

MOLECULAR DYNAMIC SIMULATION OF WATER VAPOR INTERACTION WITH VARIOUS TYPES OF PORES USING HYBRID COMPUTING STRUCTURES

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Theoretical and experimental investigations of water vapor interaction with porous materials are very needful for various fields of science and technology. Mathematical modelling plays an important role in these investigations. Conventional approaches to solve problems of mathematical research of the processes of interaction of water vapor with individual pore are the so called micro and macro approaches. The first approach is based on the use of diffusion equation for description of interaction of water vapor with a pore. The second approach is based on various particle methods like Monte-Carlo simulations, molecular dynamics (MD) etc. In MD usage of efficient calculation methods is necessary because the degree of approximation for simulating system is largely determined by the dimensionality of the system of equations being solved at every time step. Number of time steps is also quite large. In this work, a study of efficiency of various implementations algorithms for MD simulation of water vapor interaction with individual pore is carried out. It is also investigated dependence of time required for simulations on different parameters, like number of particles in the system, shape of pores, and so on. The results of parallel calculations are compared with the results obtained by serial calculations.

Keywords: porous media, molecular dynamics, macroscopic diffusion model, parallel calculations

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1. Introduction

One of the most important problem in numerical simulation based on molecular dynamics or Monte-Carlo approach of many particle systems is the need to use huge computing resources to obtain realistic simulation results. A system of water vapor and a pore is an example of such many particle systems. Theoretical and experimental investigations of water vapor interaction with porous materials are very needful for various fields of science and technology. Not only studies of the interaction of water vapor and porous material as a continuous medium, but also the study of the interaction of water vapor with individual pore is very important in these researches. Mathematical modelling occupies an important place in these investigations. Conventional approaches to solve problems of mathematical research of the processes of interaction of water vapor with individual pore are the following.

The first approach is based on the use of diffusion equation for description of interaction of water vapor with a pore. It is so called macro approach. The second approach is based on various particle methods like, for example, molecular dynamics (MD). These methods essentially consider the micro-structure of the investigated system consisting of water vapor and a pore. This second approach can be called a micro approach.

At the macro level, the influence of the arrangement structure of individual pores on the processes of water vapor interaction with porous material as a continuous medium is studied. At the micro level, it is very interesting to investigate the dependence of the characteristics of the water vapor interaction with porous media on the geometry and dimensions of the individual pore. Both approaches require the most efficient calculation methods as far as possible with the current level of development of computational technologies. Usage of efficient calculation methods is necessary because the degree of approximation for simulating system is largely determined by the dimensionality of the system of equations being solved at every time step. Number of time steps is also quite large.

In this work, a study of efficiency of various implementations algorithms for MD simulation of water vapor interaction with individual pore is carried out. A great disadvantage of MD is its requirement of a relatively large computational effort and long time in simulations. These problems can be drastically reduced by parallel calculations. In this work we investigate dependence of time required for simulations on different parameters, like number of particles in the system, shape of pores, and so on. The results of parallel calculations are compared with the results obtained by serial calculations. Two-dimensional and three-dimensional models of the pore are used for comparative analysis of parallel and serial calculations.

2. Molecular dynamics model

In classical molecular dynamics, the behavior of an individual particle is described by the Newton equations of motion [1], which can be written in the following form

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i, \quad 1)$$

where i – a particle number, $1 \leq i \leq N$, N – the total number of particles, m_i – particle mass, \vec{r}_i – coordinates of position, \vec{f}_i – the resultant of all forces acting on the particle. This resultant force has the following representation

$$\vec{f}_i = - \frac{\partial U(\vec{r}_1, \dots, \vec{r}_N)}{\partial \vec{r}_i} + \vec{f}_i^{ex}, \quad 2)$$

where U – the potential of particle interaction, \vec{f}_i^{ex} – a force caused by external fields. For a simulation of particle interaction, we use the Lennard-Jones potential [2] with $\sigma = 3.17 \text{ \AA}$ and $\varepsilon = 6.74 \cdot 10^{-3} \text{ eV}$. It is the most used to describe the evolution of water in liquid and saturated vapor phase. Equations of motion (1,2) were integrated by Velocity Verlet method [3]. Berendsen thermostat [4] is used for temperature calibration and control. The coefficient of the velocity recalculation $\lambda(t)$ at every time step t depends on the so called "rise time" of the thermostat τ_B which belongs to the interval [0.1,2] ps. τ_B describes strength of the coupling of the system to a hypothetical heat bath. For increasing τ_B , the coupling weakens, i.e. it takes longer to achieve given temperature T_0 from current

temperature $T(t)$. The Berendsen algorithm is simple to implement and it is very efficient for reaching the desired temperature from far-from-equilibrium configurations. Initial concentrations were obtained from the density of water vapor at the appropriate pressure and density at a given temperature using known tabulated data. The pressure in the pore was controlled using the formula based on virial equation [5].

$$P = \frac{1}{3V} \left(\langle 2K \rangle - \left\langle \sum_{i < j} r_{ij} \cdot f(r_{ij}) \right\rangle \right).$$

Here V is the pore volume, $\langle 2K \rangle$ is the doubled kinetic energy averaged over the ensemble, $f(r_{ij})$ is the force between particles i and j at a distance r_{ij} .

3. Computational algorithm for molecular dynamic simulation

For molecular dynamic simulation we used the code written in **CUDA C**. The program does not require a lot of memory. We only keep co-ordinates, speeds and forces for each particle. One of the main problems of molecular dynamic simulation is a large number of particles and time steps. Therefore, it is necessary to use parallel calculations. The code for our simulations was implemented on heterogeneous computing cluster *HybriLIT*.

The code contains four functions that are paralleled, and which are performed on the **GPU**. This is a function for calculating the forces (i.e., acceleration) for individual particles, which calculates the interactions between all particles (F1). There are two functions to calculate new coordinates and speeds for each particle. We need two functions to calculate them because we need forces acting on particles at two different time moments (F2 and F3). Finally, we use the Berendsen thermostat in the program that runs parallel at the **GPU** too (F4). Other calculations are performed on the host. General scheme of the calculation algorithm for two- and three-dimensional molecular dynamic simulation is shown in Figure 1.

In this paper we compare the temporal realization of these four functions F1-F4 on the **GPU** and the **CPU**. The total time of parallel computing consists of two parts, that is the time needed directly to calculate on the **GPU** (pure **GPU** time) and the time needed to complete these calculations on the **CPU** because some algorithms performed on the **GPU** must be completed by the **CPU**. In this work, total **GPU** time will indicate the sum of these two times.

4. 2D molecular dynamic simulation

For two-dimensional (2D) molecular dynamic simulation we consider 2D model of the pore in the shape of a rectangle with dimensions $l_x = 1\mu m, l_y = 1\mu m$. The outer space in this micro-model reflects is a rectangle right to the pore with $k \cdot l_x$ and $(2k + 1) \cdot l_y$ dimensions. All sides of the outer space satisfy to the periodic boundary conditions. The left pore side reflects the inner molecules due to the boundary condition [6] but also provides the periodic boundary conditions for a part of outer space.

There are 420 molecules of water vapor inside the pore which form saturated water vapor at temperature 35°C and pressure 5.62 kPa at the time $t=0$. The value of parameter $k = 3$ means that the outer space volume for calculations is 21 times larger than the pore volume. There are 1764 molecules of water vapor in outer space corresponding to 20% saturated water vapor. The integration step is 0.016 ps and evolution time is 65.3 ns.

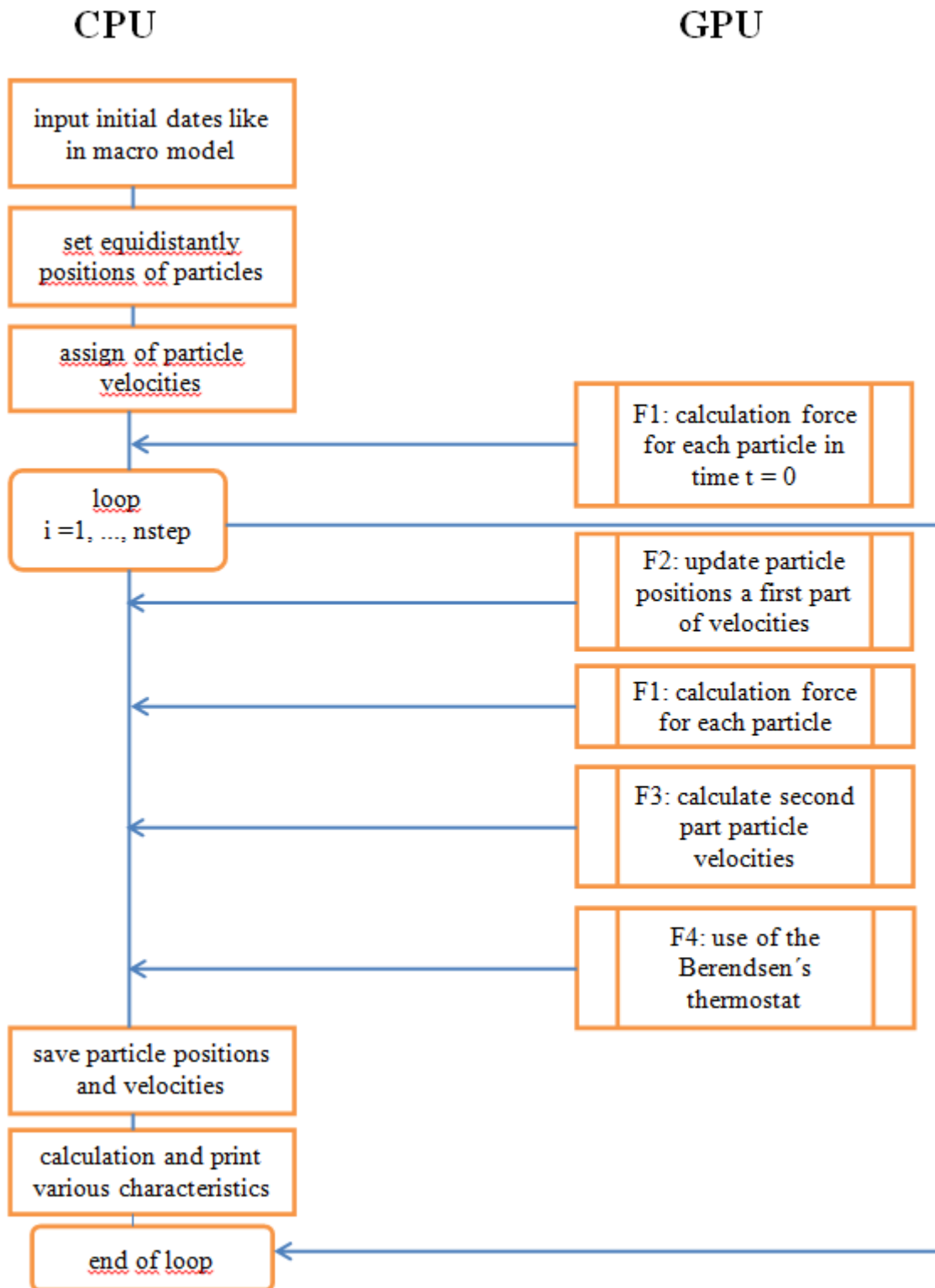


Figure 1. Parallelized algorithm for molecular dynamic simulation

5. 3D molecular dynamic simulation

In three-dimensional (3D) case [7] we made simulation for 3D model of the pore in the shape of a prism of dimensions $l_x = 500nm, l_y = 50nm, l_z = 50nm$. Five walls are isolated and so there is no exchange of particles with outer space. The sixth wall is open and connected with the external environment. The external environment is modelled by a prism which is 9 times bigger than the pore.

The big prism satisfies periodic boundary conditions. This means that the particles which pass through one wall return to the system through the opposite wall. The integration time step is 0.016 ps and evolution time is 65.3 ns.

Consequently, we have considered the following input data for the drying process. There are 1000 molecules of water vapor inside the pore which forms saturated water vapor at temperature 25°C and pressure 3.17 kPa. There are 1800 molecules of water vapor in the outer area space corresponding to 20% saturated water vapor.

6. Conclusion

For both simulations, in 2D and 3D cases, the average time t_1 required to calculate one step was calculated. To compare the two simulations, we have converted this time to one particle t_p . The results are shown in Table 1. The time required to calculate one step for one particle for 2D and 3D simulation on GPU in both cases (pure GPU time and total GPU time) especially pure GPU time is 2:3. CPU time does not keep this ratio.

Table 1. Comparison of computation times per step and for one particle for both simulations

Time	2D			3D		
	CPU	pure GPU	total GPU	CPU	pure GPU	total GPU
t_1	112.732	4.532	4.668	184.349	8.649	8.786
t_p	0.05162	0.00207	0.00214	0.06584	0.00309	0.00314

As our investigations showed for both cases of 2D and 3D simulation, when paralleling the computations, there are some optimal value of number of threads in blocks 2^7 such that the computation time becomes minimal then for other values of this number of threads. Parallelized algorithm runs about 24 times faster than the sequential one in the 2D case and about 21 times faster in the 3D case for one time step t_1 and for average time step per particle t_p . In addition, it should be noted that, when parallelizing, the cost ratio of the computation time per particle for 2D and 3D modeling is equal 2/3 with high precision.

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