A unified approach to explain thermo-fluid science concepts using interactive molecular-level simulations

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Abstract

Engineering students may possess misconceptions about topics in thermo-fluid sciences. These misconceptions, once formed, persist with students at the junior and senior levels. Educational research shows that learning is enhanced when concepts are described at the molecular level as emergent processes. A review of college textbooks used in the engineering curriculum revealed a mixed trend towards including molecular level descriptions of scientific processes. However, these descriptions are often not presented as emergent processes at the molecular level consistently when discussing topics. In support of an ongoing study, interactive molecular-level simulations have been created to help students develop an enhanced understanding of scientific processes in the thermal and fluid sciences.

Introduction

Are view of widely adopted college textbooks used in the engineering curriculum to teach introductory thermal and fluid sciences revealed a mixed trend towards including molecular level descriptions to explain fundamental concepts and processes[2,4-8,11-16,18,20,22,23,25,27,28,30]. Many of the textbooks reviewed included some molecular level descriptions, but the use of molecular level descriptions frequently did not extend across an entire subject. For instance, when discussing heat transfer many textbooks adopt a molecular level approach to describe conduction of heat by molecular vibrations in solids, but resort to a blackbody approach when discussing heat transfer by radiation. The blackbody approach introduces a hypothetical material called a blackbody that absorbs all wavelengths of radiation. Real materials are then modeled by how closely they resemble an imaginary blackbody[5,15,22,27].

Increased coverage of molecular level descriptions is encouraging because it is in line with educational research findings that suggest misconceptions about many difficult topics can be attributed to about a lack of understanding of emergent processes[9,24]. Most importantly the descriptions of difficult concepts at the molecular level as emergent processes can help students be mentally prepared to learn advanced and sophisticated concepts[29]. Emergent processes are more complicated processes than those of sequential processes. The main distinctions between the two scientific processes are the different ways the elements that make up each process interact with each other[9]. An emergent process is one that occurs by the collective actions of its individual elements. The elements operate in a continuous and disorganized fashion and have no clear beginning or end. For example, the elements in an emergent process interact with other elements in a uniform or indistinguishable and unrestricted manner, such as the molecular movement in a dye diffusing in water. A more specific example of emergence is the formation of a snowflake. The complex pattern of a snowflake is the emergent property that occurs by the disorganized actions of all of the constituent water molecules. Each water molecule bonds with its neighbors with no goal of creating a pattern and no molecule being more or less responsible for the pattern that develops. Examples of emergent processes include many of the concepts covered in engineering education (e.g., temperature, viscosity) which are due to the random interactions of atoms.

In contrast elements of a sequential process interact in a distinguishable and restricted manner such as in the process of building a skyscraper. Examples of sequential processes include most processes designed by people like machinery, software, or management hierarchies. In a car each part interacts in a predetermined with a limited number of other parts; spark plugs interact with pistons but not the tires. Each part has a specific role with an identifiable impact on the output; each gear has a quantifiable effect on the output. Sequential processes most often can be explained through macro-level observable descriptions. Emergent processes, on the other hand, require micro level descriptions of molecular movement and motions. The molecular approach towards explaining complicated scientific and emergent processes can be found in upper level textbooks such as Transport Phenomena by Bird et al[3]. Molecular level descriptions provide details about what exactly is happening within a scientific phenomenon, which students may otherwise invent the "happening" for themselves without being able to visualize the changes and interaction staking place at the molecular level. The incorrect assumptions and the happenings that students may make up without further validation could form the basis of misconceptions that are persistent and resistant to later correction[21,26].

The lack of consistent coverage of molecular level descriptions of some concepts and processes can partially be explained by the difficulty of explaining scientific processes as molecular actions with static images in a textbook. For instance, in *The Feynman Lectures on Physics*, Feynman expressed his frustration with using static images to describe concepts from an atomistic and molecular foundation[10].The increasing availability of computers and flexible software development environments enable educators to develop visually realistic simulations that can portray the complex processes at the molecular level.

We hypothesize that molecular level descriptions of foundational concepts in thermal and fluid sciences, supplemented by interactive computer simulations, can enhance student learning and help avoid forming misconceptions about these concepts. To this end, we created a series of interactive educational simulations to help convey the concepts of temperature, pressure, fluid shear stress, viscosity, and heat transfer mechanisms at the molecular level. We focused on these fundamental concepts, because educational research has identified these concepts as being particularly difficult to learn, and students develop misconceptions about these concepts that persist even after completion of upper level courses[21,26]. Our goal is to test our hypothesis on a group of first-year engineering students and quantify the effectiveness of using molecular level description approach to teaching thermal and fluid sciences with the help of interactive simulations. In this paper we discuss the design and development process of interactive computer simulations.

Background

It has been observed that some undergraduate students have difficulty understanding certain concepts in the engineering curriculum more than others. The thermal and fluid sciences are one area where misconceptions are prevalent, and persist in senior engineering students. Misconceptions in the thermal and fluid sciences also resist instruction and remedy interventions[17,19,29].

Misconceptions in thermal and fluid sciences may partly originate from the constructivist approach used to teach fundamental concepts[9]. The constructivists focus on student's current understanding of a subject as a foundation for further learning. This approach may not be useful when a student's fundamental understanding of a concept is flawed as is often observed in thermodynamics[17].A correct basis cannot always be established in a constructivist approach as students encounter some of these concepts in their daily lives and may have already formed misconceptions before encountering the subject in college. It is important to provide students with an accurate foundation on which to build, which is the purpose of introducing students to the emergent scientific process.

Scientific processes can be categorized as being emergent or sequential[9]. Some of the misconceptions encountered may be due to a fundamental mismatch in understanding of the common processes in the thermal and fluid sciences[9]. Students tend to have a strong grasp of sequential processes, because sequential processes are more visible in everyday life and more readily understood. In contrast, emergent processes possess properties that make them difficult to observe and to attribute cause and effect relationships to. Therefore students tend to have little to no understanding of emergent processes. In education it is typical to explain most concepts in the language of sequential processes. This may cause confusion about concepts in the thermal and fluid sciences that are emergent processes, because of a fundamental mismatch in the approach adopted to explain them[9]. Students may apply their knowledge of sequential processes to concepts that work in fundamentally different ways, resulting in misconceptions. These more complex and emergent concepts should be presented as emergent processes to prevent the development of misconceptions in students.

Other issues observed in education are that new concepts are typically presented in isolated sections and are not explicitly connected to a student's existing understanding by explaining the new concept's relationship with previous concepts. This can cause students to panic when presented with problems different or more complicated than example problems. For example, when we delivered a quiz in an undergraduate fluid mechanics course asking students to pick the graph that depicts the variation of shear stress within a Couette flow with a linear velocity profile, about 80% of the students failed to choose correctly. Because the information of shear stress is not being assimilated correctly, students often make their own incorrect connections, which may turn into fundamental misconceptions, and prevent students from correctly understanding the concept[9]. These misconnections, once made, are difficult to eliminate. It is important to properly introduce these concepts in a way that prevent the formation of misconceptions.

Explanation of interactive simulations

We used the Wolfram Mathematica software to create the interactive educational simulations to help students understand some difficult scientific concepts and phenomena at a micro level. Some of our simulations were adapted from the publicly available simulations at the Wolfram Demonstrations Project website[1]. The simulations we created adopt major simplifications to the underlying theory of each concept to enable interactivity while emphasizing the fundamental operations of the emergent process in a visually realistic fashion. For the purpose of our project, pairs of simulations were made to depict a process at the molecular level and to show the same process operating at the continuum level.

Temperature

In the engineering textbooks which we reviewed, they tend to discuss the history and differences between the Fahrenheit and Celsius scales[4,5,11,22,27,30]. Few textbooks included a section discussing the physical origin of temperature as the measure of molecular energy[12,25]. This type of coverage may leave students with an incomplete understanding of temperature, or even erroneous understanding as they try to apply their understanding of the gas phase to the liquid and solid phases of matter, leading to potential misconceptions in the phase change physics.

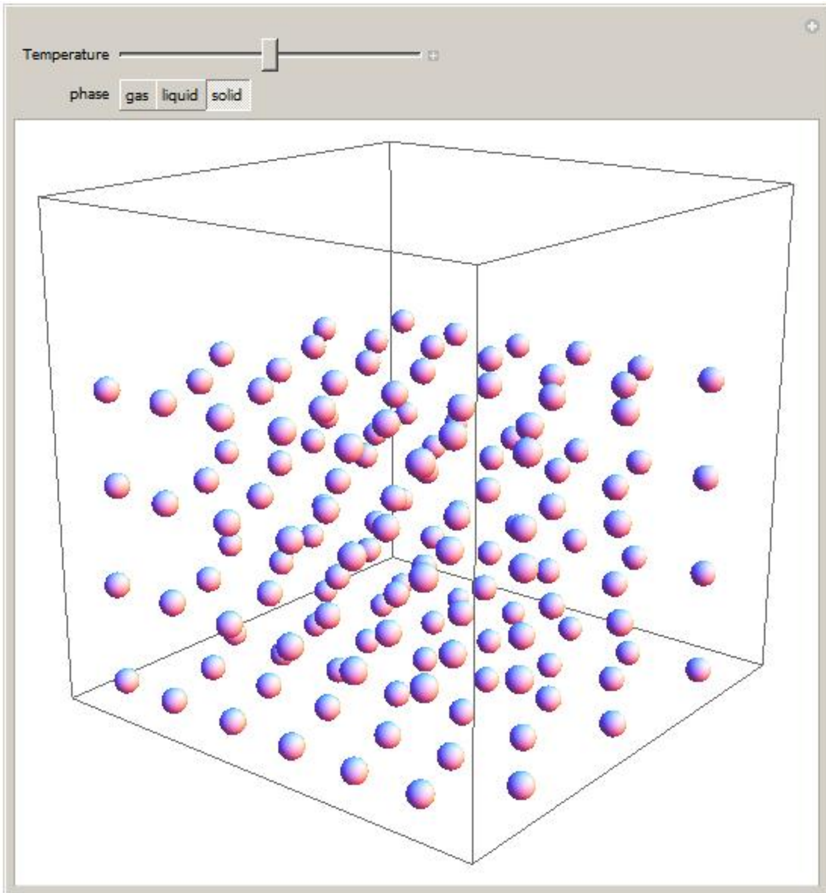

Figure 1. Screen shot of molecular motion animation in the solid phase.

In our instructional approach, temperature is explained as an ongoing process of kinetic energy transfer between molecules in the liquid and gas phases. Temperature in the solid phase is explained as a process by which individual molecular vibrations affect neighboring molecules causing vibrations throughout large areas of the structure. A change in temperature of an object is explained as being due to a change in the average molecular kinetic energy within the object.

The molecular level simulation shows the molecular motion associated with each phase of matter. The screen shot of the molecular motion simulation is shown in the solid phase in Figure 1. The phase of matter and energy of the system can be adjusted in order to demonstrate how molecular motion changes with changes in temperature. The continuum scale simulation depicts a thermometer in Fahrenheit and Celsius along with pictures of water. As the students change the temperature in the system the thermometer reads the temperature and the picture of water changes phases to illustrate how the scales were created.

Pressure

In the textbooks that we reviewed, pressure is often described at the continuum level within the context of liquid pressure due its own weight acting on a point[5,22,25]. The molecular origin of pressure tends to be discussed more often in newer editions of textbooks[12,27,30]. When the molecular origin of pressure is discussed, it is in the context of a gas in a sealed container.

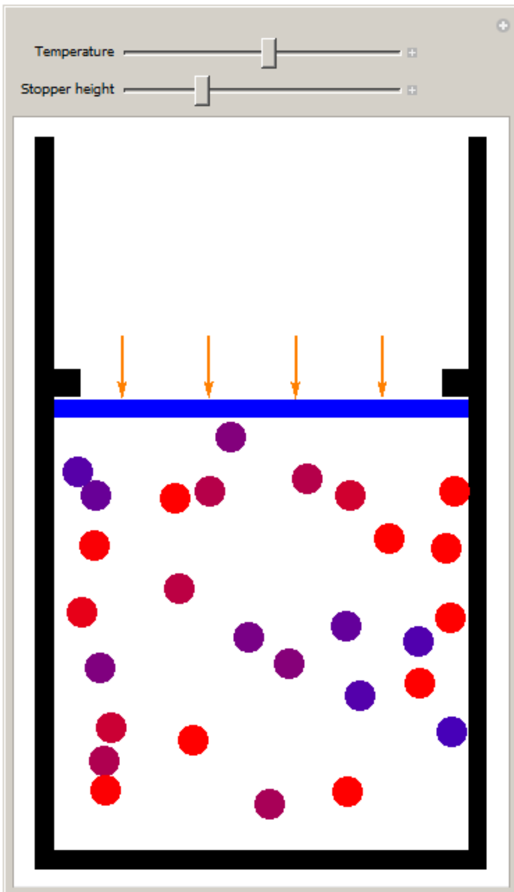

Figure 2. Molecular level animation to describe gas pressure in a piston-cylinder device

The molecular simulation of the concept of pressure is two dimensional, and depicts gas molecules inside a piston-cylinder (Fig. 2). The atmospheric molecules outside of the piston-cylinder are not shown for the sake of visual clarity. In the molecular level simulation the temperature of the molecules is shown with color; red for hot and blue for cold. The kinetic energy of the molecules follows an approximate Boltzmann distribution and is transferred between molecules during collisions. The piston deflects upwards when molecules strike it and falls otherwise. The simulation shows that pressure is due to molecular collisions, and how pressure varies with temperature and volume. Students are able to manipulate the temperature of the molecules and are able to constrain the maximum height of the piston. The continuum level simulation depicts a similar piston cylinder device with a pressure gauge that reads the absolute and gauge pressure.

Viscosity

In most of the introductory textbooks that we reviewed[8,18,27,28], the concept of viscosity is taught exclusively with the use of a simple flow example, called Couette flow, and with Newton's equation used to formulate shear stress as follows

$$\tau = \mu A \frac{du}{dy}. \quad (1)$$

One problem with this approach is that there is no explanation of why a certain velocity profile forms in a flow field, and why viscosity as a fluid property responds differently to temperature changes for gases and liquids. This approach does not delve into the origins of viscosity as the molecular transport of momentum, but describes viscosity as a measure of resistance to flow. Students are then expected to develop an understanding of fluid friction that may arise in fluids as invisible and light as air. Some students may just "accept" the concept, and develop their own interpretation of it to help in later topics, which may conflict with the core scientific principles.

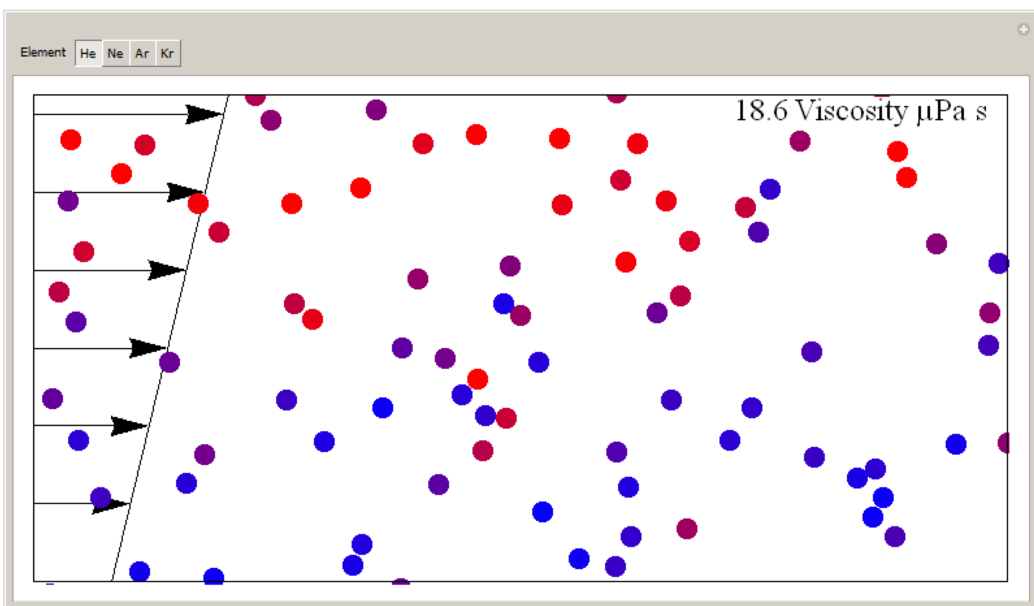

Figure 3.Animation of fluid flow illustrating the origins of viscosity.

In our study, viscosity is explained as a process of momentum transport at the molecular level, the mechanism of which is described separately for the liquid and gas phases. Viscosity and fluid friction is demonstrated with two molecular level simulations that are based on Couette flow. One viscosity simulation focuses on demonstrating viscosity as being the resistance to fluid flow. This simulation (Fig. 3) allows students to change the mass and size of molecules to observe the effects on fluid flow.

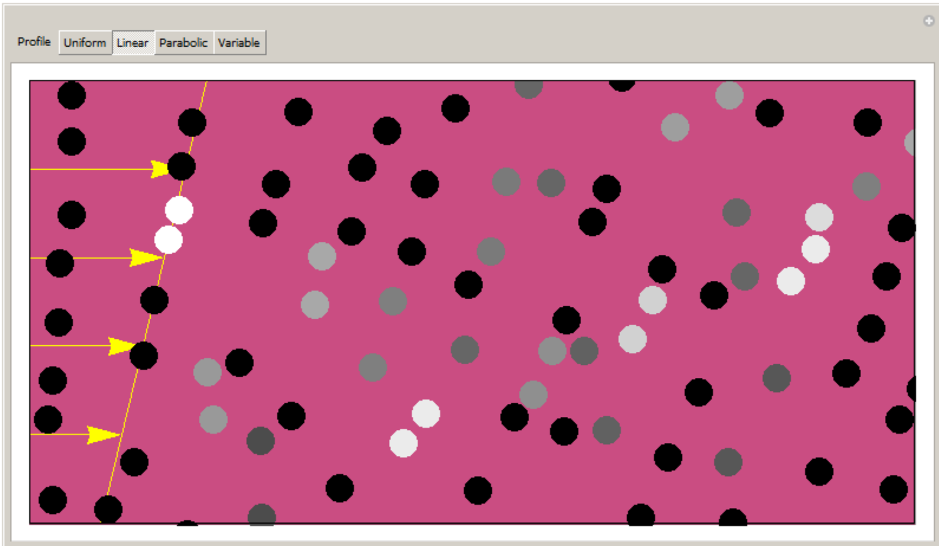

Figure 4.Animation of fluid flow illustrating the origins of fluid friction or shear stress.

The other molecular viscosity simulation focuses on illustrating the concept of fluid friction or shear stress. This shear stress simulation shown in Figure 4 allows student to vary the velocity profile of the fluid flow to observe changes in shear stress. This simulation includes four different flow profiles to provide students with a stronger basis for understanding other types of flow that is not normally provided in textbooks. The shear stress is visualized by the background color of the simulation and the color of the fluid molecules after collisions. When the fluid molecules collide their color changes briefly to highlight areas where collisions are frequent indicating areas of high momentum transfer.

Heat transfer

The heat transfer concept in our study discusses the concepts of heat, temperature, internal energy, and energy transfer by conduction, convection, and radiation. Conduction is explained as the transfer of molecular energy, and discussed separately for each phase of matter. The conduction simulation (Fig. 5) allows students to vary the temperature at one side of a non-metal solid to show the molecular motion of the solid as energy is conducted. In non-metal solids thermal conduction occurs by lattice vibrations in the structure of the solid, in metals and semiconductors thermal conduction mostly occurs by free electrons.

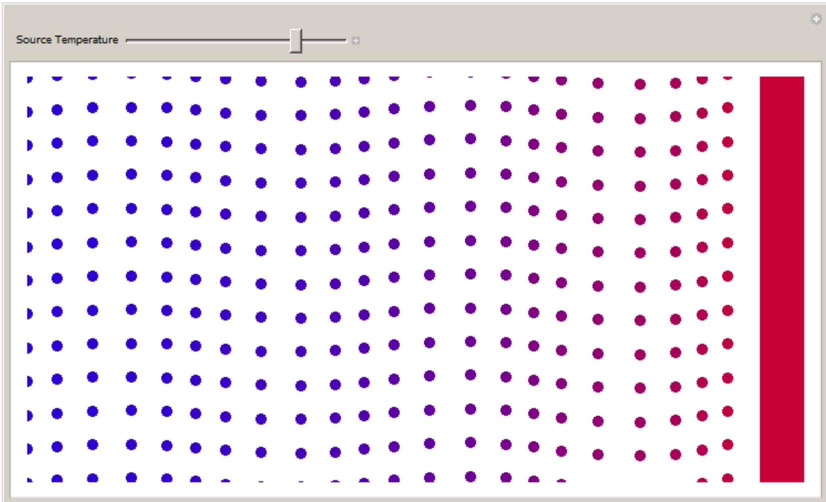

Figure 5. Molecular simulation of conduction heat transfer in a non-metallic solid

The convection concept is explained as a combination of conduction in the fluid and the bulk motion of the fluid in our study. The convection simulation (Fig. 6) shows fluid molecules removing energy from solid molecules as students vary the wind speed.

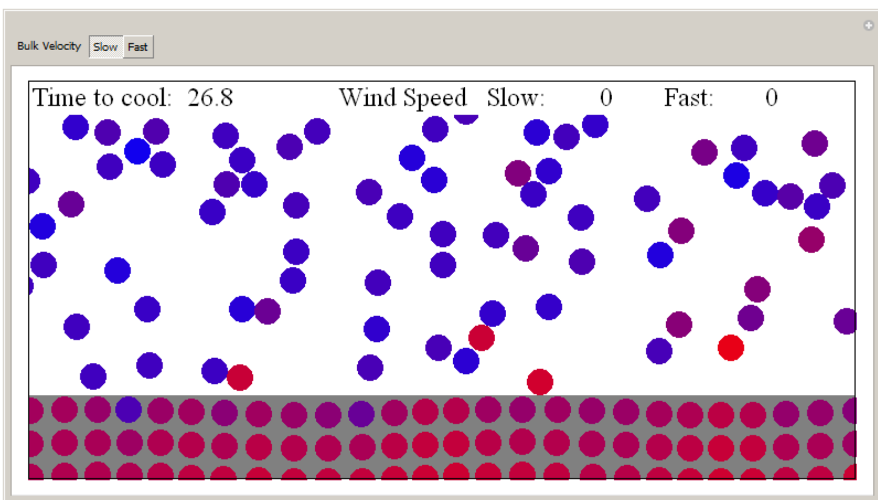

Figure 6.Molecular simulation of convection heat transfer.

The radiation module (Fig. 7) explains the concept as the interaction between molecules and photons in our study. The radiation simulation depicts a water molecule absorbing, reflecting, or being transparent to different wavelengths of radiation. Students are able to change the temperature of a solid object that acts as an energy source. As students change the temperature of the source the amount of energy emitted increases and the wavelengths of the energy change.

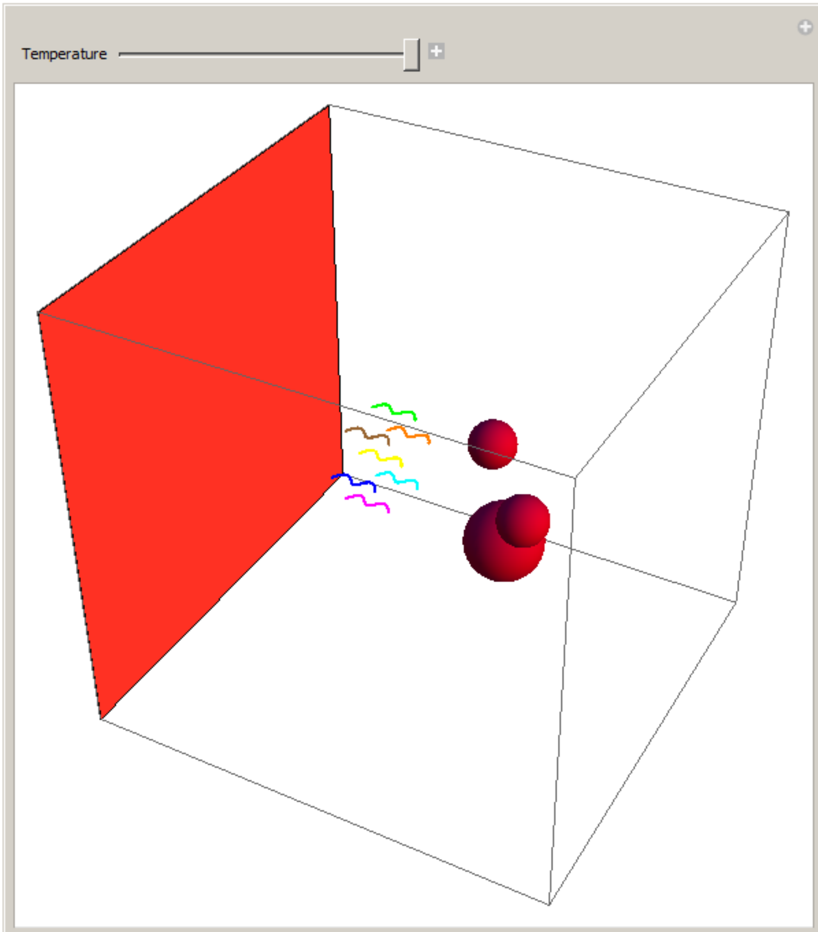

Figure 7. Molecular simulation of heat transfer by thermal radiation

Conclusion

The literature on educational research shows that student learning is enhanced when subjects are presented at the molecular level framed as emergent processes[9,17,24]. A review of popular college textbooks revealed that molecular level descriptions are becoming common in newer editions, but the coverage is not consistent across the topics. Distressingly, some textbooks define temperature as a measure of hotness and coldness of an object, and left off claiming that an explanation is difficult.

In our ongoing study we have created new educational materials to aid the teaching of subjects such as temperature, pressure, viscosity, and heat transfer. The materials were designed, in each case of the concept, starting from the molecular level and progressing to the continuum level. There are quantum effects that contribute to some of the processes, but the effect of their contribution can be explained without delving into the subject that maybe too advanced for freshman students.

Acknowledgments

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