Haptization of Molecular Dynamics Simulation with Thermal Display

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(Received 7 December 2009 / Accepted 30 March 2010)

Thermal display, which is a type of haptic display, is effective in providing intuitive information of temperature. However, in many studies, the user has assumed a sitting position during the use of these devices. In contrast, the user generally watches 3D objects while standing and walking around in large-scale virtual reality system, In addition, in scientific visualization, the response time is very important for observing physical phenomena, especially for dynamic numerical simulation. One solution is to provide two types of thermal information: information about the rate of thermal change and information about the actual temperature. We propose a thermal display with two Peltier elements which can show above two pairs of information and the result (for example energy and temperature, as thermal information) of numerical simulation. Finally, we represent an example of visualizing and haptizing the result of molecular dynamics simulation.

Keywords: haptization, visualization, molecular dynamics simulation, virtual reality

DOI: 10.1585/pfr.5.S2107

1. Introduction

Numerical representation method is very important in scientific research. Especially, visualization is widely used for representing numerical data; in particular, it is used for numerical simulation. In visualization, numerical data is represented by color contours, vector arrows, and isosurfaces; however, these representations are artificially defined and are not intuitive. On the other hand, a study has shown that representing 3D data with haptic sense promotes more realistic presentation when compared to the representation of data without haptic information in a virtual environment. Thus, the purpose of this study is to apply "haptization," that is, the addition of haptic information to representation of a numerical simulation result. We focus on thermal display since temperature is an indispensable factor in numerical simulation. Therefore, we propose a thermal display as a haptic device that can present information about both cold and warmth.

Haptic devices have been proposed for thermal and tactile display for representing object surface temperature and textures [1, 2]. In particular, many types of thermal display using Peltier elements have been proposed [3, 4]. A Peltier element has a marked advantage in that the thermal information about warmth and cold can be controlled just by changing the direction and value of the electric current. It is also easy to control the element using a computer. Therefore, in this study, we use the Peltier element for thermal display.

We have also used a large-scale immersive projection technology (IPT) display such as the CAVE [5] for scientific visualization. In the IPT, the observer is surrounded by several screens, each of which projects stereo images. This makes the user feel deeply immersive sense. This device is very effective for comprehending numerical simulation results, especially complex 3D data. However, in the IPT display environment, the observer can move freely, change his/her position frequently, and stand up. Hence, it is necessary to develop a thermal display that can be used by an observer while standing. However, the abovementioned devices use a haptic display on the basis of the assumption that the observer is sitting in front of a computer. Consequently, as the position of the observer changes, the thermal data acquired from the 3D environment (numerical simulation result) also changes. Therefore, it is also necessary to frequently update the temperature representation of the data.

Finally, this study aims at developing a thermal display that can be used in a standing position and can give the thermal information rapidly. And our primary purpose is to provide much intuitive information about numerical simulation result to the observer.

2. Configuration of Thermal Display

We propose a thermal display with the Peltier elements. This element is often used in thermal displays, however, the response time until the temperature reaches the target temperature is long. As already mentioned, fre-

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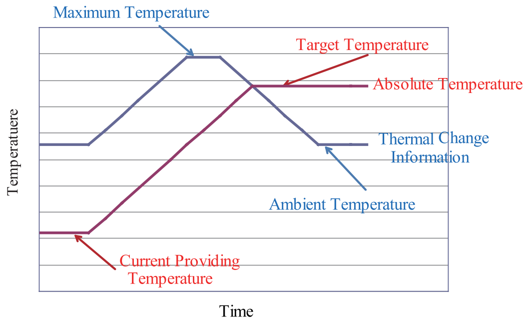

Fig. 1 Temperature Control (when temperature (numerical simulation result) rises in the virtual space).

quent changes in the position of the observer causes frequent changes of data in the IPT display. Therefore, we attached two Peltier elements for compensating this fault, the first to provide absolute thermal information and the second to provide information about thermal change, because it is important not only to provide thermal information to the observer but also to indicate thermal changes rapidly in the IPT environment. Furthermore, a study has shown that we cannot recognize small or slow changes in temperature [6].

For example, when no temperature change occurs at the observed position (device position), the element for absolute temperature provides the absolute temperature and the element for thermal change information provides no information. On the other hand, when the temperature change occurs, the information about the variation in temperature is provided by the second element, thereby enabling the users to easily recognize changes.

Figure 1 shows the procedure adopted in this study. The red line indicates one example of the absolute temperature information on the first element, and the blue line does one of the thermal change information on the second element. This figure shows that when the temperature increases, the temperature of the first element increases from the current temperature and reaches the target temperature, which is determined by the numerical simulation, and the temperature of the second element increases from the ambient temperature to the maximum temperature, which depends on the physical characteristics of the Peltier element, and vice versa. Moreover if the temperature of the second element reaches maximum temperature, we stop supplying electric current and the temperature gradually decreases. This is because if this element keeps maximum temperature, we cannot provide thermal change information in next time.

Figure 2 shows the proposed device. Two Peltier elements, which provide two types of temperature information, are fixed to a square bar of aluminum. A heat sink is inserted in the bar for transferring the temperature to the outside (Fig. 2 (c)). The surface of the aluminum bar is covered with butyl rubber, which has a low thermal conductivity and a high specific heat, for protecting the hand from heat. A magnetic sensor (Polhemus Patriot), which acquires the real-world, six degrees-of-freedom (position and rotation) data, is installed in this device.

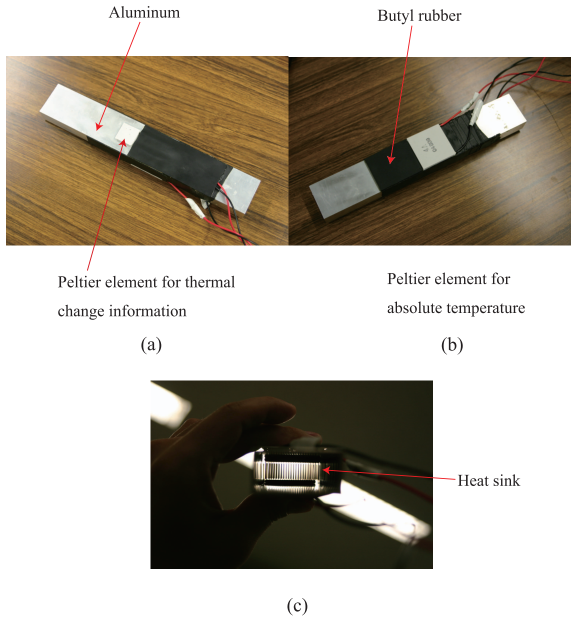

Fig. 2 Proposed thermal display (a) Peltier element for thermal change information, (b) Peltier element for absolute temperature, (c) inside the device.

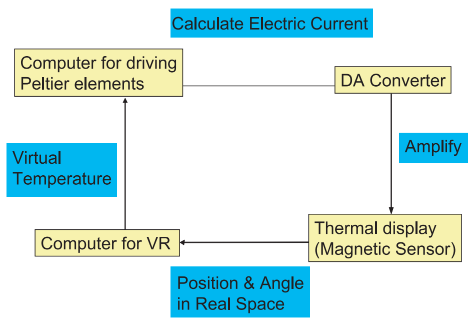

Fig. 3 Data flow between the real thermal sense and the virtual thermal data.

Figure 3 shows the system configuration. If the observer moves this device, information about the observer's position and angle is given from the magnetic sensor, and the virtual scene is translated and rotated. Subsequently, the thermal data to be presented at this point, which is determined from the result of numerical simulation, is obtained. This thermal data is translated into electric current, amplified through an analog–digital converter, and finally, represented to the user. The relationship between the electric current and the actual temperature is discussed in the following section.

3. Modeling of Haptization Device

3.1 Formulation of thermal display

For providing correct thermal information to the user, it is necessary to control the device temperature correctly. In the Peltier element, the surface temperature is controlled by the electric current, and it can be calculated theoretically. Thus, we determine the relationship between temperature and electric current.

If the Peltier device has a uniform temperature on the surface area, Eq. (1) holds,

$$C\frac{dT}{dt} = Q, \tag{1}$$

where C is the heat capacity of the whole thermal display, and t is time. Q can be calculated by the following equations

$$Q = Q_{\mathrm{M}} + Q_{\mathrm{G}}, \tag{2}$$

$$Q_{\mathrm{M}} = -ATI + \frac{1}{2}I^2R + K(T_{\mathrm{h}} - T), \tag{3}$$

$$Q_{\mathrm{G}} = K_{\mathrm{G}}(T_{\mathrm{h}} - T), \tag{4}$$

where Q_{M} is the heat absorption by itself, Q_{G} is the thermal conductivity by the atmospheric gas, A is the Seebeck coefficient of the Peltier element, I is the electric current, K is the thermal conductance of the element, K_{G} is the thermal conductance of the atmospheric gases, R is the inner resistance of the element, T_{h} is the temperature of the radiation surface, and T is the temperature of the surface in contact with the user.

Substituting the above equations into Eq. (1), C becomes

$$C\frac{dT}{dt} = -aT + b, \tag{5}$$

where

$$a = AI + K + K_{\mathrm{G}},$$

$$b = \frac{1}{2}I^2R + KT_{\mathrm{h}} + K_{\mathrm{G}}T_{\mathrm{h}}.$$

Assuming $T = T_0$ when $t = 0$, Eq. (5) becomes

$$T = \left(T_0 - \frac{b}{a}\right)\exp\left(-\frac{a}{C}t\right) + \frac{b}{a} \tag{6}$$

$$= (T_0 - T_{\mathrm{const}})\exp\left(-\frac{t}{\tau}\right) + T_{\mathrm{const}}, \tag{7}$$

where the temperature at the steady state is $T_{\mathrm{const}} = b/a$, and the time constant is $\tau = C/a$. The initial temperature and the temperature at the steady state (target temperature) are already known. We can then determine the temperature of the surface by estimating the time constant.

3.2 Estimation of applied equation

To evaluate this equation, we estimate the time constant from experimental data. The time constant can be calculated by the least square assumption by using the above-mentioned expression. Figure 4 shows one of the results obtained.

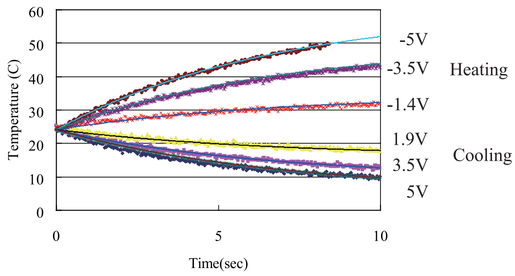

Fig. 4 Assumed time constant of the Peltier element (the initial temperature is ambient).

In this case, the time constant $\tau = 5.6$ s was obtained theoretically. The solid line is a theoretical temperature curve obtained from the equation, and the points show the obtained experimental data. This thermal data is measured by the thermal radiation sensor (FT-HT20, KEYENCE). This result shows that this equation is accurate in representing the characteristics of the thermal elements. In addition to this, this time constant is small for representing the absolute thermal information but is fast enough for showing the thermal change information [6].

The temperature of the device constantly changes due to the ambient temperature or the thermal history of the device. As a result of this, the time constant also changes. Therefore, in practical use, thermocouple is attached to this device, and the feedback from the thermocouple gives the temperature. Thus, we can control the surface temperature of the Peltier elements to estimate the continuous variations in the time constant.

4. Visualization and Haptization of Numerical Simulation Results

We simulate self-assembling behavior of amphiphilic molecules. An amphiphilic molecule is modeled as a semi-flexible chain which consists of one hydrophilic particle and three hydrophobic particles. A solvent molecule is modeled as a hydrophilic particle. We consider bond-stretching and bond-bending potentials as bonded potentials. As for non-bonded potentials, the interaction between a hydrophilic particle and a hydrophobic particle is modeled by a repulsive soft core potential and all other interactions are modeled by a Lennard-Jones potential. The equations of motion for all particles are solved numerically using the velocity Verlet algorithm at constant temperature and volume. The amphiphilic concentration is set to 0.06. Initially, we provide a randomly distributed configuration of amphiphilic molecules in solution at high temperature. The system is then quenched to lower temperature [7–10].

Figure 5 (a) shows a configuration of molecules, (b) shows isosurface of the kinetic energy of tail particles, calculated by Gaussian splatting techniques, and (c) is one example of visualizing and haptizing. In Fig. 5 (c), the isosurfaces and the color contour plane of enegy is drawn. The range of energy is from 0 to 3.85 (non-dimensional

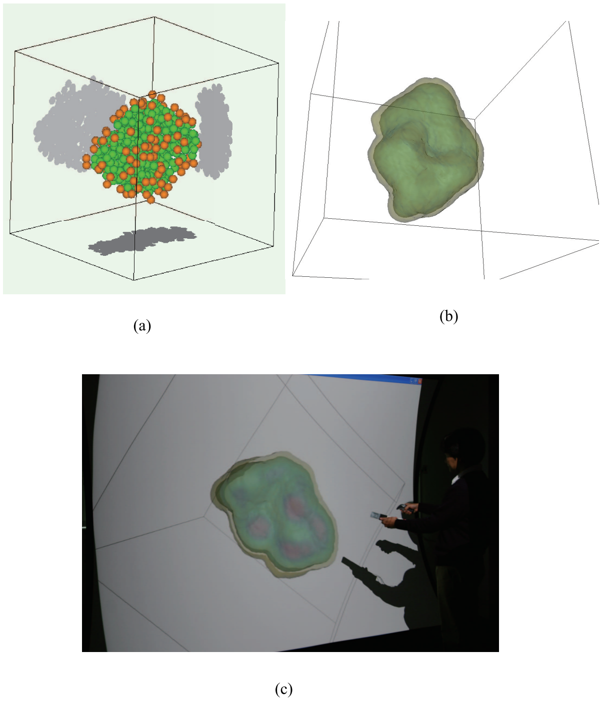

Fig. 5 Visualization and haptization of molecular dynamics simulation: (a) simulation result drawn by molecules (b) isosurfaces (c) isosurface and contour in Angle-changeable immersive display.

number). For haptizing this data, we normalized this data from 0 C to 40 C and presented the thermal information to the user. Eq. (8) shows the relationship between the absolute temperature and the temperature calculated by this numerical simulation.

$$T_{\mathrm{HapCurr}} = a(T_{\mathrm{SimCurr}} - T_{\mathrm{SimMin}}) + T_{\mathrm{HapMin}}, \qquad (8)$$
$$a = \frac{T_{\mathrm{HapMax}} - T_{\mathrm{HapMin}}}{T_{\mathrm{SimMax}} - T_{\mathrm{SimMin}}},$$

where $T_{\mathrm{HapCurr}}, T_{\mathrm{HapMax}}, T_{\mathrm{HapMin}}$ mean the temperature of haptic device. “Curr” means current temperature and “Max” and “Min” indicate maximum and minimum. $T_{\mathrm{SimCurr}}, T_{\mathrm{SimMax}}, T_{\mathrm{SimMin}}$ also mean the temperature of the numerical simulation result.

This device is able to show colder and hotter information, but we cannot stay touching the device.

This 3D image is drawn by using a general visualization tool, a Visualization Toolkit (VTK) [11], and OpenGL. A VTK is a toolkit for visualizing scientific data and has many functions. The visualized image is projected on the Angle-changeable Immersive Projection Display [12], which has been developed by us. The Angle-changeable Immersive Projection Display is a type of IPT display, and it can show stereoscopic images. Above all, this screen system can be freely moved in the vertical and horizontal directions. When we want to see the left-side image, we can physically move the screen to the left and see the image. By using this system, the observer can see 3D objects from various positions and angles.

In this system, the observer uses a 3D mouse and the proposed thermal display. The observer changes his/her position and angle by using the 3D mouse and can feel the temperature at that position.

5. Conclusion

We proposed a thermal display that can simultaneously represent temperature change information and absolute temperature. This display consists of two Peltier elements and these two elements provides absolute temperature and temperature change information. We experiment the relationship between the electric current and the temperature on the Peltier element. As a result of that, we can control the temperature of the surface correctly. By this device slow and small thermal changes can also be recognized. This device is effective in rapidly providing the thermal change information, in particular, in the IPT display environment, where the observers can move freely and the value changes frequently. Then we can intuitively feel the thermal distribution when we observe other data such as pressure and magnetic field; if the data is not visible, we can feel the data by hands or other part. Finally we apply this device for representing the result of molecular dynamics simulation.

Acknowledgment

This study was funded partly by a Grant-in-Aid for Scientific Research KAKENHI (19700122) and the Hirao Taro Foundation of the Konan University Association for Academic Research, Japan.

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