Chapter 1

Temperature and States of Matter

SENSATIONS OF TEMPERATURE ARE A PART OF EVERYDAY EXPERIENCES. My friend's hand is warm. The ice in my drink is cold. Florida in July is hot. When we quantify these sensations by measuring temperature, we usually find: the warmer the sensation the higher the temperature.

We also know from experience that temperature can affect the 'state' of matter. Water becomes ice when we put it in the freezer and steam when we boil it on the stove.

The first step towards uncovering the mystery of temperature was made more than two thousand years ago when the ancient Greek philosopher Democritus formulated the hypothesis that *all objects are made of invisibly small, constantly moving particles called atoms.* It was not until the mid-nineteenth century, that scientists built upon the ancient *atomic hypothesis* to formulate a model of what the individual atoms or molecules might be doing that could explain temperature and the state of matter.

1.1 States of Matter

Discuss the following questions:

Q1.1: What are the states of matter?

Q1.2: How are ice, liquid water, and steam similar?

Q1.3: How are ice, liquid water, and steam different?

Q1.4: Imagine that you could make a “microscopic” dive into a pool of water and see the individual water molecules. What do you see happening to the molecules as the water is cooled and ice begins to form?

Q1.5: What would you see as water is heated and begins to vaporize?

BEGIN ACTIVITY

SimuLab 2: Temperature and the State of Matter

Your objective is to:

Recognize the differences between solid, liquid, and gas from the microscopic point of view.

You will be able to:

Describe the phase transition from liquid to solid and from liquid to gas in molecular terms.

Contrast the motion of particles in the solid, liquid and gaseous phase.

Describe a liquid–gas equilibrium.

Describe the relationship between states of matter and temperature.

Q1.6: Describe, in drawings and in words, your conception of the molecular structure of a substance in the solid, liquid, and gas states.

Q1.7: Describe what happens when we heat a solid in terms of particle motions and overall structure?

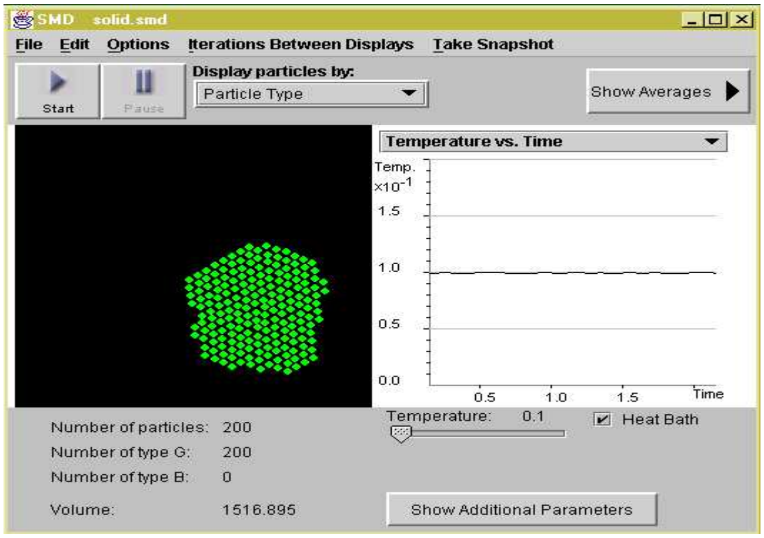
1. Open **SMDPlayer**, select **IntroStatesofMatter** from the **StatesofMatter** folder. Press **Play**. Study the captions and follow the instructions. When you are finished, select **File - Quit**

This is an introductory movie that visualizes the three states of matter at the molecular level and the effect of increasing temperature.

Q1.8: In the introductory movie we saw that as we increase the temperature, solid melts into liquid and liquid evaporates into gas. Describe, in drawings and in words, what would happen as we decrease the temperature of a gas? (Answer such questions as: Do the molecules move faster or slower? Does the gas expand or condense?)

2. Open **SMD**, select **Solid** in the **States of Matter** folder. Press **Start**. In order to speed the simulation switch **Iterations Between Displays** to 100.

In this experiment you are visualizing 200 particles at the molecular level. The particles are in the solid state at temperature $T = 0.1$ as shown in Figure 1.1. Our program uses computer units for all the parameters. You can see temperature and all the other parameters in real units by selecting **Show Averages** and then selecting **Show Real Units**.



Display particles by: Particle Type

Number of particles: 200
Number of type G: 200
Number of type B: 0
Volume: 1516.895

Temperature: 0.1

☑ Heat Bath

Figure 1.1: You see 200 particles at a temperature far below the freezing point of the substance we are simulating. The horizontal axis of the graph shows the simulation time. The vertical axis shows the temperature of the system. The particles are frozen in a triangular crystal.

3. Select **Display Particles by: Trajectories**. Wait no more than 10 time units. **Pause** the simulation. Select **Take a Snapshot** – **Screen**. When the dialog box with the **Title of the Picture** appears type in: "Solid ($T = 0.1$)" and press **Ok**.

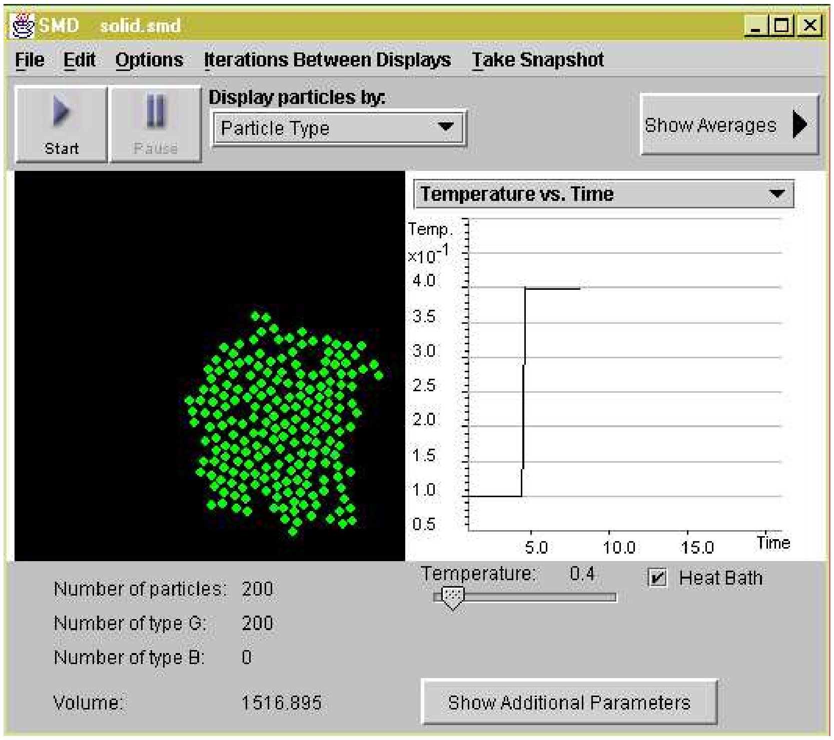
You are saving a snapshot of the trajectories of particles in the solid state for later comparison. Trajectory is another word for the path a particle travels over time.

Q1.9: Which phrase best describes the trajectories of particles. "The particles appear to be . . ."
(a) fixed in position
(b) slightly wobbling around a fixed position
(c) moving along in curved lines
(d) moving along straight lines

4. Select **Display Particles by: Particle Type**. Using the scroll-bar increase the **Temperature** to $T = 0.4$. Press **Start**. Wait at least 20 time units for the particles to spread.

As the temperature increases, the regular pattern of the solid is destroyed as shown in Figure 1.2. The molecules begin to move more freely.

Q1.10: Predict what would happen if you lower the temperature back to $T = 0.1$. Time permitting, check you prediction. Make sure you then set the temperature back to $T = 0.4$ and wait again for 20 time units before proceeding to Step 5.



Display particles by: Particle Type

Temperature: 0.4

☑ Heat Bath

Number of particles: 200

Number of type G: 200

Number of type B: 0

Volume: 1516.895

Figure 1.2: Your system undergoes a phase transition from the solid state to the liquid state. The graph shows the change in the temperature that you made in Step 4.

5. Select **Display Particles by** : **Trajectories**. Wait no more than 5 time units. **Pause** the simulation. Select **Take a Snapshot** – **Screen**. When the dialog box with the **Title of the Picture** appears type in: "Liquid ($T = 0.4$)" and press **Ok.**

You will compare the trajectories of the particles in the liquid state with trajectories of particles in the solid state.

Q1.11: Describe the differences between your snapshots of trajectories from “Solid (T=.1)” and “Liquid (T=.4).” Your descriptions should include a comparison of the particle motion between the two states.

6. Select **Edit** – **Reset Trajectories** and press **Start**. If the trajectories get too cluttered, select again **Edit** – **Reset Trajectories**.

Observe that some particles leave the liquid state and move in straight paths. These gas particles sometimes rejoin the liquid state and sometimes leave it. You are visualizing two states of matter at equilibrium.

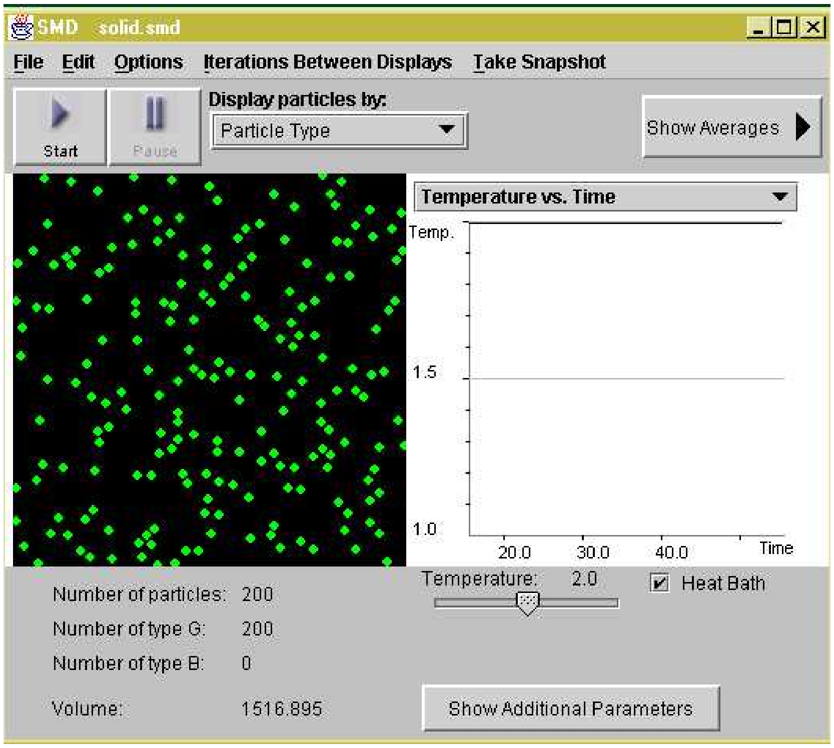
Q1.12: What real-life examples can you list where a gas and liquid co-exist in the same system?

Q1.13: Which phrase best describes the trajectories of particles in the liquid phase . “The particles appear to be . . .”
(a) fixed in position
(b) slightly wobbling around a fixed position
(c) moving along in curved lines
(d) moving along straight lines

7. **Pause** the simulation. Switch **Display particles by: Particle Type**. Using the scroll-bar increase the **Temperature** to $T = 2$. Press **Start** and wait at least 20 time units.

As the temperature is increased, the particles leave the liquid state and become gas as shown in Figure 1.3.

Q1.14: Which phrase best describes what is happening as the particles begin to fill your container. "The particles are . . ."
(a) melting
(b) freezing
(c) evaporating



Display particles by: Particle Type

Temperature vs. Time

Temperature: 2.0

☑ Heat Bath

Number of particles: 200

Number of type G: 200

Number of type B: 0

Volume: 1516.895

Figure 1.3: A snapshot visualizing the gas state.

8. Switch **Iterations Between Displays** to 5. Switch **Display Particles by:** to **Trajectories**. Wait 5 time units. **Pause** the simulation. Select **Take a Snapshot** – **Screen**. When the dialog box with the **Title of the Picture** appears type in: “Gas ($T = 2$)” and press **Ok**.

You will compare the trajectories of the particles in the gas state with trajectories of particles in the solid and liquid states.

Q1.15: What are the differences between the trajectories in the liquid and gas states? Try to explain why the trajectories are different.

Q1.16: Using your snapshot gallery, describe the differences in the three states of matter in terms of particle motion.

Q1.17: Describe in drawings and in words how the state of matter is related to temperature.

9. Switch **Iterations between Displays** to 100. Select **File-Reset Experiment**.

You can further investigate the trajectories of *individual* particles in the three states of matter.

10. Select **Edit - Select Particle** and choose one particle at the *center* of the solid. Select **Display Particles by: Selected Trajectories** and press **Start**. After 10 time units, **Pause** the simulation. Raise the **Temperature** to $T = 0.4$ and press **Start**. For approximately 20 time units, observe the changes in the trajectory of your selected particle. **Pause** the simulation and increase the **Temperature** to $T = 2$. Press **Start**. Watch the trajectory of your chosen particle for another 20 time units. Press **Pause**.

You are watching the behavior of the chosen particle at different temperatures.

Q1.18: Explain the changes observed in the particle trajectory as the temperature is raised.

11. Select **Take a Snapshot** – **Screen**. When the dialog box with the **Title of the Picture** appears, type “Center”.

You will compare this “center” particle with a particle from the “edge” of the solid.

12. **File -Reset Experiment**. Repeat the step 10 but now select particle from the *edge* of the solid.
13. Select **Take a Snapshot** – **Screen**. When the dialog box with the **Title of the Picture** appears, type “Edge”.

Q1.19: Compare your snapshots “Center” and “Edge”. Do you see any difference in the trajectories in the two different cases of initial position. Explain.

1.2 Temperature

What is temperature?

Our computer model is based on the *kinetic molecular theory* which predicts that temperature is related to the motion of a large number of particles that are continually bumping into one another. The temperature of an object is a measure of the energy of particle motion.

Energy is one of the most important concepts in science because it is essential to our existence and it cannot be destroyed. The *Law of Energy Conservation* is one of the most fundamental in nature and says that in any process, the total amount of energy is always conserved.

Energy is not at all easy to define because it exists in many forms that transform into one another in various chemical and physical processes. In fact, before the development of modern civilization, human beings knew how to utilize relatively few sources of energy.

Kinetic energy is one form of mechanical energy and is due to the motion of an object. The kinetic energy of an object depends only on the object's velocity v and mass m. In mathematical terms, kinetic energy can be defined by the equation:

$$E_k = \frac{mv^2}{2}. \tag{1.1}$$

Q1.20: Rank the following asteroids according to the amount of damage they would inflict on Earth during a head-on collision: (a) mass m, velocity v; (b) mass $2m$, velocity v; (c) mass m, velocity $2v$. Explain your answer.

According to the kinetic molecular theory the temperature, T, of a substance is proportional the *average* kinetic energy of the particles in the substance, so that:

$$T \propto (E_k)_{\text{avg}} = \left(\frac{mv^2}{2}\right)_{\text{avg}} . \tag{1.2}$$

The average kinetic energy of a large number of particles, $(E_k)_{avg}$ is equal to the sum of the kinetic energies of all the particles divided by the total number of particles. A typical laboratory sample contains about 10^{23} particles. Our computer model contains, at most, 200 particles.

Q1.21: Suppose we have a system of only 3 identical particles, each with mass $m = 1$. The first has a velocity magnitude $v_1 = 2$, the second $v_2 = 1$, and the third $v_3 = 4$. Compute the magnitude of the average kinetic energy of this system. (Note: Our model uses "computer units" where the particles are not identified as specific atoms. For exploration of units, see *Feature Tour* and *HandsOn 34: Computer versus Real Units*).

Q1.22: Now suppose we have a system of only 2 identical particles, each with mass $m = 1$. The first has a velocity magnitude $v_1 = 2$ and the second has a velocity magnitude $v_2 = 4$. After a purely elastic collision, the velocity magnitude of the first particle becomes $v_1 = 3$. What is the velocity magnitude of the second particle?

Q1.23: If we increase the temperature, what happens to the average speed of particles v? What happens to the average kinetic energy? Explain your answers.

Q1.24: Assuming the temperature remains constant, will heavier particles move faster or slower than lighter particles? Explain your answer.

Q1.25: If temperature increases by a factor of 100, by what factor will the average particle velocity increase or decrease? Explain your answer.

The temperature equation is based on the *average* kinetic energies of all particles. What about each individual particle? Whatever the temperature of a substance, the movement of its particles will be chaotic and the range of their constantly-changing velocities can be quite large. It is important to study the range of velocity values. For example, in a chemical reaction, usually only the fastest molecules react when they collide.

BEGIN ACTIVITY

HandsOn 2: Observing Particle Motion in Hot and Cold Water

Nearly fill one beaker with cold water and another with hot water. Place a drop of food coloring into each beaker near the rim.

Q1.26: Describe, in drawings and in words, what you think may be happening at the molecular level.

BEGIN ACTIVITY

SimuLab 4: Velocity Distribution

Your objective is to:

Investigate the distribution of particle velocities and its dependence on temperature and mass.

You will be able to:

Explain why, in a system at fixed temperature, particles have a wide range of velocities.

Contrast the velocity distribution of a gas at low temperature with a velocity distribution of a gas at high temperature.

Contrast the velocity distribution of heavy particles with the velocity distribution of light particles.

1. Open **SMDPlayer**, select **Temperature** from the **StatesofMatter** folder. Press **Play**. Read the captions and follow the instructions. Select **File - Quit**

In the introductory movie we see that the average kinetic energy of particles increases with temperature. We also see that velocities of the majority of particles increases with temperature.

2. Open **SMD**, select the file **Temperature1** in the **States of Matter** folder. Press **Start**

Your system represents a high density gas of 200 green particles at high temperature.

Q1.27: What is the temperature of your system?

Observe the temperature graph. Go to graph panel and switch the graph to **Kinetic Energies**.

The green line represents the average kinetic energy of the green particles.

Q1.28: What is the average kinetic energy of the green particles?

Q1.29: Does the kinetic energy graph coincide with temperature graph? Explain.

3. Switch **Display Particles by:** to **Absolute Kinetic Energies**.

The colors of the particles indicate their kinetic energies in the rainbow order: red particles have small kinetic energies, violet particles have large kinetic energies. Observe how the velocities of the particles (and their color) change as they collide.

4. Press **Pause**. Set **Iterations Between Displays** to 50. Select **Edit - Select Particles**. Choose **Select Particle(s)** and click on any particle in the display window. Press **Start**.

A white rim will appear around the selected particle. You will observe changes in the kinetic energy of this particle over time.

Q1.30: Does the kinetic energy and the velocity of the selected particle remain constant? Explain.

Q1.31: Why are the velocities of the particles not equal? Why do the colors of the particles change? Explain.

5. Set **Iterations between Displays** to 100. Switch the graph to **Velocity Distribution**.

The x-axis of the graph represents the velocity and the y-axis represents the percentage of particles with that velocity. At each update of the screen, the computer program measures the velocities of all 200 particles and adds these values to the histogram.

Q1.32: Describe what happens to the histrogram of velocities as more and more velocity updates are taken into account.

6. Wait until the velocity distribution becomes a smooth curve with a well-defined maximum which usually happens when the number of velocity updates (# of obs) reaches approximately 10000. Press **Pause** and select **Take a Snapshot** – **Graph** and **Take a Snapshot** – **Screen**. Type the name of the picture "T=4,m=1".

You will need these snapshots to compare the velocity distributions at different temperatures. This snapshot represents the particles of mass $m = 1$ and temperature $T = 4$.

Q1.33: Which velocity value corresponds to the maximum of the histogram? Predict what will happen to the velocity value for the maximum of the histogram as the temperature is lowered to $T = 0.25$ and $T = 1$

7. Hit **Pause**. Using the temperature scroll change the Temperature to $T = 0.25$, and repeat Step 6, naming the snapshots "T=.25,m=1".

8. Change the **Temperature** to $T = 1$, and repeat Step 6, naming the snapshot "T=1,m=1".

Q1.34: Do the actual positions of the maxima of the velocity distributions coincide with your predictions in Q.1.33?

9. Enlarge snapshot gallery window (by dragging bottom right hand corner). Arrange screen shots on top, velocity distributions below screen shot.

Q1.35: Compare the velocity distributions at different temperatures from the **Snapshot Gallery**. Explain how they are similar how they are different.

Q1.36: Compare the snapshots of the screen at different temperatures. Relate the range of colors of the particles in the screen snapshots and the width of the velocity distributions.

10. Select menu item **Edit - Particles**. Choose **Change all particle(s) to B** and click on the particle screen. You will not see a change in the particles because they are displayed in Absolute Kinetic energy mode but now you can vary the particle's mass. Using scroll bar for mass change **B particle mass** to 4. Set **Temperature** $T = 1$. Press **Start**.

We will investigate how the velocity distribution depends on the mass of the particle. In our program, only the blue particles have variable mass. Green particles always have mass $m = 1$. So in order to change a particle's mass, we have to change the particle type to B.

Q1.37: Predict what will happen to the histogram of particle velocities when the particles have mass: (a) $m = 4$ and (b) $m = 0.1$. Predict the positions of the maxima of the velocity distributions for each case.

11. Repeat Step 6, naming the snapshot "T=1,m=4"
12. Change **B particle mass** to 0.1. Repeat Step 6, naming the snapshot "T=1,m=0.1"

Q1.38: Compare the velocity distributions for different particle masses: $m = 1$, $m = 4$, and $m = 0.1$. Explain how they are similar and how they differ.

Q1.39: Does the actual position of the maximum of the distribution coincide with your predictions in Q.1.37? Explain any difference.

Q1.40: Compare the snapshots of the screen (colors representing kinetic energies) with the corresponding snapshots of the velocity distributions. Explain why the colors are the same while the velocity distributions are different.

1.3 Research Projects

We encourage you to pursue independent research projects. Science moves forward through research! Try the suggestion below or design your own. Or, feel free to write an essay using any of the questions throughout this chapter as inspiration.

BEGIN ACTIVITY

Research Project 2: States of Matter

See SimuLab 1

Explore how the decreasing of temperature affects the state of matter. In **SimuLab 1**, we explored how the increase of temperature lead to melting and evaporation of a substance. Is this process reversible? Will the cooling of gas leads to condensation and then to freezing? Will the process be as fast as melting and evaporation is if you just watch the movie StatesOfMatter in the opposite direction, or it will happen in a different way?

1. Open **SMD** and select **Gas** in the **StateOfMatter** folder. Decrease the **Temperature** to $T = 0.4$. and observe what happens. You have to wait for about 2000 computer time units. To speed up the process, set **Iterations Between Displays** to 1000.
2. Decrease the **Temperature** to $T = 0.25$ and observe the process for another 2000 time units.

3. Determine the condensation point temperature (the point at which the gas becomes a liquid) and the freezing point temperature (the temperature at which the liquid becomes a solid) by varying the temperature in the appropriate range and watching the changes in the order and in the motion of the particles.

BEGIN ACTIVITY

Research Project 4: Velocity Distribution

See SimuLab 3

Test if the velocity distribution depends on the state of matter or the density of the substance.

1. Open **SMD** and select **Temperature2** in the **StateOfMatter** folder.

You are visualizing a crystal of blue particles surrounded by a gas of green particles. The crystal does not melt because in this simulation the blue particles interact much stronger than the green particles. (See **Show Additional Parameters** – **BB interaction parameter**.

Q1.41: Read the values of the **Temperature** and **B particle mass** and predict if the velocity distributions of B and G particles will coincide or differ.

2. Change **Display particles by** to **Absolute Kinetic Energy**.	Observe that the colors of particles in the gas and in the crystal are similar. This means that particles in the crystal and in the gas has the same average value, hence they have same temperatures. In other words they are at thermal equilibrium with each other.
3. To save computer time, we recommend setting **Iterations Between Displays** to 100 or more. Make screen and graph snapshots.	Compare velocity distributions for particles in the gas and in the crystal using **Velocity Distribution for G** and **Velocity Distribution for B** graphs and waiting until the velocity distribution for B and G particles become smooth curves with well-defined maxima.
4. Change **particle mass** to 0.1 and then 10. Repeat Step 3.	Predict the change in the velocity distributions.
5. Restore **B particle mass** $= 1$. In the **Additional Parameters** window, Change **Density** to 0.8. Repeat Step 3.	Predict the changes in the velocity distributions.
6. Increase the **Temperature** to $T = 4$. Predict the changes in the velocity distributions. Repeat Step 3.	

Q1.42: Compare the snapshots of velocity distributions of B and G particles with the initial set and explain their differences and similarities. Do the velocity distributions depend on the density or state of matter? Explain your answer.

Q1.43: Compare the snapshots of the screen at different conditions.

BEGIN ACTIVITY

Research Project 6: Velocity Distribution II

See SimuLab 3

Investigate whether velocity the distribution depends on parameters other than temperature and mass of particles.

1. Open **SMD**, select the file **Temperature2** from the **States of Matter** folder.

2. Keep mass of particle B and temperature constant (**Heat bath on**). Set **Iterations Between Displays** to 100 or more. Vary any other parameter in the **Additional Parameters** window. For example, change density, interaction parameters, boundaries, insert piston, introduce gravity. For each set of parameters obtain smooth velocity distributions for B and G particles. Make a snapshot of screens and velocity distribution graphs for different conditions. Be sure to run the program for each parameter setting long enough so that the velocity distributions are smooth.

Q1.44: Compare the snapshots of velocity distributions of B and G particles and explain their differences and similarities. Can you conclude whether the velocity distributions depend on any parameter except temperature and mass? Explain.

Q1.45: Compare the snapshots of the particle screen at different conditions and try to relate the parameter changes to what you see.

BEGIN ACTIVITY

Research Project 8: Velocity Distribution III

See SimuLab 3

Explore how the velocity distribution aquires its shape due to particles collisions.

1. Open **SMD** using the default configuration. Change **Display particles by** to **Absolute kinetic energy**. Set **Iterations between Displays** to 100. Switch graph to **Velocity Distribution**. Press **Start**.

At the beginning all the particles are assigned the same velocity magnitude.

Q1.46: As the simulation proceeds, why does the distribution of velocities differ from the initial distribution?

BEGIN ACTIVITY

Research Project 10: Velocity Distribution IV

See SimuLab 3

Explore how two substances in contact reach thermal equilibrium.

1. Open **SMD**, select the file **Temperature3** from the **States of Matter** folder. Switch the **Display Particles by** to **Absolute Kinetic Energies**. Make a snapshot of the screen. Switch **Iterations Between Displays** to 100 and Press **Start**.

The temperature of the crystal is much smaller than that of surrounding gas.

Q1.47: Watch the graphs of the average kinetic energies of the blue and the green particles. Explain what you see on the graph and on the screen from the point of view of molecular kinetic theory.

2. **Reset** the experiment. Switch the graph to **Velocity distribution**. Collect the velocity distributions for B and G particles for 10000 observations. Make snapshots of the velocity distributions.

3. Switch the graph back to **Kinetic Energies**.

Wait until the average kinetic energies of green and blue particles become equal.

4. When the system reaches equilibrium, reset the velocity distribution by switching to **No graph** and then to velocity distribution

Collect 10000 observations. Make snapshots of the velocity distributions.

Q1.48: Collect the new set of velocity distributions. Compare them to the previous distributions from Step 2. Explain what you see from the point of view of molecular kinetic theory.