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A FORMULATION FOR THE ACTIVITY OF SIMPLE MOLECULES

Part II

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ABSTRACT

No doubt, the power of numerical simulation gives the opportunity to see the activity of molecules. And it is hoped that this may be used to advantage to observe and study the fluid molecules at different flow regimes.

In the previous paper the concern was essentially with the development of a formulation to simulate the molecular activity. The mechanical activity is restricted to spinless motion of molecules.

Though the formulationexplained in Part I may easily be used in three dimensions, presented results are obtained in two dimensions. The restricted work done to simulate many molecules in an unbounded domain is presented.

SOME PLANAR SIMULATIONS

As stated previously, nondimensional (n.d.) values are utilized in the code. Length unit (LU) is length/σ, velocity unit (VU) is velocity/U_0 and time unit (TU) is LU/VU. One TU corresponds approximately to 1 ps if the gas is Ar. Simulations shown below are conducted for 4900 parent molecules (otherwise quarantined from the rest) starting at TU = 1 and ending after 300 TU in steps of ΔT = 1TU. At the beginning of each time step, the velocity vector of each molecule is calculated and its new position is found for the end of the same time step. The molecules are placed within a square of 690LU by 690LU in an unbounded domain and are positioned randomly according to a uniform-random distribution. Their initial velocity is assigned as a Gaussian distribution with zero and finite means and a standard deviation of 3. The average velocities shown in the following figures are molecule number averaged values, n.d. as usual.

The effective zone of influence is selected with a radius of influence of 100LU. This means $I = 10^{-4}$ and NEMF ≈ 6.6% whereas the radius of the zone containing all molecules is $R_0 \approx$ 389LU. To make it clear, instead of dealing with 4900 molecules at each time step, 6.6% of it, i.e. only 324 molecules is used in the calculations. This seems to suffice to see the effect of all parent molecules on the selected molecule. Yet, it is our thought that NEMF should not be less than 10%, an arbitrary number of our own.

Figure 1 shows the initial positions of 4900 molecules (TU = 1) as explained above and is common to following cases.

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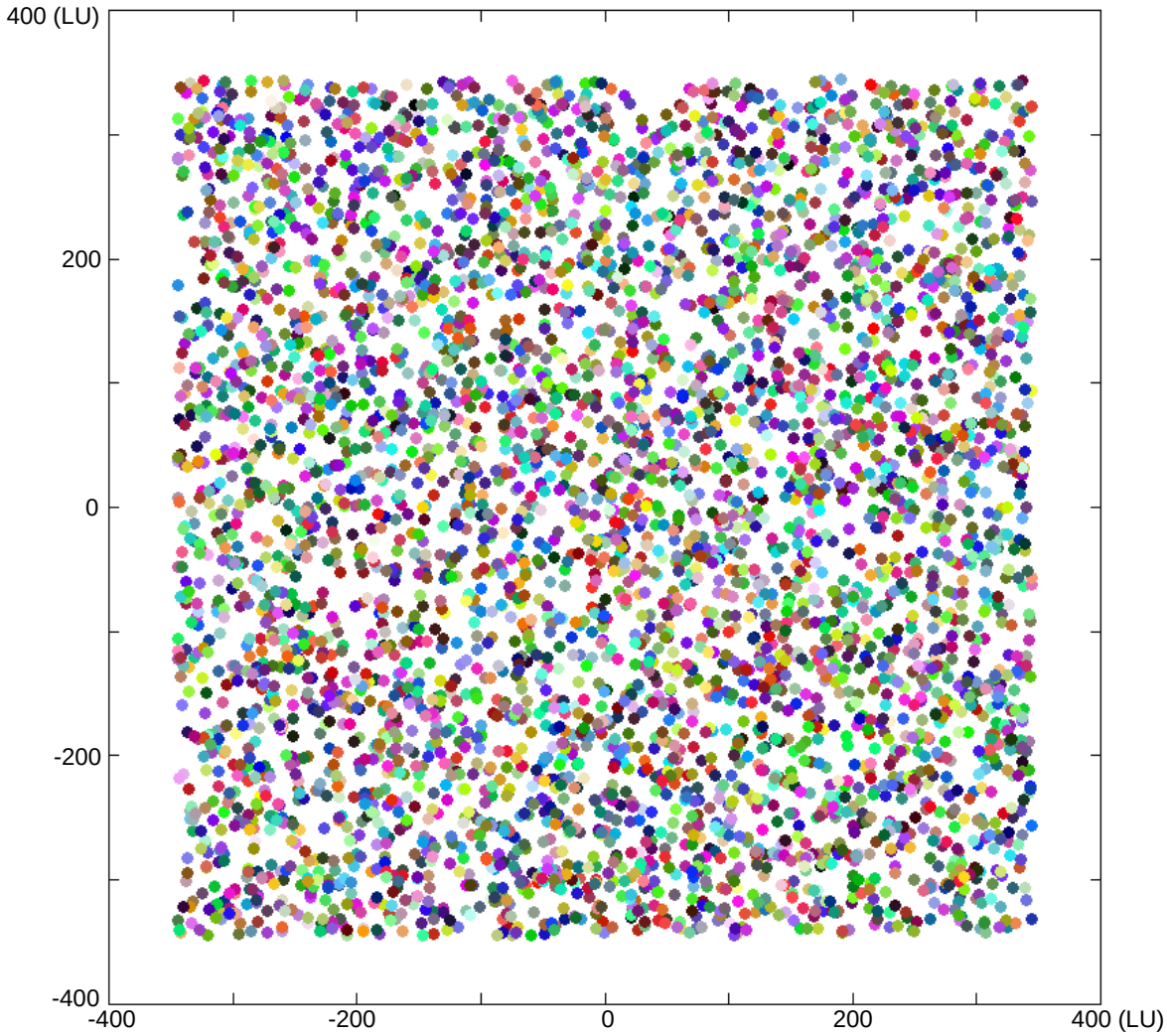

Figure 1: Initial positioning of 4900 molecules

Case 1: 4900 molecules simulation without any control

In this case, initial mean velocity = 0 and standard deviation = 3. The first three inserts of Figure 2 show positions of molecules at different times. It is clear that a strong and rapid dispersion takes place. The velocities reached by the molecules are very high as can be seen in the last insert of Figure 2. These velocities when multiplied with ΔT yield large incremental distances which cause molecules to be pushed outside of the original frame, therefore giving the impression of strong dispersion. It is also clear that these high velocities are not realistic. Hence the implementation of another molecule of some control is needed.

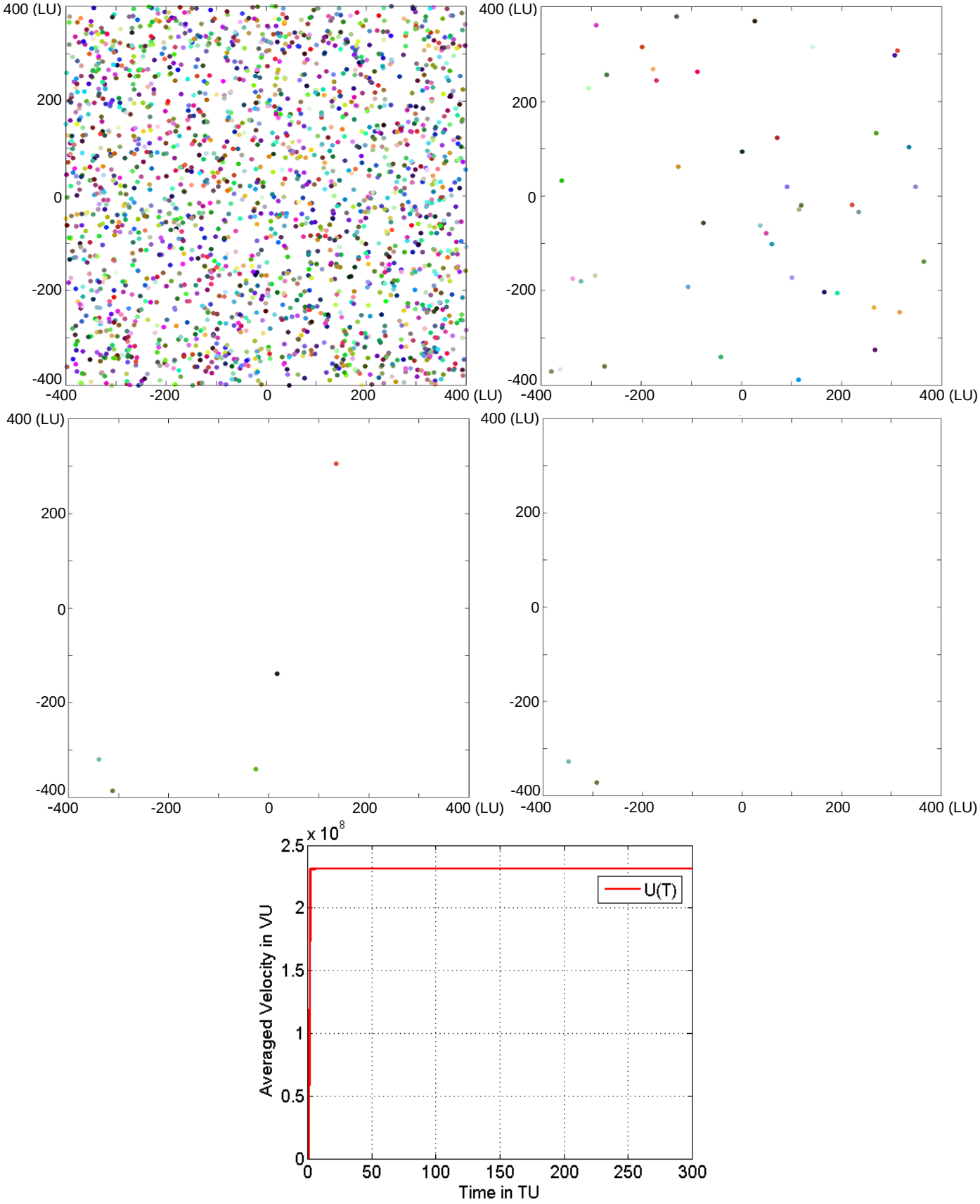

Figure 2: Positions at TU = 2 (upper left), TU = 3 (upper right), TU = 10 (middle left), TU = 50 (middle right), and Averaged velocity variation with time (bottom)

Case 2: 4900 molecules simulation with controlled energy level only

In this case, initial mean velocity = 0 and standard deviation = 3. The kinetic energy acquired at TU = 1 (called reference energy) is adjusted to remain constant at the end of each time step. This is achieved by calculating the total kinetic energy at the beginning of the time step and scaling it by a factor to the reference energy. The square root of scaling factor is used to correct the velocity of each molecule at the end of the time step.

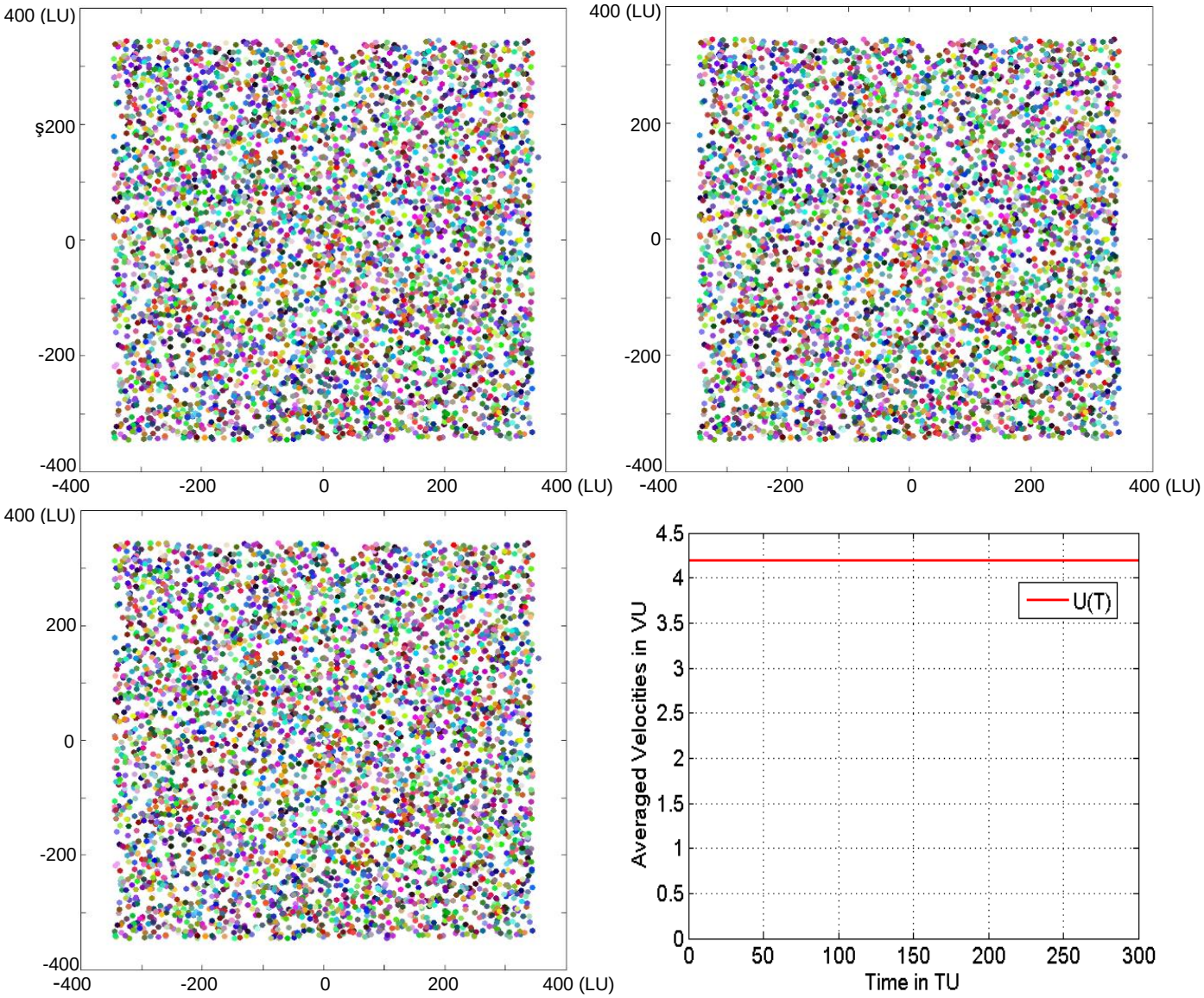

Figure 3: Positions at TU = 50 (upper left), TU = 150 (upper right), TU = 300 (middle left), Averaged velocity variation with time (middle right)

The inserts of positions of molecules in Figure 3 show that the dispersion is eliminated. Yet, the insert on velocities shows sporadic high and unrealistic velocities. They result from intrusion of some molecules into the repulsion zone of some other molecules. This observation led to intrusion control.

Case 3: 4900 molecules simulation with restricted intrusion into repulsion region only

In this case, initial mean velocity = 0 and standard deviation = 3. In Figure 4, a similar pattern is observed as in Figure 2 with the exception of the magnitude of average velocities. Their magnitudes are not as large as in Case 1, but they are still unrealistic.

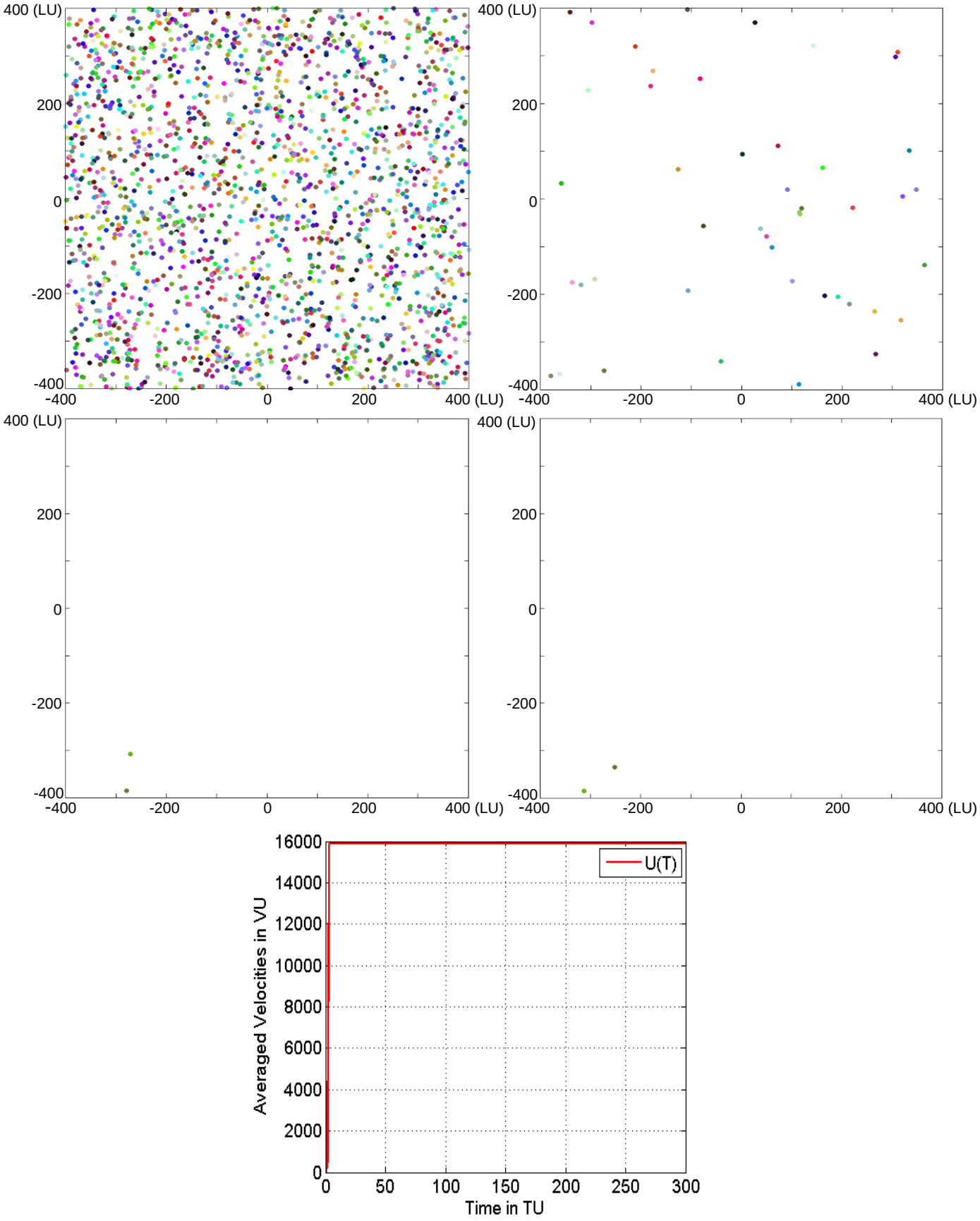

Figure 4: Positions at TU = 2 (upper left), TU = 3 (upper right), TU = 10 (middle left), TU = 50 (middle right), and Averaged velocity variation with time (bottom)

Case 4: 4900 molecules simulation with both controlled energy level and restricted intrusion into repulsion region

In this case, initial mean velocity = 0.7, standard deviation = 3 and two control mechanisms are applied together: Firstly, the energy control where the reference kinetic energy which was obtained from the initial Gaussian velocity distribution is preserved; secondly, any molecule intruding into the repulsion zone of another molecule is moved back in its coming direction to a distance (inside the repulsion zone) which creates a repulsion velocity of the order of mean velocity.

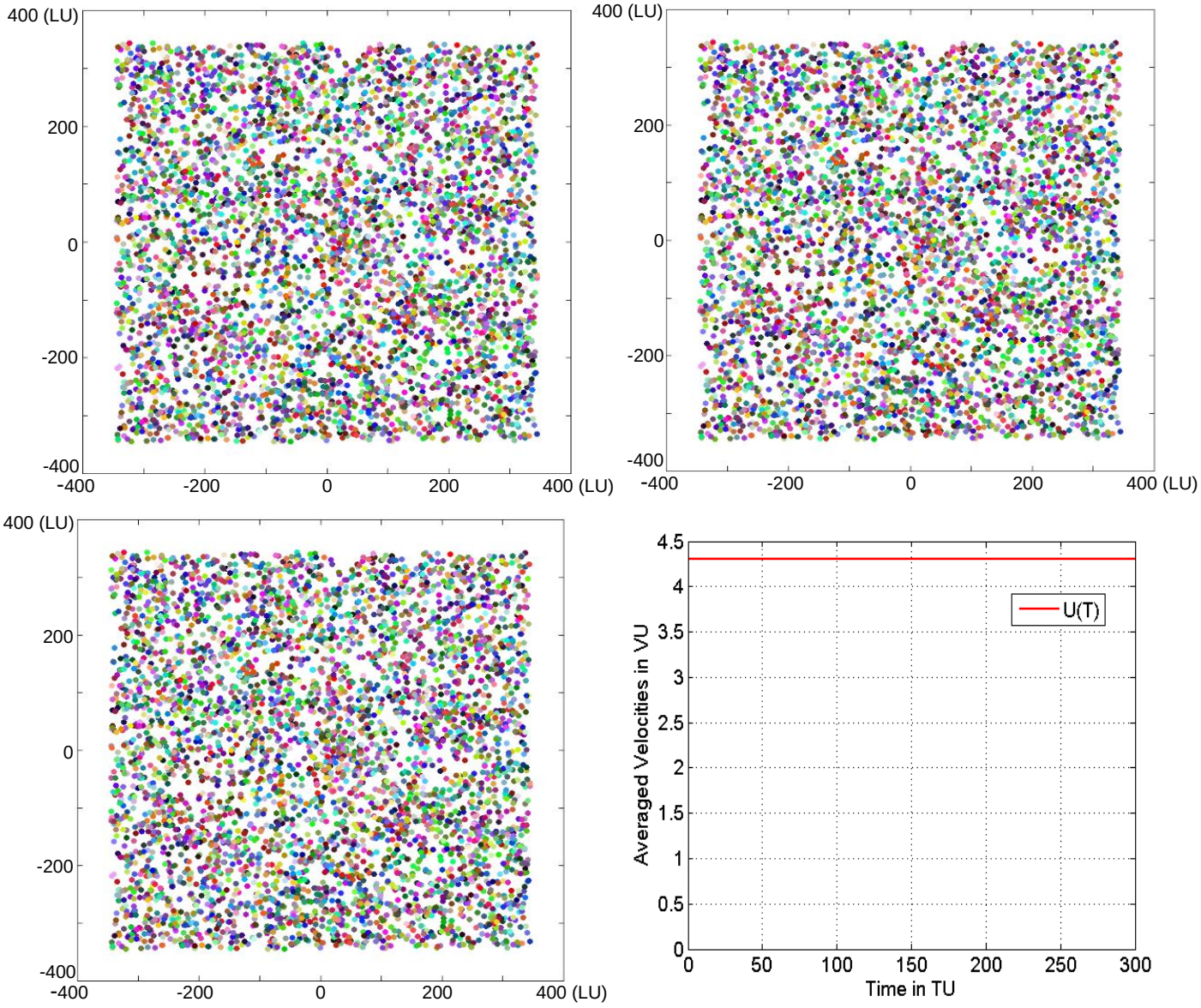

Figure 5: Positions at TU = 50 (upper left), TU = 150 (upper right), TU = 300 (middle left), Averaged velocity variation with time (middle right)

The result can be seen in Figure 5. Molecules travel in resulting directions, but they do not move far away, i.e. they stay inside the starting square. Molecules sometimes collide with each other. After a while, collisions occur only at the center region. In other words, molecules away from the center tend to slow down or perhaps stop (This is considered to be the ineffective result of NEMF in outer regions).

CONCLUSION

MATLAB version R2014a is used for all calculations and simulations. Since number of molecules is not too much, faster computation tools were not needed. Indeed, simulation with only 1 core took around 35-40 minutes whereas post processing occupied 75% of this time.

These applications gave the necessary control element to continue with the method.

In order to cope with the high memory and CPU need, FORTRAN code will be implemented with parallel computing when larger number of molecules will be used.

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