Learning by Being: Playing Particles in the MeParticle-WeMatter Simulation

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Abstract

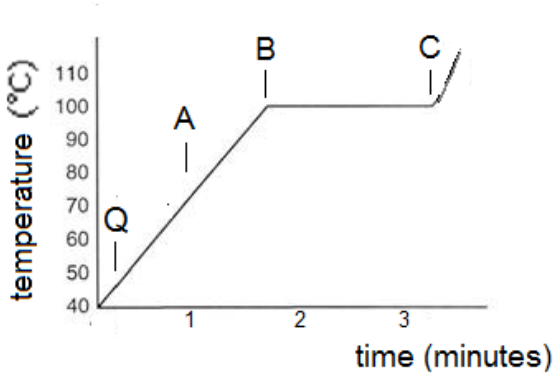
MeParticle-WeMatter is a participatory simulation in which students play the role of particles. The students "drive" their particle and navigate in a multi-particle environment, as they are pulled or pushed by Lennard-Jones forces. We have used a quasi-experimental setup to study how participating as particles in this environment contributes to learning. The study focuses on an activity in which the students "heat" the particle fluid by colliding with the surrounding particles. 9th grade classrooms were assigned to two conditions: in one group students played the role of particles, and in the other group, students observed the simulation without participating as particles. In the paper we will report on the structure of the simulation as well as the learning gains for the two conditions.

Introduction

The plateau of the temperature/time graph that appears when a substance goes through a phase transition, is one of the first emergent phenomena introduced to students in science classes. Emergent phenomena are explained using complex system models that link the macroscopic behavior to the interactions of the micro-level entities. These models are more intricate and complex than most sequential and causal models (e.g. planetary motion) that the students learn up to that point (Lehrer and Schauble 2006). Nevertheless, according to common core standards, by the end of 8^{th} or 9^{th} students are expected to explain the emerging plateau of the temperature vs heat/time graph. (A framework for K-12 Science Education 2012, pp 235-237). The expected explanation may vary from a macro-level explanation (e.g. " the temperature remains constant because the material changes from liquid to gas") to a micro level explanation of the phase change mechanism (e.g " The constant temperature means that heat is consumed in breaking the bonds between the particles and does not change their average kinetic energy"). We adopt the latter expectation – that students should be able to use particle properties to explain the macroscopic emergent phenomenon.

Many studies discuss student ideas about the particle model of matter (e.g. Johnson, 1998, Harrison and Treagust, 2002, Pozo & Gomez Crespo, 2005) and computational visualizations have become increasingly popular tools for teaching this subject (Smetana et al 2011). Many of these studies report significant effectiveness of computer simulations in shaping student ideas related to the particle model (Levy & Wilensky 2009, Stern et al., 2008, Plass et al 2012). Even though simulations have aided learning of the particle model, research reports indicate that it is difficult for students to fully use its richness for explanations of macroscopic phenomena. For example, after finishing a computer based "phase change" module, high-school students were asked to answer the following question:

A sample of water is heated from a liquid at 40^0C to a gas at 110^0C. The heating curve is shown below:



Which section of the graph shows a phase change in the water sample?

(i) QA (ii) AB (iii) BC

Explain your choice. In your explanation, include what is happening to the water molecules.

Figure 1: Phase change questionnaire item (adapted from D. Levy, 2013)

Only 5% of about 600 students in grades 9^{th}-12^{th} mentioned that the phase change that occurs in the section BC on the graph is related to a change in inter-particle bonding(D. Levy, 2013). This shows that learning about phase change using simulations and animations can still be improved. We suggest that using a model that provides a better acquaintance with the particle level interactions, and enables explicating the global properties, can be a powerful learning tool for learning about phase change. The model is implemented in a novel learning environment "MeParticle WeMatter" that puts the students in the shoes of particles that interact via Lennard-Jones forces. We discuss the structure of the simulation and its use for producing the emergent plateau in the temperature graph. Finally, we report some student learning outcomes that demonstrate how the environment enables a deeper awareness of the local particle interactions for explaining the emergence of the plateau in temperature-time graph.

Learning about phase change using dynamic computer simulations.

Modeling phase change through a complex systems perspective mandates a learning environment that is different from most current educational technologies. Let us examine the common template of simulations that were developed to promote understanding of the micro and macro levels of processes such as phase change. As an example, we examine the simulations used in previous studies (Xie & Pallant 2011, Plass et al., 2012). Most these simulations utilize an interface similar to the one in Figure 2:

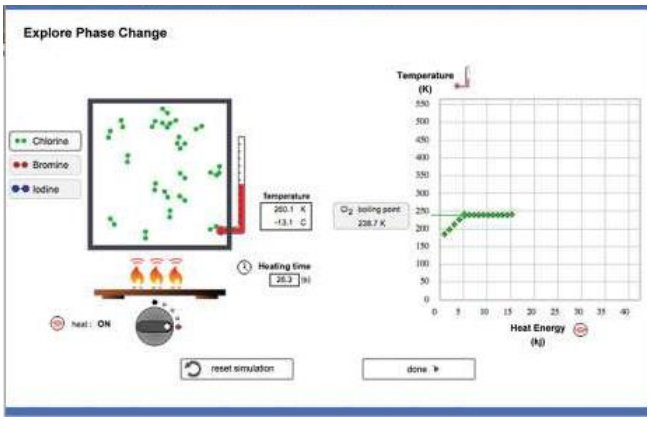


Figure 2: Simulation interface screenshot (reproduced with permission from Plass et al., 2012

The first common feature of the simulation is a display, which usually includes a particle level representation on one side and a macroscopic descriptor on the other. In the Figure 2: the macroscopic descriptor is the temperature/heat graph that is correlated with the animation of the moving particles by simultaneously updating the two representations.

Another common characteristic of these simulations concerns the mode of students' participation. In most simulations, students participate as observers of the process and can manipulate some of its features such as the heating rate or the type of materials that are being heated. Learning about emergent phenomena involves careful attention to individual behaviors, their local interactions, including heuristics such as mid-level construction (Levy & Wilensky, 2008) to reason about interactions in close range, and their extrapolation to global changes to the system. Shifting the focus to a framework of emergent behaviors requires an examination of the opportunities provided by the simulation to explore the local particle perspective and to bridge the particle perspective and that of the macro phenomenon.

The choice of representation in educational simulations is designed to facilitate cognitive processing of the visual information by using iconic symbols that are straightforward to interpret and dynamics that are easy to follow (Plass et al., 2009, Akaygun & Jones 2013). For example, the simulation in Figure 2 portrays relatively few particles (~20 diatomic molecules). Both representations – that of the particles in the vessel and the temperature graph are updated simultaneously on the screen to show their connection.

However, this representation entails a serious idealization of the real equivalent system that is not made explicit to the students. It is clear that measuring the temperature of a real system made of 20 molecules during heating would not produce a smooth temperature vs. time graph. 20 particles would produce a fluctuating bumpy graph that does not quite yield the horizontal plateau. Therefore, we can assume that the points on the graph in Figure 2 are not derived from average velocities produced by the commonly used molecular dynamics algorithm. If the temperature display would have been derived from the average of the square of the particles' velocities, it would not produce a smooth plateau as the one in figure 2 rather a much 'messier' and bumpy graph such as the one in figure 5 below. To obtain a smooth graph one has to simulate the behavior of a very large amount of particles, which requires substantial calculation power, not afforded by standard computers. Given the fact that the temperature vs. time graphs of the educational simulations that usually contain a small number of particles, cannot produce the smooth plateau, it is not

surprising that these simulations avoid displaying the simulation averages to the students and replace those with fabricated ones.

These animated representations may be easier for connecting the textbook concepts and the dynamic simulations, reducing the students' cognitive load (Sweller 1999) which would be required for the interpretation of a more fuzzy and detailed graph. However, by preferring the simplicity of the fabricated representations over the genuine simulation averages students may lose an opportunity to learn. System averages derived from computational models can facilitate sophisticated micro-macro connections of the behavior of the system among regular secondary school students (Wilensky 2003). Framing the phenomenon as emergent requires more awareness to the micro-macro connections in the computational model. Thus, when engaging students in learning about phase change should entail the examination of real time, simulation averages.

Table 1: Comparison of approaches and related simulations that build upon traditional versus an emergence perspective

	Quantification of macroscopic properties	Student perspective and control
Traditional dynamic simulations	Idealized, not derived from simulation averages	Observe the particle level visualization, control macroscopic properties only
Emergent phenomena approach	Messy, based on the simulation's statistical averages	Observe the particle level visualization, partial control over particle level occurrences

The second aspect of the simulations that differs in our approach is the students' mode of participation. In most simulations, students act as observers and manipulate the macroscopic properties of the model. Rarely do students focus on the local interactions of individual particles, and attribute the local occurrences of the particles to macroscopic changes in the system. One way to achieve deeper awareness of the particle level interactions is through engagement in programing the model itself (Wilensky and Reisman 2006, Blikstein and Wilensky 2009). However, constructing computational models requires background knowledge in programing. Introducing students to the particle perspective without requiring students to construct the model themselves can be achieved through participatory simulations.

Participatory simulations are computational environments in which the collaborative behavior of individual actors produces a global pattern. For example, in the "Disease" participatory simulation (Wilensky and Stroup 1999; Colella 2000) students move in a room, and one of them carries a virus. The disease then propagates in the room as other students get 'infected' and the emergent phenomenon is the propagation dynamics, i.e. the amount of infected people vs. time. The students in the participatory simulation gain an individual perspective by playing people moving about when one of them gets infected, and are experience the propagation of disease both at as individuals (interactions between healthy and sick people) and as the group's disease propagation dynamics.

Learning about phase change using a participatory simulation

We suggest that emergent processes such as the plateau in the temperature/time graph of Figure 1. could be better understood if students participate as individual particle-agents in the simulation. In order to

explore this avenue, we developed a participatory simulation, MeParticle-WeMatter (Roller et al., 2014) 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 (Wilensky, 1999) and the server-client HubNet platform (Wilensky & Stroup, 1999), allows students to navigate their particle-avatar in a multi-particle environment in which computer-controlled particles move according to Lennard-Jones forces using a molecular-dynamics algorithm (Verlet, 1967).

Explaining vaporization relies on three linkages between particles' (agent) level properties and the global, macro aspects of the phenomenon: 1. Temperature (global feature) is a measure of the average kinetic energies of the particles. 2. Heat transfer (global feature) results from particle collisions and momentum transfer that increases the average kinetic energy of the particles in the liquid. 3. During phase change, the density of the material changes drastically (global feature) which entails a sharp increase in the average inter-particle distances. When particles move away from the liquid, they slow down because the inter-particle forces hold them back, therefore for some of the particles the average energy decreases. In the MeParticle WeMatter simulation, students can induce phase change in the system by colliding with the computer-controlled particles. The collisions can either increase the other particle's velocity or break the intermolecular bonds between them. The temperature versus time graph is then directly related to the collective behavior of the students-particles in the simulation. Various aspects of the emergent pattern such as changing the amount of the fluid (computer-controlled) particles, the bond strength between the particles and other properties of the system could then be explored. Similar to most other educational simulations we use a two dimensional model which is more straightforward. The particles are represent by circles with an arrow indicating the particle's direction of motion, and the inter-particle attractive forces are represented as dashed lines with varying width that represent their strength. (Figure 5). The force cutoff is taken to be 2.5 times the radius of the particle which is common practice for Lennard-Jones models (Frenkel and Smit 2002).

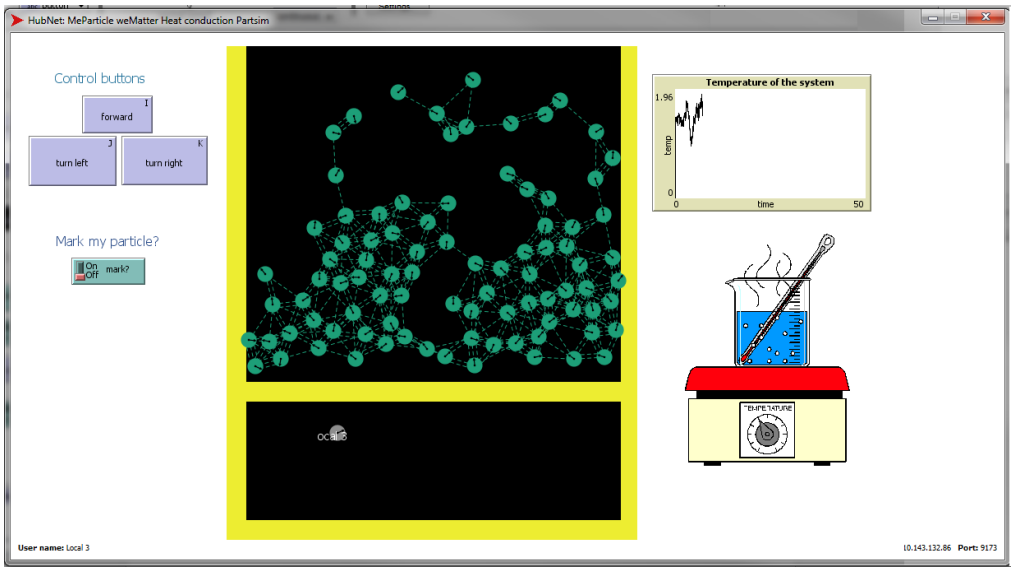


Figure 3: the participatory simulation screenshot. The turquoise particles are controlled by the computer and the grey particle at the bottom is an avatar controlled by a student. The control keys

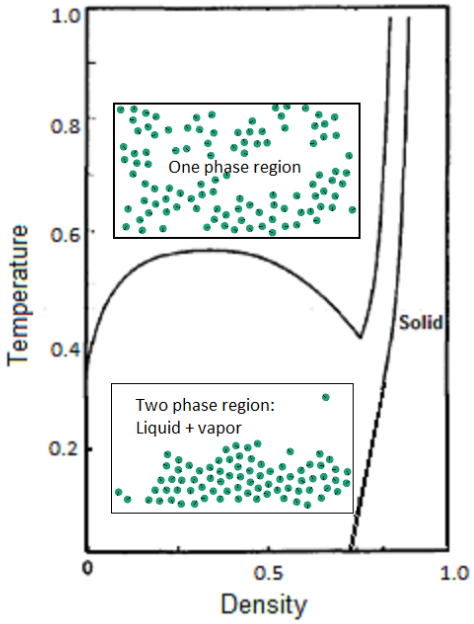
are shown on the left side of the simulated system and the macroscopic equivalent of the system and the temperature graph are shown on the right.

The simulation can be used in two modes: in the 'heat conduction' mode student particles lie outside the area of the computer-controlled particle fluid as shown in figure 3. In the 'heat radiation/convection' mode, student particles are inside the liquid and represent particles that absorb radiation energy and transfer it to their neighboring particles. The two modes serve complementary purposes: the "in liquid" radiation/convection mode engages students in experiencing the difficulty of moving inside a dense fluid, hindered by attraction forces. The heat conduction mode is better for realizing the cascading collision motion among the liquid particles that may lead to the release of particles from the upper surface.

One may question the scientific correctness of this setup. How can particles that are operated by rational players represent a phenomenon that is in reality stochastic? In the next sections we discuss the structure of the simulation code and show that it produces an emergent plateau during vaporization. We also explain how the student participation induces results bare similarity to the results of simulating a random heating process despite some deviations.

The 2D Lennard-Jones Fluid.

Models of a 3D system of particles interacting through the Lennard-Jones system produces a phase behavior that agrees with measured properties of Noble gases such as Argon (Verlet 1967). By contrast, the 2D Lennard-Jones fluid model is probably too simplistic to predict the behavior of experimentally observable 2D systems[1]. The phase diagram of the 2D Lennard-Jones system is show in figure 4:



[1] 2D systems of particles are either adsorbed on surface or kept at a liquid-gas interface. A Lennard Jones model is not appropriate for modeling these systems since does not account for interactions of the monolayer with the substrate or for capillary waves in the liquid.

Figure 4: Phase diagram of the 2D Lennard Jones fluid (based on Abraham, 1981)

Since in this paper we study the process of vaporization, we are interested in the transition between the two-phase liquid + gas region and the one-phase vapor region above it. The phase diagram of the 2D system indicates that the transition from the two phase Liquid+Gas region into the gas region occurs at a reduced temperature value of around $T \sim 0.4 - 0.55$ depending on the density of the fluid (for densities below 0.7).

The molecular dynamics algorithm for the 2D Lennard Jones fluid, is the same as the 3D model proposed by Verlet (1967). However, the force and the displacement are calculated for only two axes instead of three:

$$F_x(r_{ij}) = \frac{24\varepsilon}{\sigma^2}(x_i - x_j)\left[2\left(\frac{\sigma}{r_{ij}}\right)^{14} - \left(\frac{\sigma}{r_{ij}}\right)^{8}\right]$$

Here σ is the effective diameter of the particle (the inter-particle distance at which the potential is zero) and ε is the energy at the minimum of the potential well and r_{ij} is the distance between the centers of two particles i,j. The acceleration of a given particle *i* is calculated from a sum of all the forces induced on the particle by its j neighboring particles:

$$a_{ix} = \frac{1}{m}\sum_j F_x(r_{ij})$$

The Verlet integration algorithm, assigns the new particle position according to the previous positions and the acceleration. An introduction to molecular dynamics simulations and specifically to the Verlet algorithm and its advantages can be found in Lamberti et al 2002, a more comprehensive discussion can be found in Frenkel and Smit (2002).

At the initialization of the program, the computer-controlled particles are distributed either randomly or in a form of a hexagonal lattice with a separation distance of 1.1σ at which the potential is almost at its minimum value. The particles are assigned random velocities according to the given temperature of the system. The particles controlled by the students are either distributed among the computer-controlled particles or in a compartment below the simulated liquid as shown in figure 3. The students can then move their particles but their control is partial since their particles are also influenced by the forces induced by neighboring particles. If students direct their particle to bump into a computer controlled particle, an elastic collision algorithm is executed and the particles collide and bounce off so that their overall momenta is conserved. The collision algorithm was chosen since it provides an immediate change in velocity in both particles that is congruent with students' previous experience with a head-on collisions.

In order to conserve momentum, the velocity of the particle is then updated according to the initial velocities and direction of the two particles without changing their current position. The student particles have an upper limit velocity in order to ensure that the perturbation in the velocity of the computer controlled particle won't move the particle in a way that would create an overlap between particles thereby inducing an extremely high repulsion force and acceleration.

Comparison of student controlled evaporation and simulated evaporation dynamics

Does the student behavior indeed produce a pattern that resembles the macroscopic temperature/ time plateau? First, we checked whether this pattern is observable when we introduce random "heating of a 2D fluid". In order to simulate evaporation of a fluid, we initialize the program with the particles arranged in a hexagonal lattice at the bottom of the vessel. We implement a rule in the program that when a particle reaches the upper boundary of the container it disappears and its location is no longer considered when calculating the forces and the average velocity. We also impose a constant downward acceleration on all particles to prevent the entire bulk of the fluid from moving upward at once. The simulation is initiated with a temperature of T=0.25 and runs until 25% of the particles "die off" at the upper boundary. The time step is set to $\Delta t=0.01$ and heat is added every 100 time steps by increasing the velocity of two, randomly picked particles by $\Delta v=1$. When considering 200 particles, this perturbation should lead to an increase of $\Delta T=0.01$ per one unit of time. However, due to the Lennard-Jones interactions, some of the energy is consumed in loosening the bonds and the heating rate is not constant. After reaching a transition temperature, many particles are no longer bound to the bulk and the ones with higher velocities start to leave the system. Every time a fast molecule leaves the fluid, the temperature which corresponds to the average square of the velocities decreases. This leads to an emergent plateau in temperature/time graph which can be seen in the graphs of figure 5. The temperature at which the plateau occurs, and the time interval at which 25% of the 200 particles "evaporate" both increase when the bond energy ("Epsilon") increases as shown in figure 5.

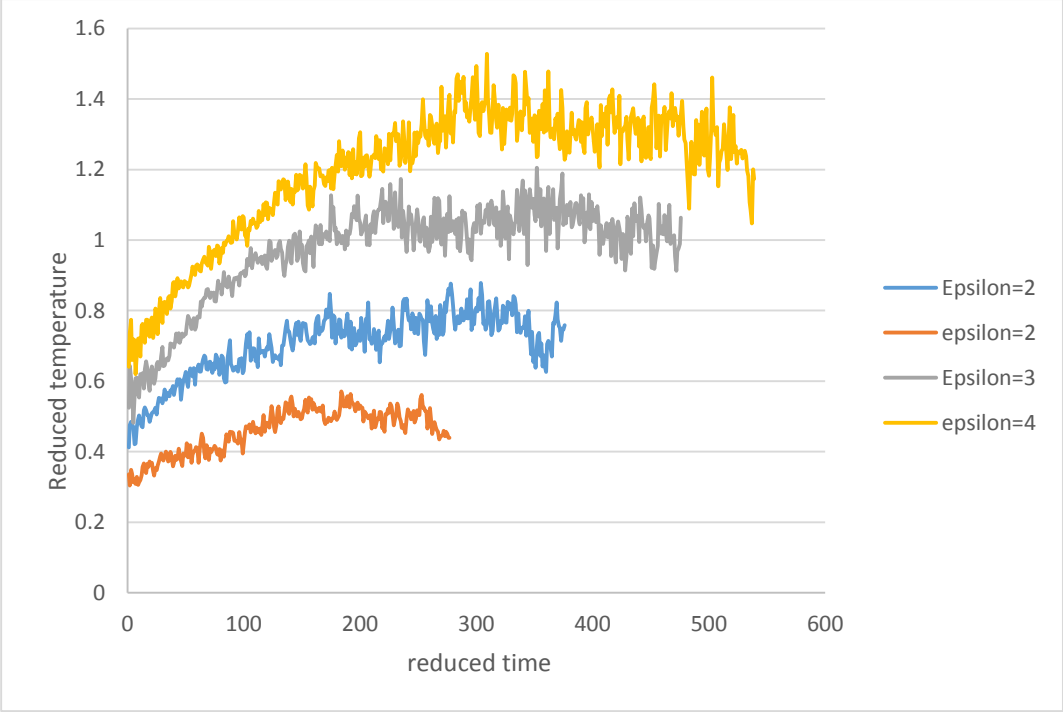


Figure 5: Variation of heating curves with the strength of the interaction for N=200 particles. The plateau in the $\varepsilon = 1$ curve occurs at approximately T=0.5 which is similar to the value for the liquid to gas transition indicated in figure 4.

The collisions of the student controlled particles with computer controlled particles do not occur at constant a rate nor do they hit a particle randomly, however, the pattern of the temperature/time graph produced by the students is similar to the graph in figure 5, but the temperature reached in the simulation is much higher than the one observed in the randomly simulated heating. A possible explanation for this difference is rooted in the fact that students tend to hit the same particle multiple times, thereby increasing its velocity much more than the random heating algorithm. In addition, the number of particles in the system is 50 (versus N=200 in figure 5), which gives more weight to the velocity of the individual particles. However, the overall emergent pattern of the temperature / time graph is similar and once the fast moving particle leaves the system the average velocity squared of the particles in the system decreases.

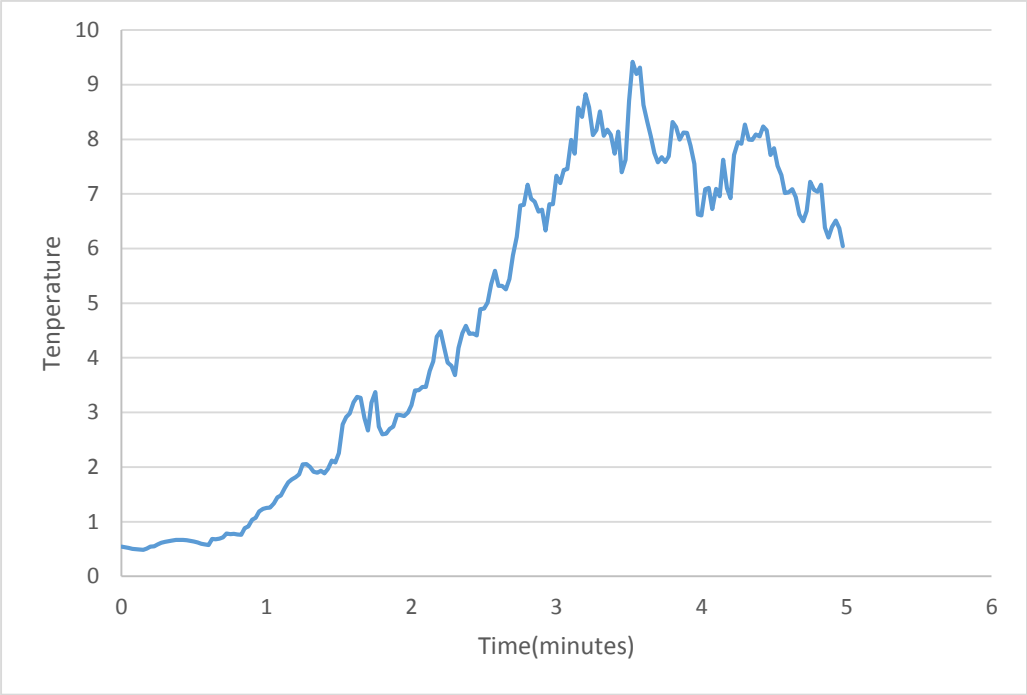


Figure 6: The temperature of the simulation when particles are heated by students in a classroom with N=24 computers. During the initiall 40 seconds, student control was disabled so that the system could equilibrate.

Implementation of the participatory simulation in the classroom

The effect of student participation as particles in the simulation, has been studies in 9th-grade classrooms in a public school in the US. The simulation had been introduced after a demonstrating the difference in evaporation rate of water and acetone using a digital scale. The variables that influence evaporation rate was discussed in whole classroom forum, and then the model was briefly presented to the entire class. In the next lesson, the study group played the role of particles and simulated evaporation under various conditions (number of fluid particles, strength of bonds) while a different group only observed the model on the board. We used pre/post questionnaires to compare the performance of a classroom who just observed the model, to students who role-played particles in the simulation. The classroom who merely observed the model was an honors classroom while the classroom in which the students role-played was a regular classroom. The study revealed that the average pre-test scores of the control (honors) classroom

were higher than the score of the regular one and a higher gain of the participating group in relating macroscopic features to the behavior of the particles. The percent of correct responses on the post test, i when relating temperature to particle motion, than when relating the plateau in the graph to the bonds as shown in figure 7.

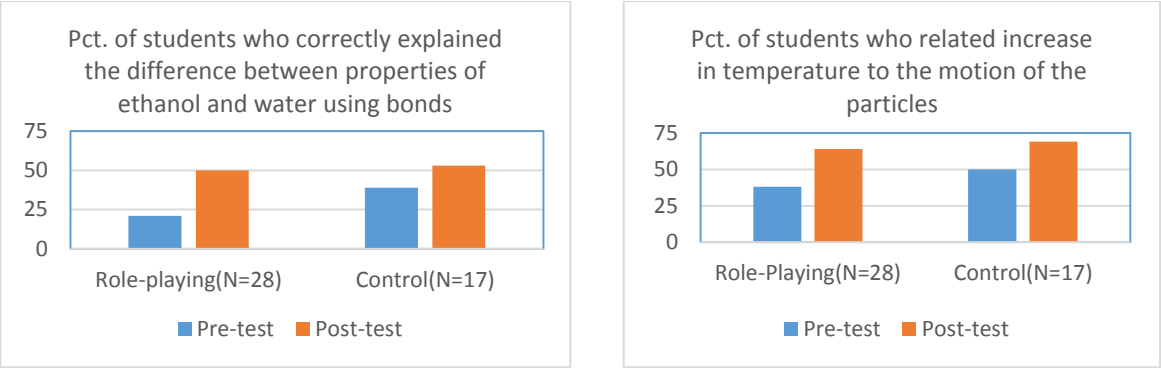


Figure 7: student performance on questions that require to explain macro-scale behavior to particle level properties.

Summary

Our findings show that the participatory simulation in which student play the role of particles in a liquid improves student abilities to explain macroscopic phenomena using particle level properties. However, the results are far from being satisfying, with almost 50% of the classroom giving incorrect, or partial responses. The mediocre results reflect the time allotted for the unit - a two period sequence - which is probably too short for capturing the intricacies of the three dimensions of the explanation mentioned above: the relation between temperature and kinetic energy, understanding heat transfer as a propagation of collisions and the slowing down effect due to bond breaking. In addition, the comparison is problematic, since these two groups have different characteristics (honors and regular classes), and in addition the learning time in each group was not identical – the role-playing group spent more time learning than the honors group. In a subsequent study we extended the classroom unit into a three lesson sequence and made sure that the groups were balanced and were spending the same time on learning the topic. We hope to analyze the data and report on the results soon.

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