

Haptization of molecular dynamics simulation with thermal display

Y. Tamura, S. Fujiwara^a, H. Nakamura^b

Konan University, 8-9-1 Okamoto, Higashinada-ku, Kobe 658-8501, Japan

^a*Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*

^b*National Institute for Fusion Science, 322-6 Oroshi-cho, Toki 509-5292, Japan*

tamura@konan-u.ac.jp

Visualization is often used for representing numerical data, especially numerical simulation result. In visualization, numerical data is shown as color contour, vector arrows, isosurfaces, etc, but these expressions are not intuitive. By contrast, a research shows that representing 3D data with haptic sense promote reality more than without haptic information, on a virtual environment.

Our purpose of this study is to apply haptization, which means to add haptic information, to represent molecular dynamic simulation result. As one haptic device, we made a thermal sense display that can present both cool and warm information by control electric current.

Thermal sense displays have been researched [1][2], but the most of them are used in a sitting position. We have used a large-scale IPT (Immersive Projection Technology) display, like the CAVE (CAVE Automatic Virtual Environment) [3], for scientific visualization, and this device is very useful for comprehending complex phenomena. But in the IPT display, observer commonly watches and controls 3D objects in a standing position. Thus we developed a thermal sense display that can be used in a standing position. This thermal device consists of Peltier devices. The numerical data is translated to the electric voltage and this drives Peltier device and provide thermal information to the observer.

In scientific data representation, the response time is very important to observe physical phenomena. We provide two pieces of information to the thermal sense display; one is the information about the rate of thermal change, and the other is about real temperature. By these information, we can receive information the absolute value of temperature and the rate of thermal change at same time. We installed this device to show the result (for example energy and temperature, as thermal information) of the molecular dynamics simulation.

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