

configuration, open the File menu in the control window and choose Save As.... A dialog box will open so that you can choose a name for the file, which will have the extension xml. To read a previously saved configuration, choose Read in the File menu. Notice that in LJParticlesLoader, the loadObject makes a call to the computeAcceleration and resetAverages methods of LJParticles, so that the simulation can be run starting from the newly loaded configuration by next clicking the Start button. The syntax for saving a model's configuration is described in more detail in Appendix 8A.

Listing 8.11 The LJParticlesApp target class.

```
package org.opensourcephysics.sip.ch08.md;
import org.opensourcephysics.controls.*;
import org.opensourcephysics.frames.*;
import org.opensourcephysics.display.GUIUtils;

public class LJParticlesApp extends AbstractSimulation {
    LJParticles md = new LJParticles();
    PlotFrame pressureData =
        new PlotFrame("time", "PA/NKT", "Mean pressure");
    PlotFrame temperatureData =
        new PlotFrame("time", "temperature", "Mean temperature");
    HistogramFrame xVelocityHistogram =
        new HistogramFrame("vx", "H(vx)", "Velocity histogram");
    DisplayFrame display =
        new DisplayFrame("x", "y", "Lennard-Jones system");

    public void initialize() {
        md.nx = control.getInt("nx"); // number of particles per row
        md.ny = control.getInt("ny"); // number of particles per column
        md.initialKineticEnergy =
            control.getDouble("initial kinetic energy per particle");
        md.Lx = control.getDouble("Lx");
        md.Ly = control.getDouble("Ly");
        md.initialConfiguration =
            control.getString("initial configuration");
        md.dt = control.getDouble("dt");
        md.initialize();
        display.addDrawable(md);
        // assumes vmax = 2*initialTemp and bin width = Vmax/N
        display.setPreferredMinMax(0, md.Lx, 0, md.Ly);
        xVelocityHistogram.setBinWidth(2*md.initialKineticEnergy/md.N);
    }

    public void doStep() {
        md.step(xVelocityHistogram);
        pressureData.append(0, md.t, md.getMeanPressure());
        temperatureData.append(0, md.t, md.getMeanTemperature());
    }

    public void stop() {
        control.println("Density = "+decimalFormat.format(md.rho));
        control.println("Number of time steps = "+md.steps);
        control.println("Time step dt = "+decimalFormat.format(md.dt));
        control.println("<T>= "
            +decimalFormat.format(md.getMeanTemperature()));
        control.println("<E> = "
            +decimalFormat.format(md.getMeanEnergy()));
    }
}
```

```
control.println("Heat capacity = "
    +decimalFormat.format(md.getHeatCapacity()));
control.println("<PA/NKT> = "
    +decimalFormat.format(md.getMeanPressure()));
}

public void startRunning() {
    md.dt = control.getDouble("dt");
    double Lx = control.getDouble("Lx");
    double Ly = control.getDouble("Ly");
    if((Lx!=md.Lx)|| (Ly!=md.Ly)) {
        md.Lx = Lx;
        md.Ly = Ly;
        md.computeAcceleration();
        display.setPreferredMinMax(0, Lx, 0, Ly);
        resetData();
    }
}

public void reset() {
    control.setValue("nx", 8);
    control.setValue("ny", 8);
    control.setAdjustableValue("Lx", 20.0);
    control.setAdjustableValue("Ly", 15.0);
    control.setValue("initial kinetic energy per particle", 1.0);
    control.setAdjustableValue("dt", 0.01);
    control.setValue("initial configuration", "rectangular");
    enableStepsPerDisplay(true);
    // draw configurations every 10 steps
    super.setStepsPerDisplay(10);
    // particles will appear as circular disks
    display.setSquareAspect(true);
}

public void resetData() {
    md.resetAverages();
    // clears old data from the plot frames
    GUIUtils.clearDrawingFrameData(false);
}

public static XML.ObjectLoader getLoader() {
    return new LJParticlesLoader();
}

public static void main(String[] args) {
    SimulationControl control =
        SimulationControl.createApp(new LJParticlesApp());
    control.addButton("resetData", "Reset Data");
}
}
```

Listing 8.12 The LJParticlesLoader class for saving configurations.

```
package org.opensourcephysics.sip.ch08.md;
import org.opensourcephysics.controls.*;
import org.opensourcephysics.display.GUIUtils;

public class LJParticlesLoader implements XML.ObjectLoader {
```