§31. Direct Visualization of Multi-Million Particles System via Molecular Dynamics Simulation

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Molecular dynamics (MD) simulation is one of the most powerful tools in numerical simulation, in which the motion of particles at the scale of atomistic, molecular, and even for coarse grained ones can be resolved directly. The one of great advantage of MD is that we can analyze spatial collective motion of particles in time, which is directly related to the results obtained in the continuum field simulations at the coarse grained level. The special heterogeneity or collective motions in the microscopic region often affect the trigger of the global phenomena such as phase transition or bifurcation. Therefore, to visualize detail of particle motion is important task to understand and clarify the mechanisms of global phenomena for wide hierarchal levels. These mechanisms might be considered as universal even for understanding the plasma physics.

In general, conventional scheme for visualization of many particles by computer graphics is quite simple; Points, circles or polyhedrons which are composed of triangles (called by "polygon") are assigned at the locations corresponding to each particle configuration on computer display. In case of drawing multi-million particles, since much computational cost is needed, one of conventional visualization technique is often used. At first, the field values on the spatial grids are evaluated from particle configuration (or velocity) data via coarse-graining scheme. Then, those values are drawn by using color or contour map. Above grid coarse-graining scheme enables to visualize the particle's information much faster than the direct drawing method on the display. The internal structure of system can be visualized as the cross sectional view. However, it is difficult to find the special structures regarding on the dynamical motion of local excitations in 3D spaces by analyzing the static 2D cross sectional view.

In this project, we improved the novel and powerful visualization tool for many particles system "AIScope"[1] so as to analyze the dynamical internal structure of the system, in which we can easily observe dynamical structures even for the multi-million particle system in 3D. In our strategy, we don't use spatial grids as conventional method, but we use semitransparent points for particle drawings. Actual scheme is described as follows: When we render the particles to display, the positions of whole particles are projected into 2D surface parallel to the display. Since the drawn points must be discretized on the pixel (resolution) of display, we use this character to improve efficiency. Many drawn points for particles are overlapped within one pixel with each other, which cannot be identified separately at least within one pixel on the display. Therefore, we assigned the semitransparent colors to each drawn particle. In this method, if many particles are overlapped within the same pixel, it is colored by the superposition of semitransparent colors for particles. In case of dense in a certain pixel, it is colored as "light". On the contrary, in case of sparse, it is colored as "dark". Note that if the drawn points are completely opaque, the almost area on the display becomes single color. Therefore, the system with the resolution of pixel on the display is drawn as "see-through". Based on above scheme, we can easily recognize the internal dynamical structure of the system via the concentration of color within the resolution of the display, which is actually probed to be very efficient.

Figure 1 shows one of example of the visualized particles by AIScope. In this case, the system includes 2,097,152 particles, which are obtained via the Event-Driven MD [2] numerically. We can identify the internal (void) structure clearly.

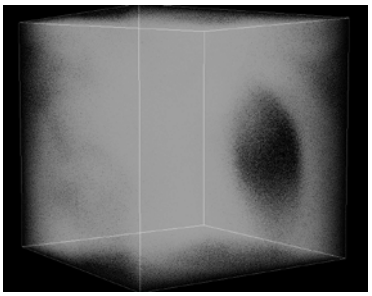

Fig. 1. The visualized particles by AIScope. The 2,097,152 particles were drawn as semitransparent white points on the black background display.

Present rendering of visualization by the AIScope is using two application programming interfaces (APIs) for graphic processer unit(GPU)(i.e., OpenGL and DirectX). In our scheme, the "real time" rendering for multi-particles system can be realized by using shader programming on the GPU, since we can compute all required information for visualization. By using the shader programming, we can avoid time-consuming calculation for drawing high quality computer graphic image such as video game.

Acknowledgement

The present works were supported by NIFS Collaboration Research program (NIFS09KNSS002 and NIFS11KNTS008), and NINS Program for Cross-Disciplinary Study. The particle configurations for visualization were generated by Event-Driven MD, which was performed by the Plasma Simulator in the facility of National Institute for Fusion Science.

1) http://www-fps.nifs.ac.jp/ito/

2) M. Isobe, Int. J. Mod. Phys. C, 23 (2012) 1250032.