Quick Start and Troubleshooting Guide

Boltzmann 3D is educational software developed and offered by the BYU Department of Chemistry & Biochemistry. Written in Java, with OpenGL graphics libraries and Windows, Mac, and Linux options, Boltzmann 3D is a kinetic theory demonstrator.

This guide explains how to get started quickly in and troubleshoot Boltzmann 3D.

Author: Randall B. Shirts
Department of Chemistry and Biochemistry
Brigham Young University
Provo, Utah 84602
Programmers: Scott R. Burt, Benjamin J. Lemmon
Additional programming: Jared Duke, Derek Manwaring, Aaron Stewart, Dustin Carr

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Go to the Boltzmann 3D Main Page and follow the instructions. You may also have to download the Java2 runtime environment from http://www.java.com (or software update for Mac users).

What is Boltzmann 3D doing?

Boltzmann 3D solves Newton's equations in real time for the classical motion of N hard spheres, displays the motion on the computer screen, and keeps track of important statistical quantities including velocity, energy, collision rate, free path and time between collisions, and pressure. You can choose container size, number of particles, particle size and mass, temperature, dimension (1, 2 or 3), colors used, five different choices of boundary modes, and a range of display options.

What is Boltzmann 3D for?

Use **Boltzmann 3D** for in-class demonstration of the principles of kinetic theory or as a hands-on exploration tool. It can be used in education from high school to graduate statistical mechanics. Use set files supplied with **Boltzmann 3D** or your own saved demonstrations to illustrate various principles of chemistry, physics, kinetic theory, or statistical mechanics. Suggestions for using these files are in Section II of the manual.

Screen resolution and window size

Adjust the size of your **Boltzmann 3D** window by dragging the lower right corner of the window or by using the manual settings under **options** in the **simulation** menu. For lower resolution, you will need a smaller arena. If the controls do not fit vertically in the left-hand-side window, a scroll bar will appear. Control areas can be minimized by clicking on the - sign left of the label. You can also adjust the magnification of items in the arena using the Zoom function.

Changing dimension and viewing angle

Simulations can be in 1D, 2D or 3D. Select your preference using **dimension** in the simulation menu. Change viewing perspective in 3D by clicking on the vertical or the horizontal ruler and then using the direction keys right of the keyboard.

Speeding up and smoothing motion

Use the **simulation speed** control under the clock to adjust the appearance of motion. If this is not satisfactory, use 2D, try fewer particles and turn shading off.

Starting a simulation

Click the **restart** button at bottom left. This starts N (as shown in the # of particles box) red particles, all with the mass and radius displayed, and all with rms velocity appropriate for the temperature displayed in its box. A restart also zeros the clock and all cumulative distributions.

Adding particles with the same or different mass and radius

New particles can only be added if you have selected **both** or **blue** at upper left. Particles added after a restart are blue. Adjust the displayed mass and/or size of new particles before you add them. Then, enter a number in the number box, click the + button right of the number box, or click the screen where you want a new particle to appear.

Pause, play, single frame advance, and reverse

Pause a simulation by clicking the **Pause** button, resume by clicking **Play**. When paused, you can advance one frame at a time using the single frame **Advance** button. You can also **Reverse** the motion of all particles.

Reporting bugs and making suggestions

Most reported problems involve incompatibilities with outdated video card drivers, so please download manufacturer's updates for your video card before reporting bugs. Detailed descriptions of problems should be directed to boltzhelp@chem.byu.edu. We also welcome suggestions and reports of success or failure. Please send examples of worksheets or labs used and explain how you used **Boltzmann 3D**.

The walls in 3D mode appear broken up

This was due to a bug in the graphics drivers for ATI video cards. Update your Boltzmann #3D version to resolve this issue.

The program runs fine in 1D and 2D, but the display is black in 3D mode

This is most likely due to lack of video memory. The 3D display may require more video memory than you currently have. There are 2 workarounds to this issue.

- **Lower your screen resolution**: Lowering the screen resolution can free up some of your video memory for use by **Boltzmann 3D**. This can be done in Windows by right-clicking the desktop, then choosing properties. Under the settings tab there is a box labeled *Screen resolution*. Slide the bar there to the left to lower the resolution. Usually one to two notches is enough.
- **Disable hardware acceleration**: By disabling hardware acceleration, main memory is used rather than video memory.

- Some models will let you control advanced graphics options to solve the problem. Do this by right-clicking the desktop, then selecting *properties*. Under the *settings* tab, press the *advanced* button. If there is an OpenGL tab in this window, select it, then select the checkbox labeled *Enable page flipping* and also the check box labeled *Force 16-bit Z-buffer*. If the OpenGL tab is absent, try updating your graphics drivers.
- The next best solution is to disable hardware acceleration in Windows by right clicking the desktop, then choosing properties. Under the settings tab click the *Advanced* button. In that window, select the *Troubleshoot* tab. The slider bar in the middle of the window controls hardware acceleration. Sliding it all the way to the left will disable hardware acceleration. Disabling hardware acceleration may slow down graphics intensive programs like **Boltzmann 3D**, but it will offload graphics processing to the CPU and avoid incompatibilities between the graphics card and the OpenGL libraries. If you need to enable it later for another program, just go to that same window and slide the bar back to the right.

Distributions

Up to 16 different distributions can be chosen for display from the drop-down menu above the histogram graph. Most can be compared to a theoretical curve (black line). Abscissa limits are adjustable. Instantaneous averages for the displayed distribution are shown in green with predicted values in orange. RMS deviations (widths) can be selected for display instead.

Boundary modes

Choose **Box will Walls** (default), **Periodic Boundaries**, **Divided Box**, **Divided Box with a Hole** (for effusion or equilibration), or **Piston** (for experimenting with isothermal or adiabatic compressions/expansions) by selecting the appropriate icon in the particle control area.

Pressure readings

The pressure exerted by wall collisions is displayed for the left and right walls in a text box above the arena. Momentum transfer is averaged over 60 ps, but the averaging time can be changed using **options** in the **simulation** menu. A pressure prediction (using ideal gas law or the virial expansion) is also displayed. Using periodic boundary conditions, the pressure is calculated using the virial. Separate pressures are displayed when the box is divided.

Load a saved file

Select **load** from the **file** menu to load a saved file, whether supplied with **Boltzmann 3D** or saved by the user.

Saving a demonstration for later use

Use **save** from the **file** menu to save only the parameters (basic option) or else parameters as well as particle positions and velocities (complete option) to rerun a simulation.

Change the color scheme

Pick your own colors using the **view** menu or turn off shading to speed up calculations.

Cumulative distributions and histories

Click **cumulative** or **history** to see a cumulative distribution or the recent history of a variable.

Output of distributions, cumulative distributions, or trajectories

Use the **Advanced** area check box to output cumulative distributions, statistical averages or coordinates at uniform intervals. Click the box again to turn off output. Stored data can be analyzed in a spreadsheet.

Can anything other than hard spheres be simulated with Boltzmann 3D?

Java is too slow to include realistic attractive forces in a real-time visualization. Look for a future program written in C to visualize particles interacting with a Lennard-Jones potential.