NEW MODEL OF CONVECTION BASED ON PARTICLE APPROACH

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Abstract. A new model for thermal convection simulations using molecular dynamics (MD) approach is reported briefly. Preliminary results are presented. Development of the method is discussed in short.

1. Introduction

In the modeling of physical processes of many body systems one can choose between continuous and discrete models. Continuous models represented by partial differential equations (such as Navier-Stokes equations) have been traditionally applied to the simulation of macroscopic systems. On the contrary, particle approach, especially molecular dynamics, represented by systems of mutually interacting particles described by set of simple Newton equations of motion, has been traditionally restricted to microscopic, atomic systems.

Continuous methods are well established in science and engineering practice, however face certain problems when discontinuities (such as cracks), instabilities or deep non-linearities appear. Modeling of these phenomena is natural in particle systems, e.g. breaks in the simulated system simply mean moving one group of particles from another. Such modeling needs a large number of particles, however, rapid increase of computational power considerably increased the size of simulated systems [1] and enlarged the area of molecular dynamics (MD) applications. Maximum number of particles available now in MD simulations reaches 10^9. This cannot be compared with Avogadro number, but enables the investigation of various non-equilibrium processes in microscale. Results obtained with this approach are obviously valid when applied to particles representing atoms, and interacting via well established interatomic forces. But the idea of using MD in this new environment is

to treat particles as model elements of the system in mesoscopic or even macroscopic scale.

Among important directions of development are non-equilibrium simulations of microhydrodynamic phenomena, especially when instabilities and non-linearity occur. Simulation of convection is one of them and there have been attempts to investigate it via MD several years ago [2]. Qualitative similarity of microscopic results to those in macroscale, encourage to build macroscopic models based on particle approach [3]. Large computational power needed for this class of simulations and high efficiency of parallel MD algorithms make this approach ideal for high performance computing. Calculations for the presented work have been performed on different computers including IBM SP-2 and SGI Power Challenge.

In the presented paper we introduce a new model of thermal convection process simulated by MD method. The origin of the model is based on our previous MD simulations of convection driven by sedimentation [4,5], and Rayleigh-Taylor instabilities [6,7]. In those simulations of 2-D Lennard-Jones systems, we have found that different σ parameters in Lennard-Jones potential, applied for interaction of different types of particles, have great influence for creation and development of instabilities and convection patterns.

In the current model we have made a step forward in this direction and, assuming that σ roughly represents the radii of interacting particles ($\sigma_{12} = r_1 + r_2$), we have added varying size of each particle, as well as the new macroscopic interpretation of the system behaviour. We still use Lennard-Jones potential with other system parameters (such as particle mass or time step) of atomic scale. However due to new assumptions the microscopic interpretation is no longer valid. We assume that the heated particle increases its σ, which can be interpreted as thermal expansivity in mesoscopic or macroscopic scale

With this simple model, using large number of molecules and very long simulation times we have obtained clear convection patterns.

2. Computational particle model of convection

We assume two dimensional system of Lennard-Jones particles placed in a rectangular box with gravity field applied vertically. Periodic boundary conditions are used for vertical walls, while horizontal ones reflect particles. All particles have equal masses and initially are placed on regular mesh. Also their potential parameters: σ and ε are initially the same.

There are two basic models we have under consideration.

The first one is maximally simplified, yet it gives clear and suggestive results. For the simulation of convection within this model we introduce two horizontal layers on top and bottom of the box, which thickness may vary from 0 up to the half of box height. We assume that in the lower layer particles are heated, while cooled in the upper one. According to our interpretation heated particles increase their radii, which

in terms of Lennard-Jones potential, means the change of σ in certain interaction. We have assumed that particle radii change in discrete levels. Cooling/heating rate in this model simply means the time spent in one of the layers, necessary to change the particle type. When particle reaches its maximal radius value being in the lower layer, (or minimal - in the upper) it doesn't change any longer. The particles also don't change during their flow between the layers.

In the second, more sophisticated model, we assume quasi continuous changes of σ parameter due to interactions with nearest neighbours. As every particle represents its own type and keeps its individual radius, a number of different interaction types is $N(N+1)/2$ and tabulated potential can not be used any longer. Particles change their r_i and r_j parameters in pairs, so as to keep $r_i^2+r_j^2$ constant; the velocity of radii changes depend on the distance between particles. Changes of radius coming from different interactions are accumulated for every particle first and global update is made after all interactions have been checked. External cooling/heating is realized only by interactions with horizontal walls.

In the above model the heat-exchange mechanism is still oversimplified - otherwise a system of partial differential equations describing dynamic heat distribution with particles treated as sources of heat, should be resolved. But this weak point - the local heat exchange - in the case of convection is compensated by the particles motion.

3. Simulations and Results

For comprehensive set of simulations several parameters, such as: number of particles changing from 10^4 up to 10^6, varying aspect ratio of the computational box, thickness of thermal layers changing from one tenth to half of the box, maximal and minimal values of parameter and cooling/heating rate have to be examined. The results presented below should be treated as preliminary. They are quite promising however and show how the model works. Other simulations are in progress. We have used the model with discrete σ levels (8 particles types and 36 σ levels). Minimal and maximal σ values have been set to 0.3 nm and 0.36 nm respectively. Thickness of upper and lower layers in the square computational box has been set to 20% and 25% of the box height. Cooling/heating rate has been set to 1 per 100 timesteps. Initially all particles has been of one type (of the average radius). Figure 1 shows the number of three chosen types of particles: the average (initial type), the smallest and the largest. It can be seen that eventually after $6 \cdot 10^5$ timesteps the initial type disappears, and the number of particles of the latter two types remains more or less constant. At the same time particles change their types with a constant speed, which can be seen in Figure 2. This means that they migrate continuously between upper and lower layers, and the efficiency of this process remains constant. Sample snapshots of particle coordinates forming convection columns in subsequent timesteps for different width of thermalization layers are presented in Figures 3 and 4.

The most stable patterns have been obtained for the second case with the layers thickness equal to 0.2 of the box height.

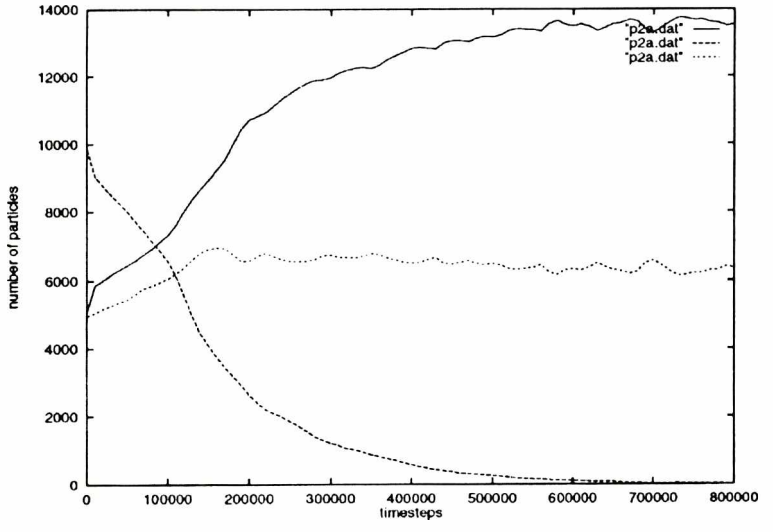

Figure 1. Number of particles of selected types in subsequent timesteps: the lower, dashed line represent the average size particles, middle, dotted line - the smallest, generated in upper layer, continuous line - the largest, generated in lower layer.

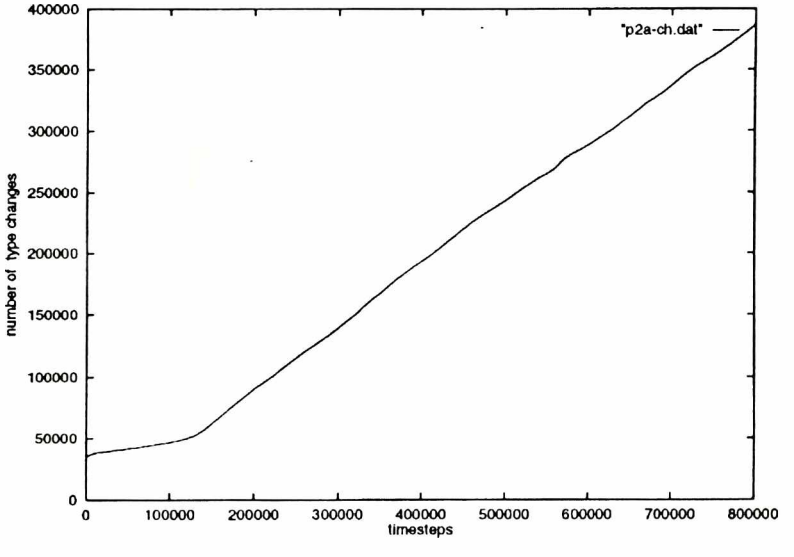

Figure 2. Total number of changes of particle types cumulated in subsequent timesteps. The slope is proportional to the particles migration between the layers. Starting from step 150000 the efficiency of convection process remains constant.

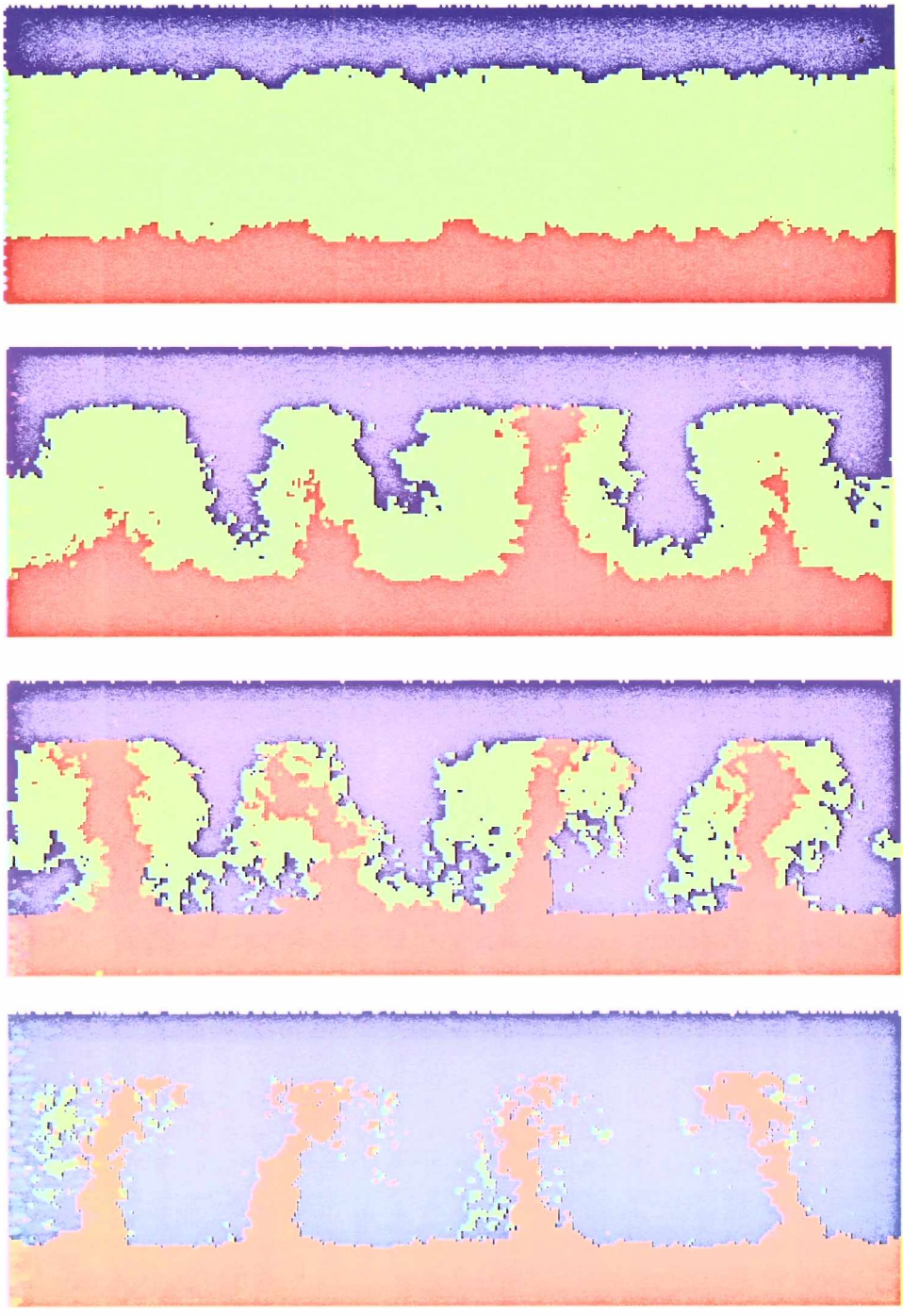

Figure 3. Snapshot of larger (red) and smaller (blue) particles forming convection columns. Initial, middle-size particles (green) disappear as the process develops. Heating/cooling layers equal to 25% of the box height

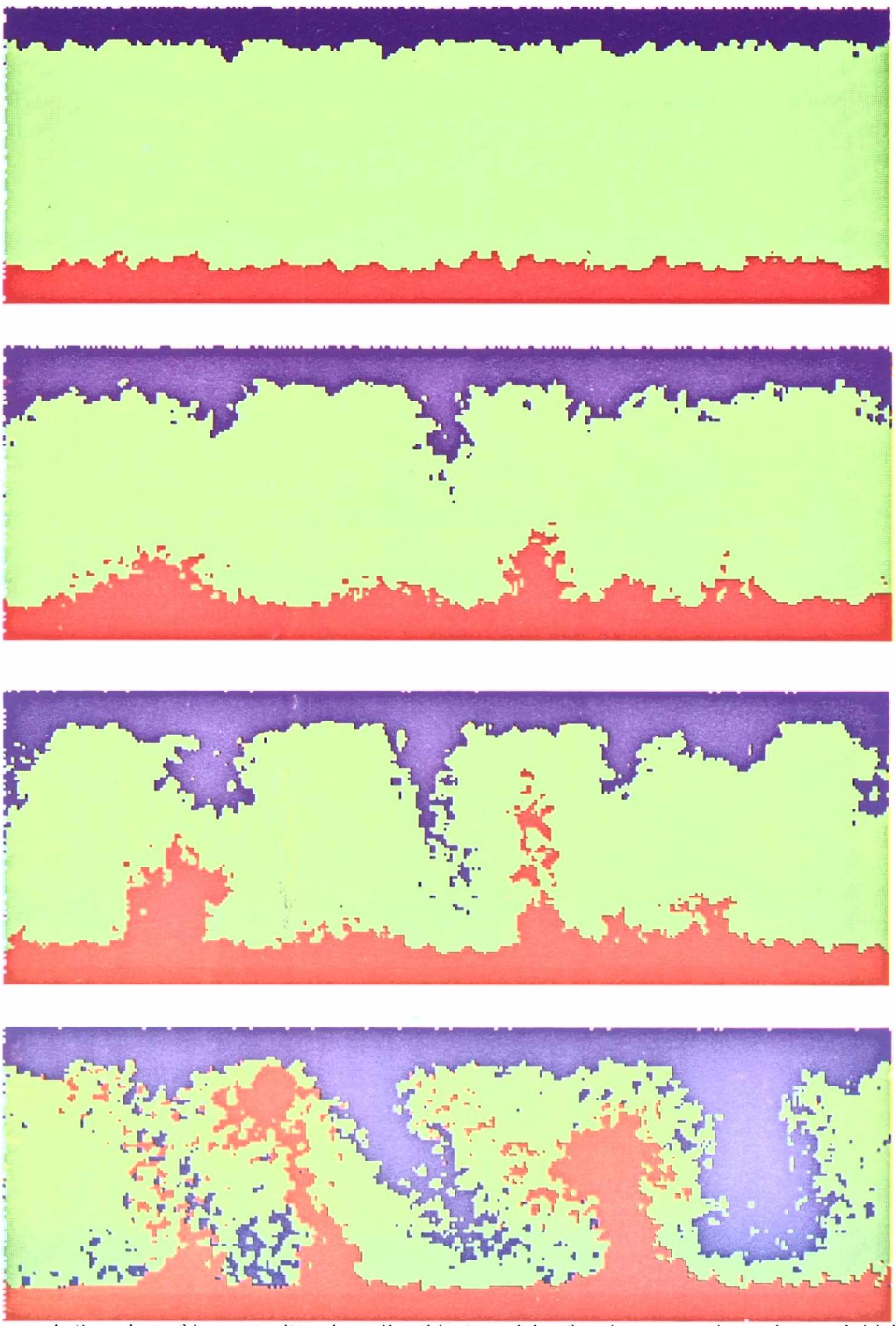

Figure 4. Snapshot of larger (red) and smaller (blue) particles forming convection columns. Initial, middle-size particles (green) disappear as the process develops. Heating/cooling layer equal to 20% of the box height.

4. Conclusions

In the presented paper we introduce a new model for simulation of convection. Despite its simplicity, the model allows to obtain convection patterns easily. The authors are aware of the weak parts of the model and plan to remove them. One of the promising approach for the future investigations is the usage of granular dynamics with contact interactions only and smooth changes of particle properties due to the interactions with neighbours.

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