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Communication

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ConfChem Conference on Interactive Visualizations for Chemistry Teaching and Learning: Learning by Being—Playing Particles in the MeParticle–WeMatter Simulation

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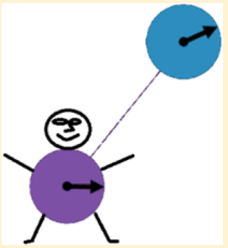
Supporting Information

ABSTRACT: MeParticle–WeMatter is a participatory simulation in which students play the role of particles to learn about the structure and properties of matter. The students navigate their particle in a multiparticle environment, as they are pulled or pushed by Lennard-Jones forces. We show how the student control of the particles resembles a random heating algorithm and describe a quasi-experimental setup to study how participating as particles in this environment contributes to learning. This communication summarizes one of the invited papers to the ConfChem online conference Interactive Visualizations for Chemistry Teaching and Learning, held from May 8 to June 4, 2015 and hosted by the American Chemical Society Division of Chemical Education Committee on Computers in Chemical Education.



KEYWORDS: *Elementary/Middle School Science, Computer-Based Learning*

PARTICIPATORY SIMULATIONS

In most educational dynamic simulations of particle models, students act as observers of the model and can manipulate only its macroscopic properties.[1,2] We suggest that emergent phenomena such as phase change could be better understood if students participate as individual particle-agents in the simulation. The idea of participation as student-agents who induce phase change exemplifies a class of role-playing simulations named participatory simulations. Participatory simulations are computational environments in which the collaborative behavior of individual actors produces a global pattern.[3,4]

We developed a participatory simulation, MeParticle–WeMatter[5] in which students play the role of particles in a 2D Lennard-Jones fluid. The simulation, which was created with the agent-based modeling environment NetLogo[6] and the server-client HubNet platform,[3] allows students to navigate their particle-avatar in a multiparticle environment in which both computer-controlled particles and student-controlled ones are interacting through Lennard-Jones forces. The position and velocity of the particles is updated using a molecular dynamics algorithm.[7] Particles are represented by circles with arrows indicating the particle's direction of motion. The interparticle attractive forces are indicated by dashed lines with varying width that represent their relative strength (Figure 1).

IMPLEMENTING THE SIMULATION

In the MeParticle–WeMatter simulation, students control the motion of their particle using control buttons. Each click of the "Forward" button moves the particle forward by a fixed displacement, and the "Left" and "Right" buttons change its heading by a fixed angle.[8] However, the calculation of the new position is also influenced by the acceleration, which is calculated from the interparticle Lennard-Jones forces. The students are told their task is to induce phase change as particles that are excited by an external source of energy (e.g., radiation) and transfer energy to other particles.

The temperature is calculated as an average of the kinetic energies of the particles. The temperature–time graph is then directly related to the collective behavior of the students-particles in the simulation. Boiling is represented as the dissociation of the dense local particle structure, and the appearance of a homogeneous, loose configuration such as the one shown in Figure 1. Various aspects of the shape of the graph (e.g., "boiling" temperature, slope of the graph while heating) can be examined by changing the amount of the computer-controlled particles, the interaction strength between the particles, and other properties of the system.

The pattern of the temperature–time graph during phase change for a stochastic "heating" of a system of 200 particles at a constant rate[9] yields a linear (although "bumpy") ascending temperature–time slope initially and then a plateau. Varying the interparticle interaction strength changes both the computational boiling point and the latent heat of vaporization, as evident in the graphs of Figure 2.

The overall emergent pattern of the temperature–time graph is also apparent when students move the particles themselves and heat the liquid by pushing the computer-controlled particles, as shown in Figure 3.

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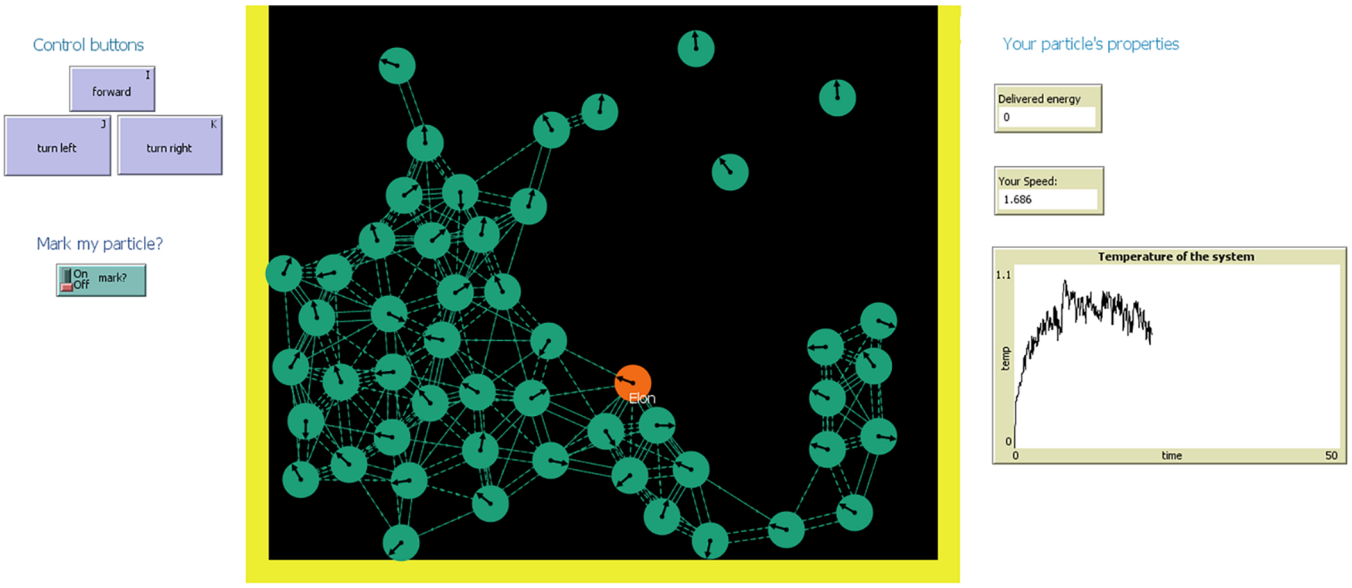

Figure 1. Screenshot of the participatory simulation. Turquoise-colored particles are controlled by the computer; the orange particle at the bottom is controlled by a student. Control buttons are shown on the left side of the simulated system; the temperature−time graph on the right. When several students are using the simulation together; "Mark my particle?" is used to discern their own particle from the rest.

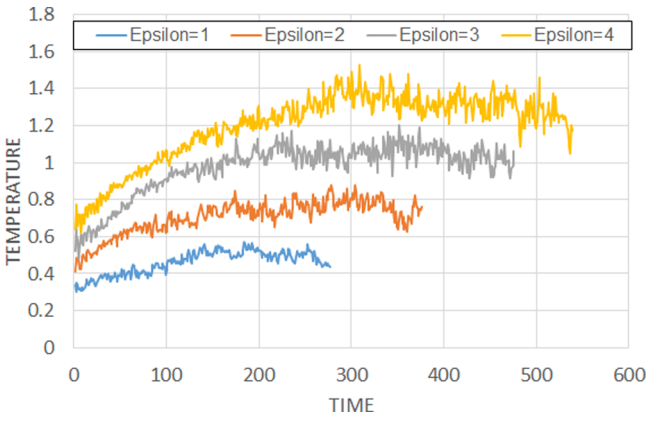

Figure 2. Variation of heating curves with the strength of the interparticle interaction (represented in the Lennard-Jones potential as the variable Epsilon) for N = 200 particles. Temperature and time units are model-based units, which can be related to real units using a straightforward calculation.[7]

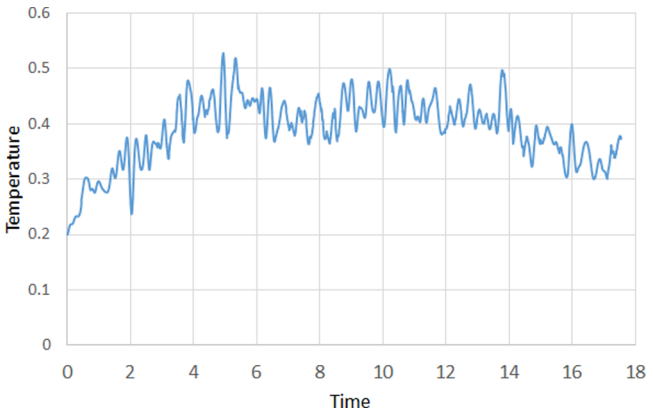

Figure 3. Temperature trend of heating N = 50 computer-controlled particles by one student-controlled particle.

To examine the effect of participation on learning with the MeParticle−WeMatter simulation, we conducted several pilot studies in 9th grade classrooms. We compared learning using the participatory simulation with learning by merely observing the stochastic heating process implemented by the simulation algorithm (which produces the pattern of Figure 2). The lesson began with a physical experiment highlighting the difference in vaporization rates of similar amounts of ethanol and water at room temperature. Then, the simulation was used to introduce the particle model explanation of vaporization. In the "observation" classroom, the simulation was controlled by the teacher and projected on a screen, showing the particle configuration and the heating curves. In a second "participatory" classroom, students actively "played" the role of particles that "push" other particles and induce their vaporization. Pretest and posttest questionnaires showed that the students in the participatory classroom had, on average, larger learning gains than their counterparts in the "observation" classroom. The difference was significant in understanding the relation between particle motion and temperature, and linking the evaporation rate to intermolecular bond strength. A more controlled study of the effect of participation as particles is currently in preparation.

THE CONFCHEM DISCUSSION

The ConfChem discussion on the paper (see the Supporting Information) allowed participants to post several queries on both technical aspects of the simulation (e.g., the relation of the simulation's temperature to measurable temperatures) as well as possibilities for implementation of the simulation in the classroom. Participants in the forum[10] questioned the advantage of a computer simulation over a "whole body" showmanship of the model by students moving themselves in the classroom. We presented our position that the advantage of playing particles in this computational simulation as compared with a physical role-playing simulation is the inclusion of information regarding the interparticle forces and a dual local-global view of the system. Attending to these two aspects—the

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electronic pulls and pushes as well as the particle's environment—is important for linking the local interactions and the global pattern that emerges. Other questions addressed the way students perceive their control over the particles and the social interactions among the students who enact their particle in the same particle environment. In response, we argued that students perceive their particle as a tool they can use to change the system without personally identifying with it. However, students are allowed to pick a "particle name", which creates a social stir, as students pick humorous and sometimes provocative nicknames. The social aspect of the activity will be studied in the near future.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00443.

The ConfChem paper and discussion (PDF)

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Notes

The authors declare no competing financial interest.

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(8) We chose a polar coordinate system (displacement, angle) rather than a Cartesian one, in order to encourage a 'looking-forward' perspective.

(9) The time step is set to $\Delta t = 0.01$. Energy is added every 100 time steps by increasing the velocity of two randomly picked particles by $\Delta v = 1$.

(10) American Chemical Society, Division of Chemical Education, Committee on Computers in Chemical Education. 2015 Spring ConfChem: Interactive Visualizations for Chemistry Teaching and Learning. http://confchem.ccce.divched.org/2015SpringConfChem (accessed Dec 2015).

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