§38. Scientific Visualization of Particle Simulation Results

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In the conventional visualization analysis, we use so called "visualization software" on graphic workstations. Because the complex particle orbits and three-dimensional (3-D) structure of vector fields are shown on a two-dimensional plane through the workstation monitor, it is difficult to grasp the spatial structure of the orbits and 3-D vector fields. In order to understand the role of the complex orbits of particles and vector fields, it is indispensable to analyze them in 3-D space by scientific visualization technology. For visualizing particle simulation data, a deep immersion into the VR world is needed. One of the most successful immersive VR systems is CAVE [1]. The CAVE system can produce three important views: stereo view, immersive view, and interactive view.

For scientific VR visualization using the CAVE system, we develop two pieces of software to analyze the results of the plasma particle simulation and the molecular dynamics simulation, respectively.

First, we report about the software for the plasma particle simulation [2]. Kageyama and Ohno has developed general purpose VR visualization software "VFIVE" [3,4]. This software can show vector fields as lines or arrows, and scalar fields as isosurface, contour, and volume rendering. It can also trace particle motion following the flow field of simulation data; however, it cannot deal with particle motion in the electromagnetic field of simulation data. We improve VFIVE to trace the trajectories of plasma particles in the electromagnetic field obtained in the particle simulation to analyze the reconnection phenomenon in the VR world. The equation of motion for a single particle is given by the Newton−Lorentz equation. You can point at the position in the VR world as the initial position of particle by the 3-D mouse "Wand." The initial velocity is given by the Box−Muller method [5] with the same average velocity as the flow velocity, which is given by simulation data. Figure 1 displays magnetic structure (lines), ion temperature (contours in the xy plane), trajectories of ions (white lines) and ion flow velocity (arrows) near the reconnection region. From the distribution of arrow lengths, it is found that flow velocity is higher in the reconnection and downstream regions. Ions enter the system from the upstream boundary and exit through the downstream boundary.

Next we explain the software "AI-scope" for molecular dynamics simulation [6]. This software can display the dynamics of molecules in VR space according to the time-sequential molecular simulation results. You can look out over the simulation region with a wide viewing angle far away in the distance (Fig. 2), because CAVE system is room-sized, cubic-shaped VR system and stereo images are projected onto 3m×3m screens of the walls and the floor. From these reasons, you can analyze the low-density particle simulation results in the extensive wide space. In the high-density particle simulation, for example crystal lattice, on the other hand, you can grasp the whole spatial structure intuitively, because the VR space is 3-D space and the viewer can move around the visualized objects.

Scientific visualization by VR in the CAVE system is a powerful tool for analysis of particle simulation data.

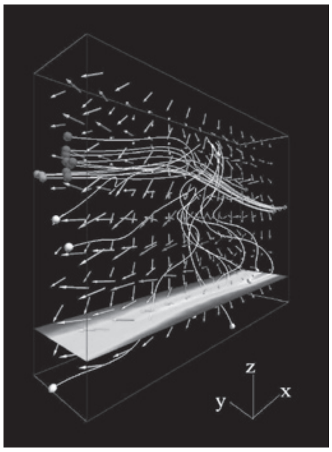

Fig. 1. CAVE visualization of plasma particle simulation results.

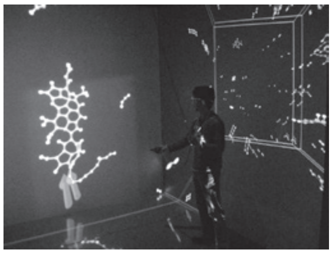

Fig. 2. CAVE visualization of molecular dynamics simulation results.

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