particle methods such as molecular and granular dynamics.

The idea for coexistence of continuous and particle approach in this paper is mainly based on works of Schwarzer *et al.* [2–4], however new elements have been added to the method and original simulations have been performed. The *Finite Difference Method* used by Schwarzer has been replaced by *Finite Elements* in order to increase the flexibility of boundary conditions. The particle-particle interaction scheme has been accelerated by applying fast algorithms extracted from *Molecular Dynamics* (MD) method. The method is valid in both 3D and 2D system, however the authors decided to limit themselves to 2D models only, mainly due to limitations in computer power.

Two-phase flow, which is an important scientific and technological task, has been intensively investigated using other approaches as well. Let us mention here similar methods developed by Hu *et al.* [5], Johnson and Tezduyar [6, 7], and Glowinski *et al.* [8, 9]. The above, highly advanced methods, base on precise calculation of particle-fluid interactions, and thus need remeshing in every step in which a particle is moved.

Completely different approaches often used for flows through porous medium problems, based on particle representation only, are such methods as: *Cellular Automata* [10], *Lattice Gas* [11, 12] and *Lattice Boltzmann Gas* [13, 14].

2. Basic elements of the model

2.1. Description of the computer experiment

The model of the computer experiment assumes two phase flow through porous medium. The fluid flow is calculated using Navier-Stokes and continuity equations. We assume stationary, laminar flow of Newtonian incompressible, viscous fluid for small values of Reynolds number.

The simulation consists of subsequent time steps for which stationary Navier-Stokes equations are solved. The dynamics of the system is modified due to particles, which move according to the Newton equations and their distribution is changed in every time step.

Boundary conditions are kept constant during the entire simulation and no free fluid surface is allowed. The particles are completely dipped in the fluid. Boundary conditions

are periodic at the source and the outflow of the fluid, while reflection walls are applied along the flow. Particles reflect from the walls without energy dissipation.

Two types of particles are allowed: immobile and/or moving along the flow stream or due to gravity force. Both types are treated equally in their interactions with fluid, except that unmovable particles keep constant positions and zero velocities.

Every particle interacts with the fluid locally, *i.e.* in the element in which it is placed. In the similar way the fluid acts on the particle with the reaction force and additionally with the lubrication force. Local interaction means that the particle has to be enclosed completely in a single element. However it is possible to introduce larger obstacles built up of several particles.

Particles interact with each other with visco-elastic forces. All the particles have the same density, mass and other physical parameters.

2.2. The algorithm

Initial calculations are done before the first step of simulation is started. The main parameters of the flow, such as vertical and horizontal velocities, as well as the pressure, are initially calculated in the absence of particles, with constant boundary conditions, using FEM method. In the next step, the particles are included. The forces between particles and fluid are calculated and considering these interactions the FEM is recalculated.

From this moment two phases are repeated alternately. The first one is the dynamics of particles performed in, what can be called, molecular dynamics (MD) steps which are much shorter than the time steps used in FEM calculations. In every MD step, particle-particle and particle-fluid interactions are computed. Particles are moved due to the resultant forces, while all fluid flow parameters are kept constant. The number of MD steps should be adjusted so as to assure that the particle displacement is smaller than the element size. Changes of velocity and pressure of the fluid produced by a single step particle motion are negligibly small. Thus a new FEM step (a second phase), in which new velocities and pressures are calculated, is done after several MD steps have been completed.

2.3. Model of the fluid

The fluid is described by classical Navier-Stokes equations for incompressible case:

$$(\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{1}{\rho} \nabla p - \frac{\eta}{\rho} \Delta \mathbf{v} = \frac{1}{\rho} \mathbf{f}, \quad (1)$$

$$\nabla \cdot \mathbf{v} = 0, \quad (2)$$

where η is kinematic viscosity, while ρ is fluid density.

Coupling of particles with the fluid is based on three main assumptions. First the particles are represented by spheres which occupy certain volume. Distribution of volume ratio of fluid contained in finite element to the volume of particles enclosed in it, is given by a scalar field $\varepsilon(\mathbf{r})$:

$$\varepsilon(\mathbf{r}) = \frac{V_e - V_p}{V_e}, \quad (3)$$

where \mathbf{r} points coordinates on xy plane, V_e is a finite element volume and V_p is the volume of the particles. The above distribution is normalized to $[0, 1]$ interval and says what fraction of the finite element is not occupied by particles.

According to the second assumption we add a factor responsible for particle fluid interaction to the external force field density vector \mathbf{f} in the Equation (1). Let us denote it $\mathbf{f}_p(\mathbf{r})$ and define as:

$$\mathbf{f}_p(\mathbf{r}) = \sum_{i=1}^n \mathbf{F}_i^d \cdot \frac{1}{V_e(\mathbf{r})\varepsilon(\mathbf{r})} \delta(\mathbf{r} - \mathbf{r}_i), \quad (4)$$

where n is the number of particles in the system, \mathbf{F}_i^d is the force of particle i acting on surrounding fluid, $V_e(\mathbf{r})$ is the volume of a finite element to which the particle belongs and \mathbf{r}_i is coordinate vector of particle i . Two values, $V_e(\mathbf{r})$ and $\bar{\mathbf{v}}_e(\mathbf{r})$ – mean fluid velocity in the element – are calculated for every element with at least one particle inside.

Momentum exchange between particles and surrounding fluid is, in general, a very complicated task, even for a single particle. In the presented model a considerable simplification has been made, assuming that the interaction is calculated for single, isolated particle [4] and that a particle is entirely contained in a finite element [1]. Force between particle i and the fluid is expressed by the *Stokes formula*:

$$\mathbf{F}_i^d = -6\pi\eta r_i[\mathbf{v}_i - \bar{\mathbf{v}}_e(\mathbf{r})], \quad (5)$$

where η is the kinematic viscosity of the fluid from Equation (1), r_i is the radius of the particle i and \mathbf{v}_i is its velocity.

The third assumption accounts for local change of fluid density. Navier-Stokes equations are introduced for incompressible flows, however locally, whenever a particle appears, the density in this very element decreases, due to the fluid volume displaced by the particle. Such a change of density can be defined as $\rho' = \varepsilon(\mathbf{r})\rho$. However, due to the fact that flow velocity is much lower than sound velocity, we can assume the flow of incompressible fluid and use the following equation [2]:

$$\frac{\partial \varepsilon \rho}{\partial t} + \nabla \cdot (\varepsilon \rho \mathbf{v}) = 0. \quad (6)$$

2.4. Dynamics of particles

The particles are treated as spheres with radius r_i and mass m_i . The motion of every particle is reduced to the center of mass coordinates changes, while particle rotation is neglected. The model under consideration is 2D, however particles are treated as 3D spheres with centers moving on one plane. Thus the particle mass is defined as $m_i = (4/3)\pi r_i^3 \rho_p$, where ρ_p is the density of each particle.

Two-body interactions between particles, as well as particle-liquid and particle-boundary interactions have been introduced in the model. Resultant force acting on particle i is equal to:

$$\mathbf{F}_i = \mathbf{F}_i^w + \mathbf{F}_i^b + \mathbf{F}_i^d + \sum_j (\mathbf{F}_{ij}^s + \mathbf{F}_{ij}^n), \quad (7)$$

where \mathbf{F}_i^w is the buoyancy force, \mathbf{F}_i^b – the force due to boundaries, \mathbf{F}_i^d – the drag force, \mathbf{F}_{ij}^s and \mathbf{F}_{ij}^n are the forces in tangential and radial directions respectively. The buoyancy force acting on particle i defined as:

$$\mathbf{F}_i^w = \frac{4}{3}\pi r_i^3 (\rho_p - \rho_l) \mathbf{g}, \quad (8)$$

where ρ_p is the density of particles, ρ_l – the density of liquid and \mathbf{g} is gravity. Drag force, \mathbf{F}_i^d is the reaction force between particle and the liquid, the same as in (5). If mean velocity

of a liquid in a finite element is bigger than the particle velocity in the same direction, then \mathbf{F}_i^d would increase the speed of particle, otherwise it would slow the particle down.

The normal force, \mathbf{F}_{ij}^n , can be split into two components – contact and lubrication forces:

$$\mathbf{F}_{ij}^n = \mathbf{F}_{ij}^{cs} + \mathbf{F}_{ij}^{lr}. \quad (9)$$

The contact force can be presented as a sum of two forces, an elastic response force \mathbf{F}_{ij}^{el} and dissipative force \mathbf{F}_{ij}^{di} :

$$\mathbf{F}_{ij}^{cs} = \mathbf{F}_{ij}^{el} + \mathbf{F}_{ij}^{di}. \quad (10)$$

The elastic response force is defined as:

$$\mathbf{F}_{ij}^{el} = -k\xi_{ij}\mathbf{n}_{ij}, \text{ for } \xi_{ij} > 0, \quad (11)$$

where k is the stiffness of the contact set to $10^4 g/s^2$, \mathbf{n}_{ij} – the unit vector in $i-j$ direction and ξ_{ij} is so called virtual overlap equal to:

$$\xi_{ij} \equiv (\sigma_i + \sigma_j) - |\mathbf{r}_i - \mathbf{r}_j|. \quad (12)$$

The elastic force acts repulsively only when overlap occurs ($\xi_{ij} > 0$) and vanishes otherwise.

The dissipative force can be formulated as:

$$\mathbf{F}_{ij}^{di} = -\gamma m_{red} [(\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{n}_{ij}] \mathbf{n}_{ij}, \quad (13)$$

where γ is a dissipation coefficient, set in our simulations to 50 s^{-1} , $m_{red} \equiv \frac{m_i m_j}{m_i + m_j}$ is the reduced mass of the pair in contact. The other radial force component, the lubrication force is defined as:

$$\mathbf{F}_{ij}^{lr} = -6\pi\eta \frac{\sigma_{red}^2}{(-\xi_{ij})} [(\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{n}_{ij}] \mathbf{n}_{ij}, \quad (14)$$

where η is the shear viscosity and $\sigma_{red} \equiv \frac{\sigma_i \sigma_j}{\sigma_i + \sigma_j}$ is the reduced radius of the contacting pair. Finally the radial force consists of three elements:

$$\mathbf{F}_{ij}^r = \mathbf{F}_{ij}^{el} + \mathbf{F}_{ij}^{di} + \mathbf{F}_{ij}^{lr} \quad (15)$$

which after applying (9), (13) and (14) eventually give:

$$\mathbf{F}_{ij}^r = \begin{cases} 0, & \xi_{ij} < -\sigma_{red} \\ [-6\pi\eta\sigma_{red}^2(\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{n}_{ij}] \left[\frac{1}{-\xi_{ij} + \delta\sigma_{red}} - \frac{1}{(1+\delta)\sigma_{red}} \right] \mathbf{n}_{ij}, & -\sigma_{red} < \xi_{ij} < 0. \\ [-k\xi_{ij} - \gamma m_{red}(\mathbf{v}_j - \mathbf{v}_i) \cdot \mathbf{n}_{ij}] \mathbf{n}_{ij}, & \xi_{ij} > 0 \end{cases} \quad (16)$$

The radial force between two particles is equal to 0 until the particle surfaces get closer to one another than σ_{red} . Below this critical distance the lubrication force \mathbf{F}_{ij}^{lr} starts to attract particles. This is in order to model the process of attraction of the particles due to lower pressure between them, caused by higher velocity of liquid flowing through the gap. When an overlap occurs, the lubrication force vanishes, while particles interact by elastic and dissipative forces. Elastic restoring force is always repulsive, while the dissipative force acts in the opposite direction to the relative motion of particles: it is repulsive when particles get closer and attractive otherwise.

In the case when two particles contact each other with their surfaces (virtual overlap is close to 0) numerical instability can occur for calculated lubrication force. To avoid it, an extra factor in the form $\frac{1}{-\xi_{ij} + \delta\sigma_{red}} - \frac{1}{(1+\delta)\sigma_{red}}$ in the second part of (16), with δ set to 0.1, replaces $\frac{1}{-\xi_{ij}}$ from Equation (14).

The tangential force, \mathbf{F}_{ij}^t is acting perpendicular to the radial force and is based on Coulomb law of sliding friction. It is assumed that \mathbf{F}_{ij}^t is proportional to \mathbf{F}_{ij}^r , always acting in the opposite direction to the relative motion:

$$|\mathbf{F}_{ij}^t| = \varphi |\mathbf{F}_{ij}^r|, \quad (17)$$

where φ is a sliding friction coefficient with a value from [0.05, 0.5] interval. In the case of central impact *i.e.* when radial force is large, tangential force can be too large even for small values of φ , which can cause numerical instabilities. To avoid them, Equation (17) is replaced by:

$$\mathbf{F}_{ij}^t = -\min(\varphi |\mathbf{F}_{ij}^r|, \zeta |\mathbf{v}_{ij}^n|) \frac{\mathbf{v}_{ij}^n}{|\mathbf{v}_{ij}^n|}, \quad (18)$$

where ζ is a constant set arbitrary to 80 s^{-1} , while \mathbf{v}_{ij}^n is a relative tangential velocity defined as:

$$\mathbf{v}_{ij}^n = (\mathbf{v}_i - \mathbf{v}_j) - [(\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}_{ij}] \cdot \mathbf{n}_{ij}. \quad (19)$$

With the above assumptions tangential force direction is opposite to the relative velocity of pairs of particles.

3. Simulation results

3.1. Sample systems

Several different simulations have been performed for both immobile particles which gave a simple model of porous medium as well as moving which can model sedimentation and/or convection of particles. In all simulations except the last one flow is forced from left to right by the pressure difference. To allow the flow, periodic boundary conditions are established on vertical box edges, while horizontal boundaries are set as a reflecting wall, not dissipating energy.

In the table below we present the range of main simulation parameters.

Parameter	Symbol	Value range
Coordinates of mesh nodes and particles	x, y	0 ... 10 cm
Time step for FEM calculations		$2.0 \times 10^{-1} \text{ s}$
Time step for MD calculations		$1.0 \times 10^{-5} \text{ s}$
Horizontal and vertical velocities	u, v	-0.1 ... 0.1 cm/s
Pressure	p	1 ... 3 g/(cm · s ²)
Kinematic viscosity	η	$4 \times 10^{-1} \text{ cm}^2/\text{s}$
Fluid density	ρ_f	1 g/cm ³
Particle densities	ρ_p	1.1 ... 1.7 g/cm ³
Particle radius	r_i	10^{-1} cm

Particle densities have been set to 1.1 g/cm^3 in the convection flow, while value 1.7 g/cm^3 has been chosen for the sedimentation simulation.

3.2. Flow through porous medium

The first simulation shows the dependence of the flow velocity through the straight tube versus thickness of the porous material. Porous obstacle is built of particles set up in 5 to 25 rows. Figure 1 shows the distribution of pressure and total velocity for extreme cases.

Colors in this figure, as well as in the subsequent pressure and velocity maps give only qualitative information of the process and they are always scaled to current minimal/maximal value. In Figure 2a one can see the velocity profile taken along the vertical cut in the middle of the box for different porous material thickness. Obviously the thicker obstacle slows down the flow velocity, but it also deflects the profile from a parabolic one. However, it appears that the average velocity versus obstacle thickness is practically linear in log-log scale (Figure 2b).

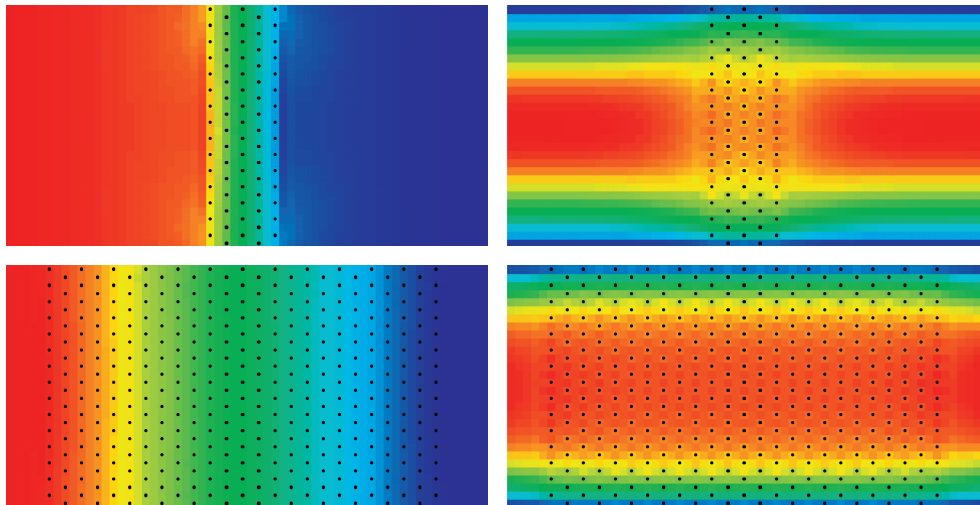


Figure 1. Distribution of pressure (left side) and total velocity (right side) for two porous obstacles built of 5 and 25 rows (75 and 375) particles

In the model presented, it is also possible to combine immobile and moving particles as it has been done in the following simulation in which 15 particles convected by the flow, penetrate the 75-particle obstacle. Velocity distribution in two time instants are shown in Figure 3.

Another example in this series is the flow through curved pipe with immobile particles inside distributed on random, shown in Figure 4. Certain irregularities of the velocity distribution due to the presence of particles is seen in Figure 4a.

3.3. Convection around the obstacle

The next experiment has been designed to show particles convection around solid obstacle of an arbitrary shape. The simulation has been performed on the mesh built of 1680 elements with 150 particles added. Distribution of pressure density and total velocity together with particles coordinates are shown in Figures 5 and 6. It can be clearly seen how the group of particles split into three parts: one passing by the obstacle on the top very fast, second moving more slowly around the bottom, and the third – staying in the niche of 0 pressure gradient.

3.4. Sedimentation example

The last computer simulation is the modeling of particle sedimentation in the fluid, in the presence of gravitational field. Density of particles is 70% larger than the fluid. Contrary to the previous simulations no fluid flow is forced. Its motion is caused by the

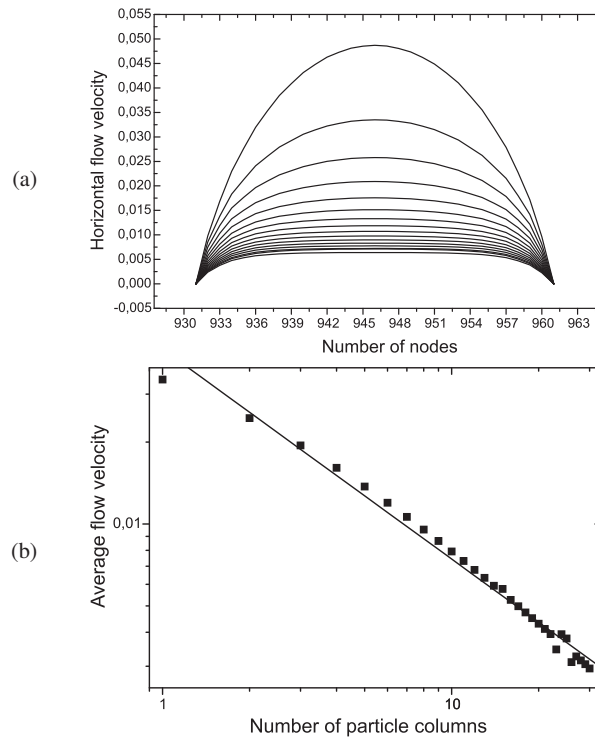


Figure 2. Vertical profiles of horizontal velocity (a) and average flow velocity (b) versus obstacle thickness

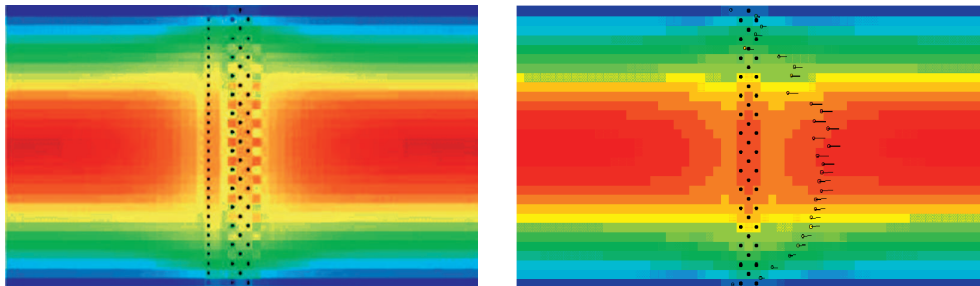


Figure 3. Velocity distribution for flow with particles penetrating porous obstacle after 2 and 27 FEM time steps

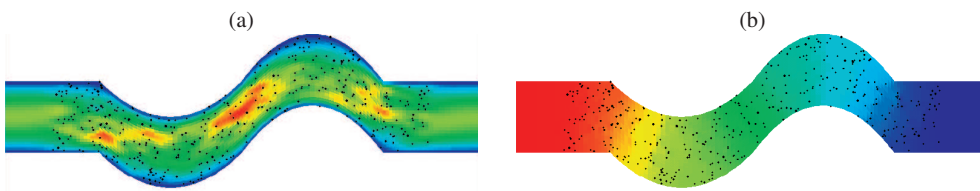


Figure 4. Distribution of total velocity (a) and pressure (b) in the flow through S shaped pipe filled with 400 particles



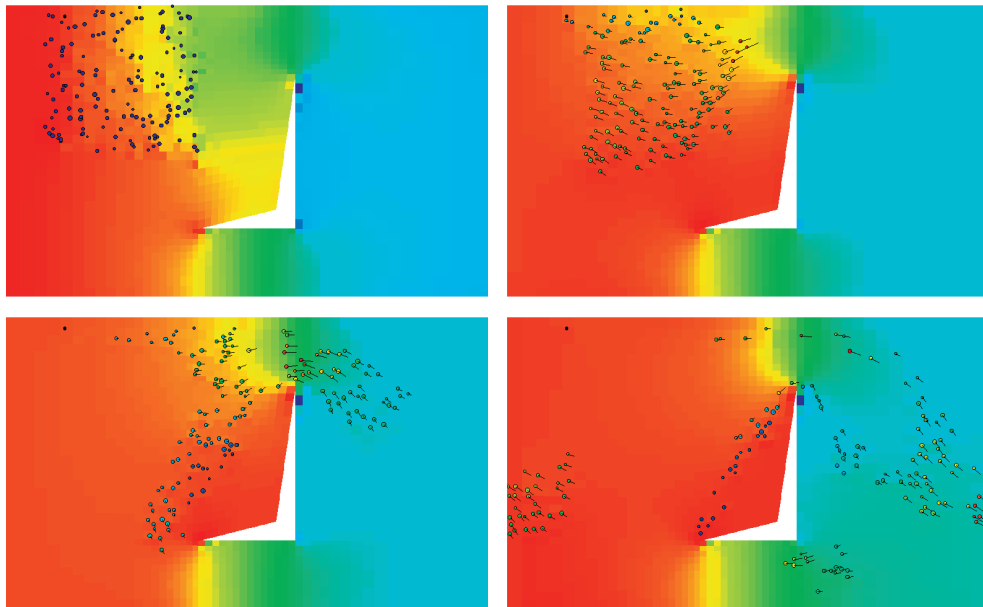


Figure 5. Pressure distribution around the obstacle

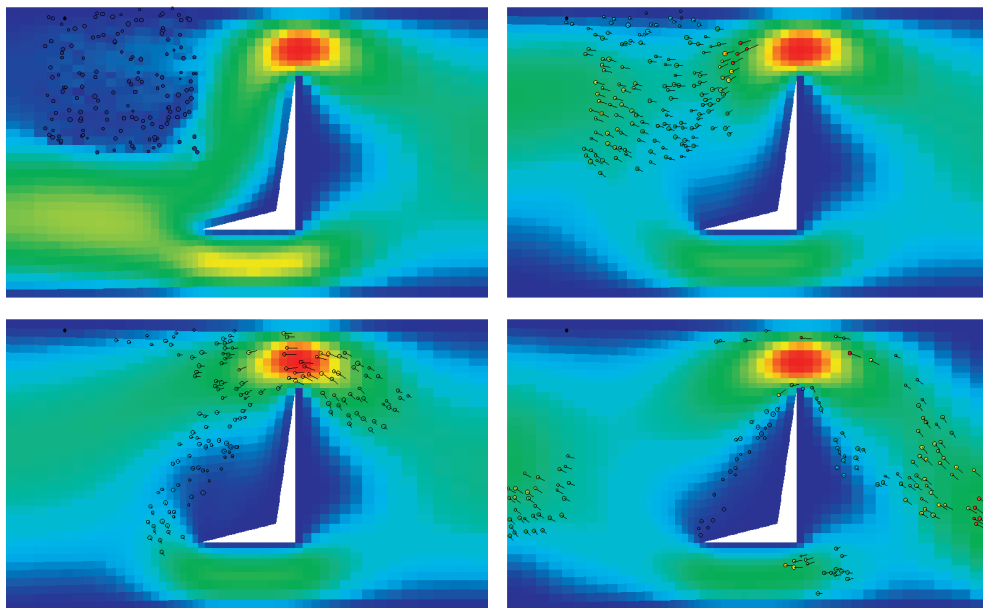


Figure 6. Total velocity distribution around the obstacle

particles only. The FEM mesh contains of 1800 elements and 300 moving particles are introduced. Boundary conditions are periodic on vertical edges and defined as reflecting walls on horizontal. Initially fluid velocity in the entire box is set to 0, while particles are distributed uniformly at random. Particle sedimentation due to gravitational field forces the fluid motion. In Figure 7 the distribution of vertical velocity of the fluid is presented

in two subsequent time steps. Red color denote upward movement, while the blue color indicates the flow in the opposite direction. In the central part of the box we can see a rising convection column. Two columns with downward flow are placed on its both sides. This convection induced by sedimentation is a well known experimental effect (*e.g.* [15], which is still in the area of interest of computational modeling.

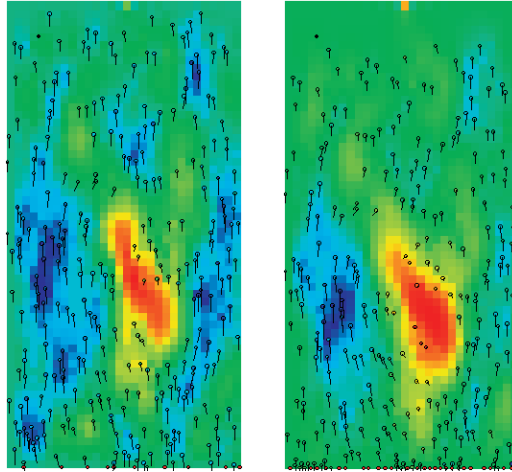


Figure 7. Convection driven by sedimentation at FEM steps 10 and 40

4. Conclusions

In the paper we have presented a combined approach for modeling fluid flow in the presence of particles. The flow is calculated using FEM method with particle-fluid and particle-particle interactions added. Due to simplification of particle representation and particle-fluid interaction reduced to a single particle Stokes formula, the method enabled to calculate medium size models with moderate computer requirements.

The method can be enhanced in many ways. The problems under consideration are: the parallel version of the program to enable calculate larger systems, ability to introduce free fluid surface (which needs remeshing in every FEM time step) and adding the time dependent Navier-Stokes equations.

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References

- [1] Soo S L 1967 *Fluid Dynamics of Multiphase Flow*, Blaisdell Publishing Company, Waltham (Massachusetts), Toronto, London
- [2] Schwarzer S 1995 *Phys. Rev.* **E52** 6461
- [3] Schwarzer S 1998 in *Physics of Dry Granular Media* Kluwer Academic, Dordrecht
- [4] Lalthoff W, Schwarzer S, Ristow G and Herrmann H 1996 *Int. J. Mod. Phys.* **C7** 883
- [5] Hu H H, Joseph D D and Crochet M J 1992 *Theor. Comp. Fluid Dyn.* **3** 285
- [6] Johnson A A and Tezduyar T E 1998 University of Minnesota, Supercomputing Institute Research Report UMSI 98/23

- [7] Johnson A A and Tezduyar T E 1998 University of Minnesota, Supercomputing Institute Research Report UMSI 98/53
- [8] Glowinski R, Pan T-W and Periaux 1997 in J R Whiteman (Ed.) *The Mathematics of Finite Elements and Applications*, Highlight 1996, John Wiley and Sons, Chichester, England
- [9] Glowinski R, Pan T-W and Periaux 1998 *Comp. Meth. Appl. Mech. Eng.* **151** 181
- [10] Travis B J, Eggert K G, Chen S Y and Doolen G 1993 *Calculating Flow and Transport in Porous/Fractured Media using the Cellular Automata Approach*, SIAM Series on Frontiers in Applied Mathematics
- [11] Chen S, Diemer K, Doolen G D, Eggert K, Fu C, Gutman S and Travis B 1991 *Physica* **D47** 72
- [12] Coveney P V, Maillet J-B, Wilson J L, Fowler P W, Al-Mushadani O and Boghosian B M 1998 *Int. J. Mod. Phys.* **C9** 1479
- [13] Freed D M 1998 *Int. J. Mod. Phys.* **C9** 1491
- [14] Koponen A, Kataja M, Timonen J and Kandhai D 1998 *Int. J. Mod. Phys.* **C9** 1505
- [15] Huppert H E, Kerr R C, Lister J R and Turner J S 1991 *J. Phys. Fluid* **226** 349

