

CE 412 Molecular Modeling

Simulation Lecture 3

Object-Oriented Programming and Etomica

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Object-Oriented Programming

- Programming accomplished through the actions and interactions of objects
 - *everything is an object*
- Forces abstract thinking about the structure and activities of a program
- Promotes re-use of code and extension to new applications
- Good design is difficult to develop
 - *requires thorough understanding of application*
 - *conversely, its use facilitates a better understanding of application*
- It's fun!
 - presents a good vehicle for teaching

What is an Object?

○ A fancy variable

- *stores data*
- *can perform operations using the data*

○ Every object has a type, or “class”

- *analogous to real, integer, etc.*

Fortran: **real x, y, z**

Java: **Atom a1, a2;**

- *you define types (classes) as needed to solve your problems*

```
public class Atom {  
    double mass;  
    Vector r, p;  
}
```

- *types differ in the data they hold and the actions they can perform on it*
- *every object is an “instance of a class”*

```
a1 = new Atom();
```

Makeup of an Object

○ Fields (data)

- *primitive types (integer, float, double, boolean, etc.)*
- *handles to other objects*
 - *complex objects are composed from simpler objects (composition)*

○ Methods (actions)

- *“subroutines and functions”*
- *may take arguments and return values*
- *have complete access to all fields of object*

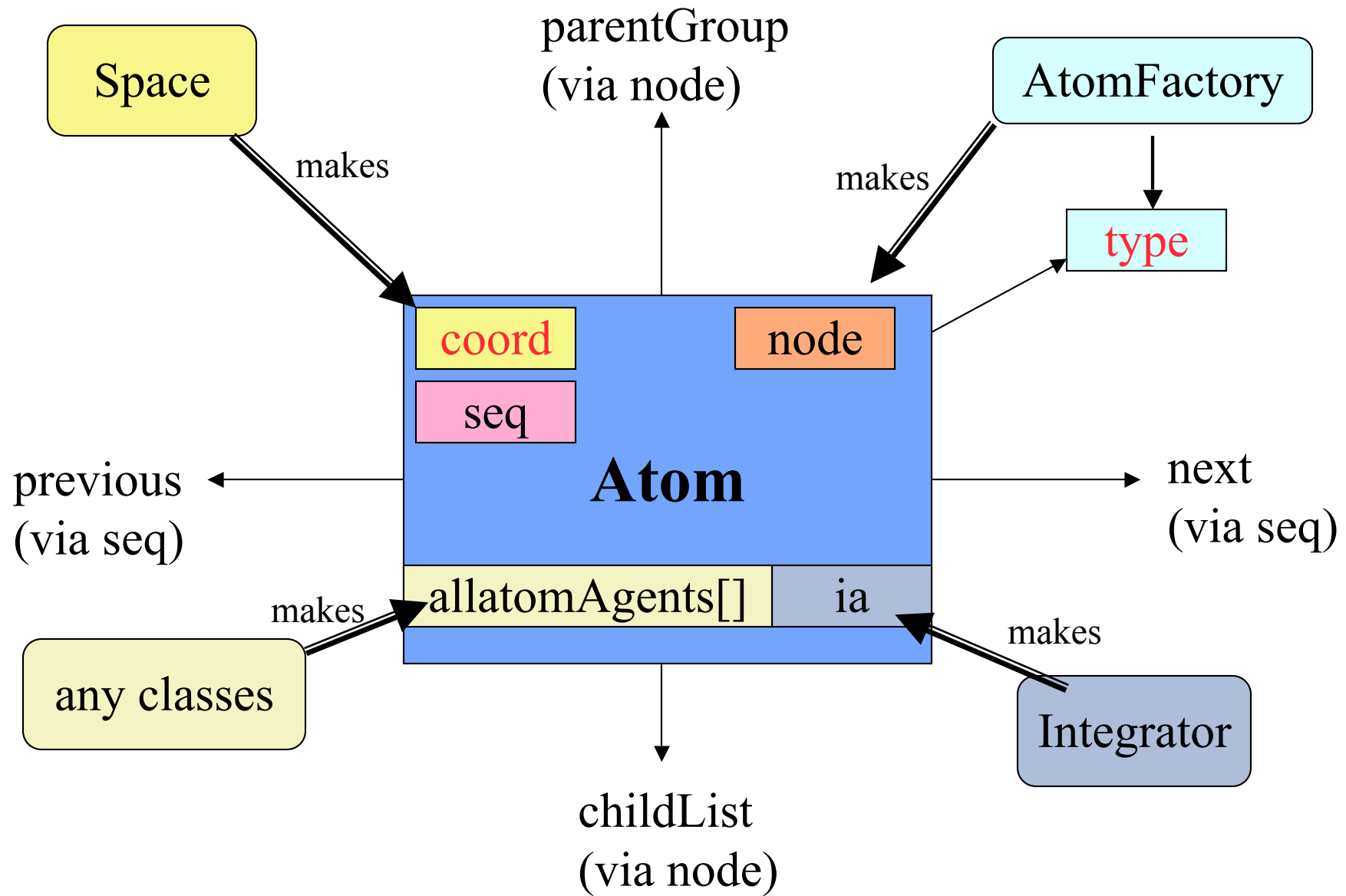
○ A class has an interface

- *what the object presents to enable its manipulation*
- *implementation (how it accomplishes its operations) can be hidden*
- *object is viewed in terms of its “actions” and not its “thoughts”*

○ Inheritance

- *can define subclasses which inherit features of parent class*
- *same interface, but different implementations*
- *subclasses can be used anywhere parent class is expected*
- *mechanism to change behavior of simulation*

Detailed Look: Atom

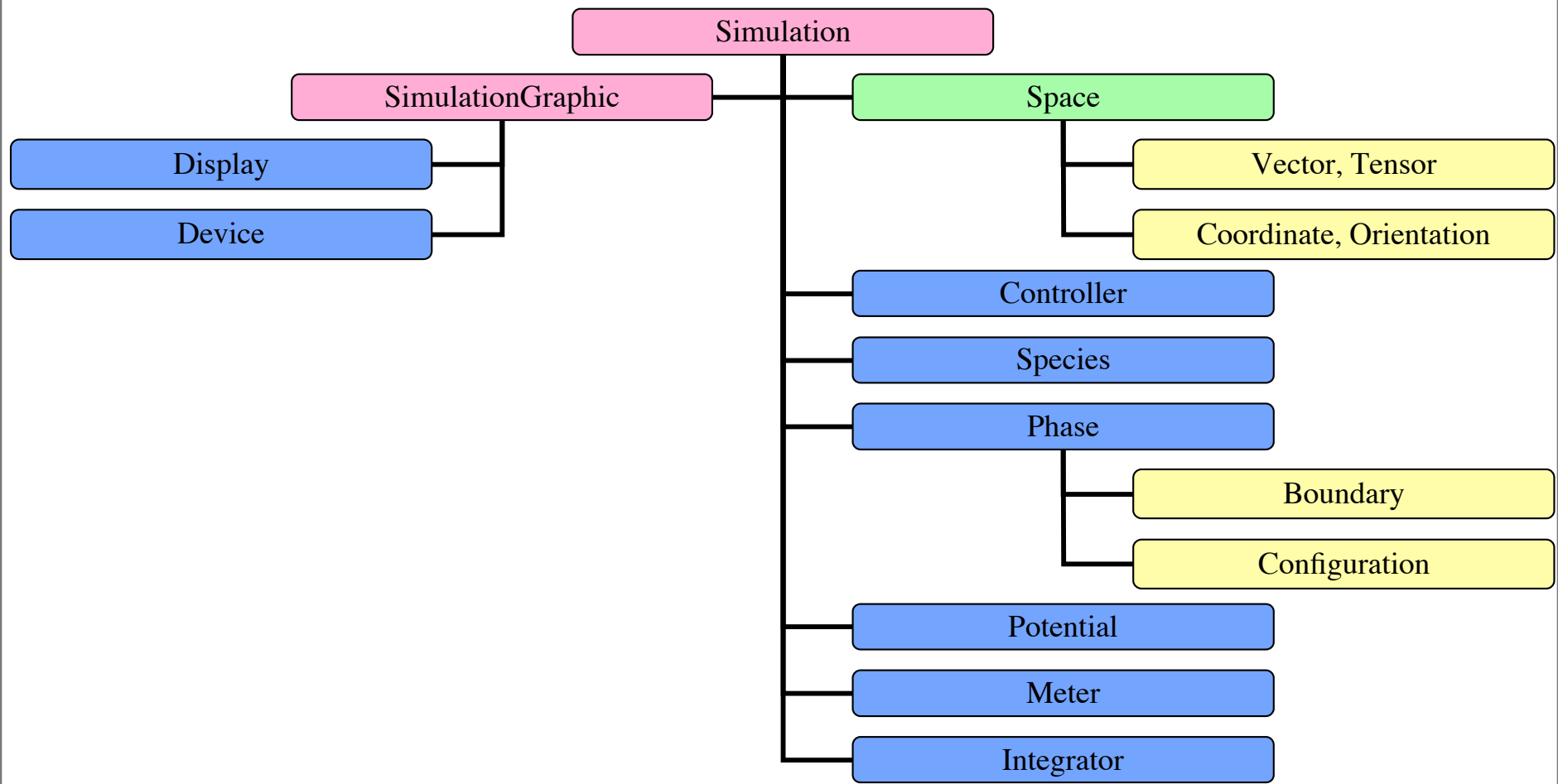


○ [Click here](#) for the complete API specification

Etomica

- Application Programming Interface (API)
 - *Library of components used to assemble a simulation*
 - *Can be used independent of development environment*
Invoked in code programmed using Emacs (for example)
- GUI-based development environment
 - *Simulation is constructed by piecing together elements*
 - *No programming required*
 - *Result can be exported to run stand-alone as applet or application*
- Written in Java
 - *Widely used and platform independent*
 - *Features of a modern programming language*
 - *Object-oriented*
- Vehicle for presentation of molecular simulation methods

Etomica API



Simulation Elements: Simulation

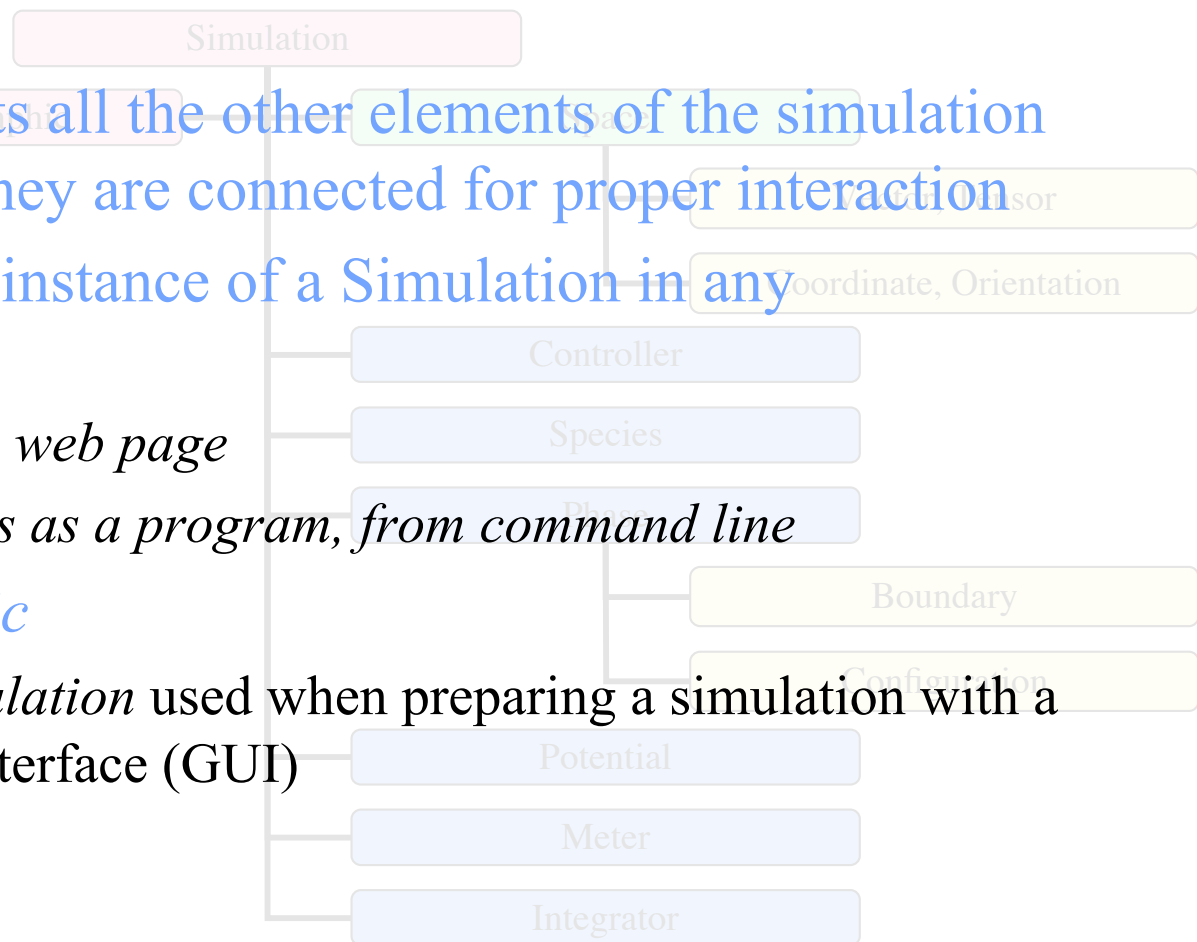
- Simulation collects all the other elements of the simulation and ensures that they are connected for proper interaction

- There is only one instance of a Simulation in any applet/application

- *Applet: runs in a web page*
- *Application: runs as a program, from command line*

- *SimulationGraphic*

- Subclass of *Simulation* used when preparing a simulation with a graphical user interface (GUI)



Simulation Elements: Space

- Space defines properties of the physical space in which the simulation is performed

- Dimensionality (1D, 2D, 3D, etc.); continuum vs. lattice
- Construction of vectors, tensors
- Makes Coordinate for placement in each Atom position and momentum vector
- CoordinatePair defines how distances are computed
- Constructs various types of Boundary for placement in each Phase

- Concrete classes

- Space1D
- Space2D
- Space3D

Simulation

SimulationGraphic

Display

Device

Controller

Species

Phase

Potential

Meter

Integrator

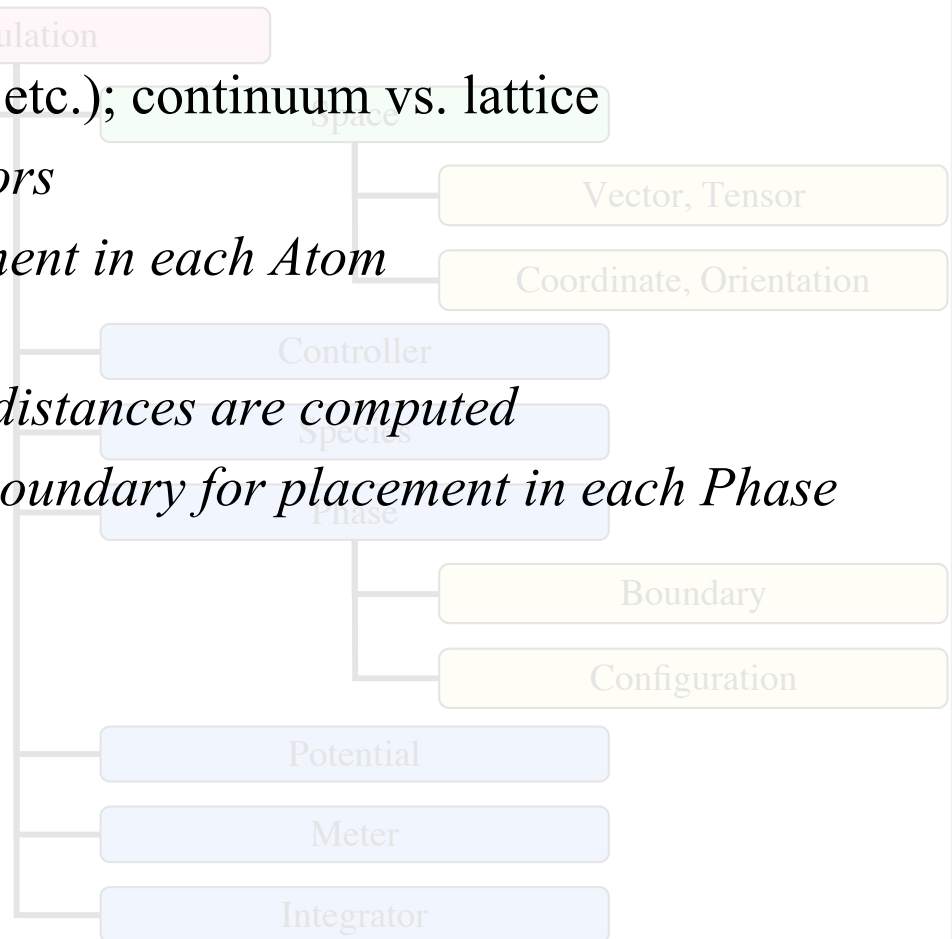
Space

Vector, Tensor

Coordinate, Orientation

Boundary

Configuration



Simulation Elements: Controller

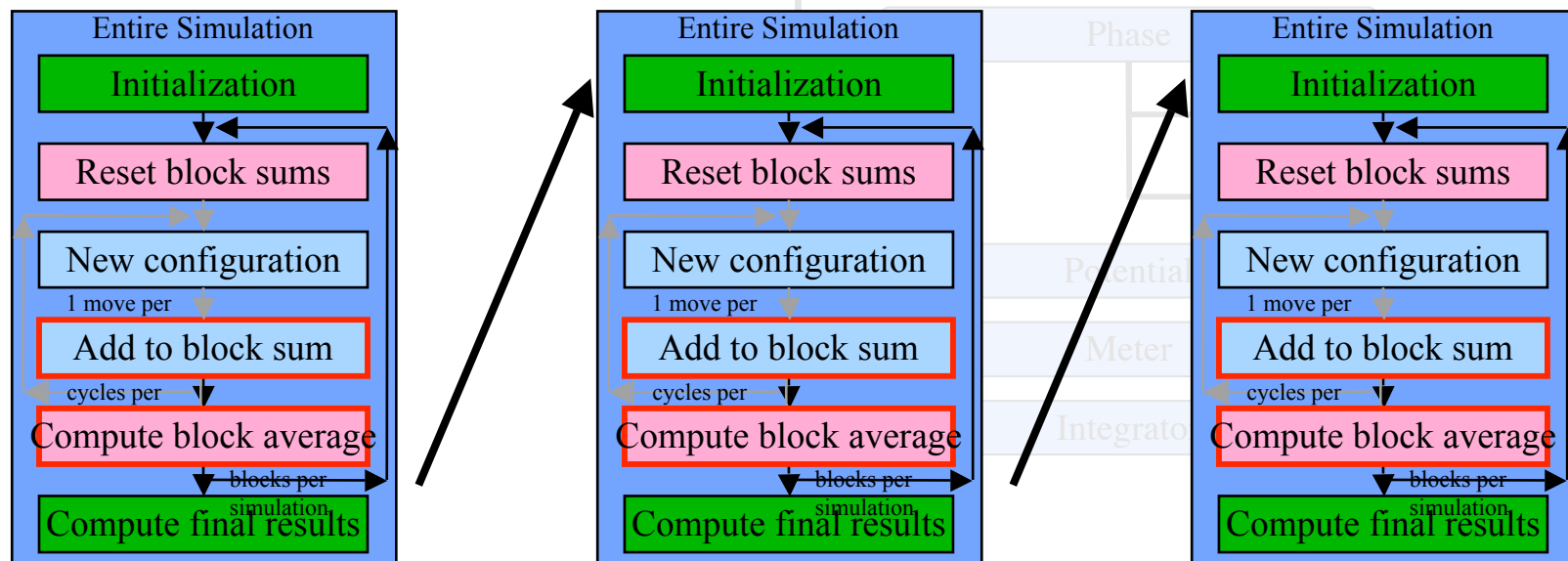
○ Governs general plan of action for simulation

- *For example:*

- run forever, as controlled by an interactive Stop/Resume button
- run a fixed number of relaxation/production cycles, then quit
- run over a series of state conditions for a fixed duration at each

○ Oversees activities of Integrator

- *Makes connections between Integrator and other elements to ensure proper functioning*
- *Turns Integrator on and off according to plan of action*



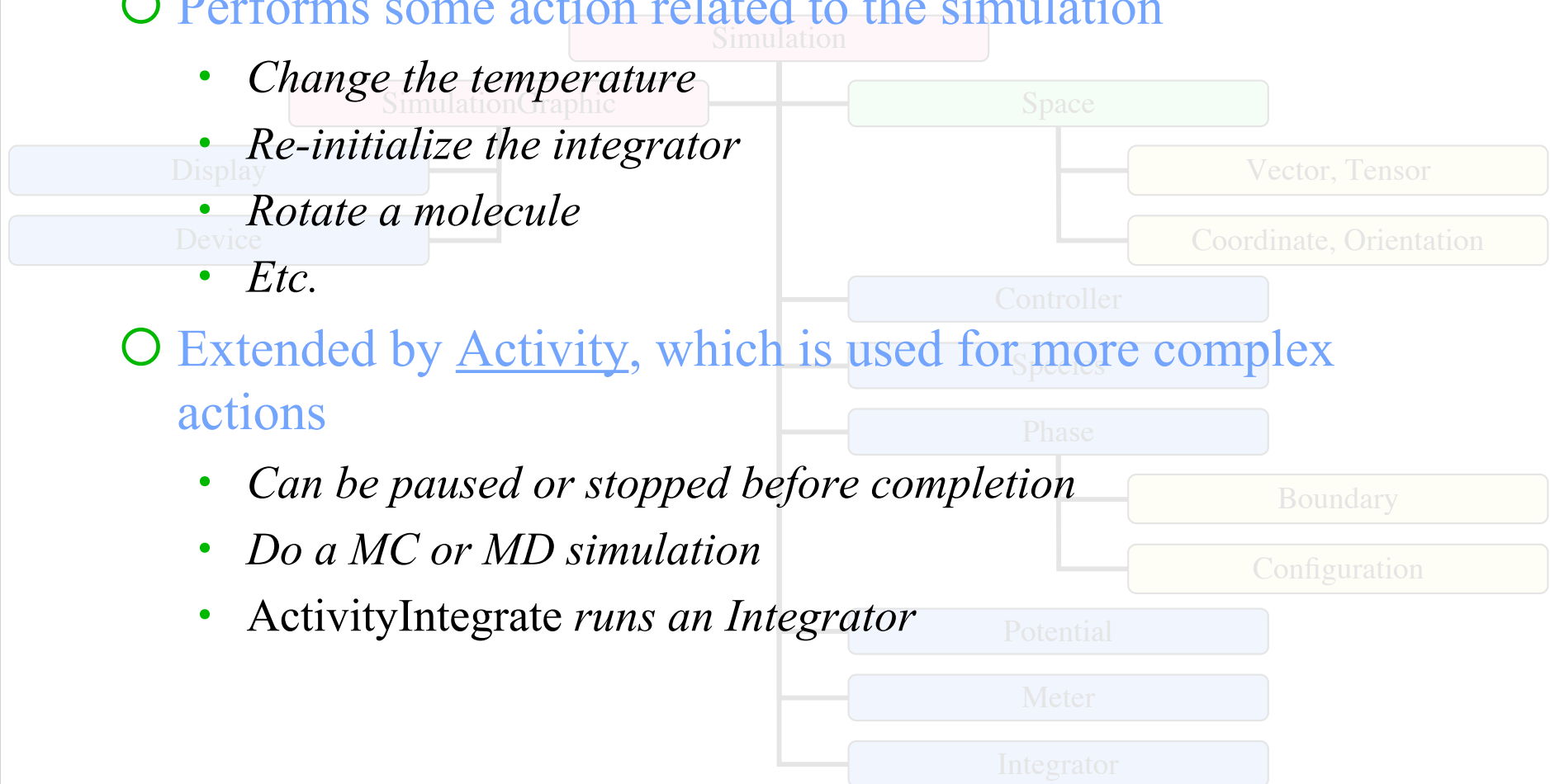
Simulation Elements: Action

○ Performs some action related to the simulation

- *Change the temperature*
- *Re-initialize the integrator*
- *Rotate a molecule*
- *Etc.*

○ Extended by Activity, which is used for more complex actions

- *Can be paused or stopped before completion*
- *Do a MC or MD simulation*
- *ActivityIntegrate runs an Integrator*



Simulation Elements: Integrator

- Adds the physics needed to generate configurations properly

- *various integration schemes introduced by developing a new integrator*

- *Molecular dynamics integrators*

hard-potential dynamics

various kinds of soft-potential integrator

- *Monte Carlo integrators*

more later

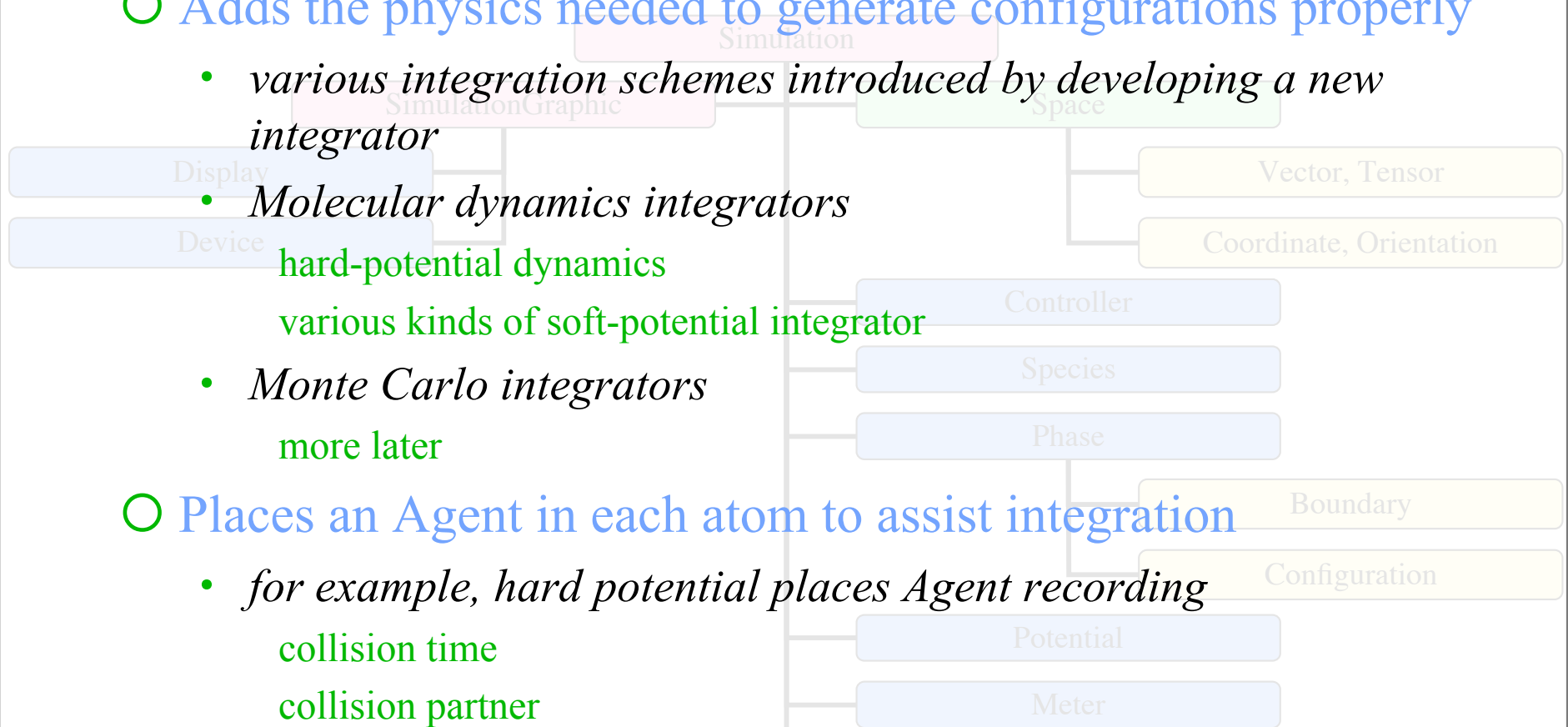
- Places an Agent in each atom to assist integration

- *for example, hard potential places Agent recording*

collision time

collision partner

- Fires IntegratorIntervalEvent to notify listeners that simulation has proceeded one step



Simulation Elements: Integrator

○ *run* method for top-level Integrator class



```

public void run() {
    stepCount = 0;
    int iieCount = interval+1;
    while(stepCount < maxSteps) {
        while(pauseRequested) doWait();
        if(resetRequested) {doReset(); resetRequested = false;}
        if(haltRequested) break;
        doStep(); //abstract method in Integrator. subclasses implement algorithms (MD/MC)
        if(--iieCount == 0) { //count down to determine when a cycle is completed
            fireIntervalEvent(intervalEvent); //notify listeners of completion of cycle
            iieCount = interval;
        }
        if(doSleep) { //slow down simulation so display can keep up
            try { Thread.sleep(sleepPeriod); }
            catch (InterruptedException e) { }
        }
        stepCount++;
    } //end of while loop
    fireIntervalEvent(new IntervalEvent(this, IntervalEvent.DONE));
} //end of run method

```

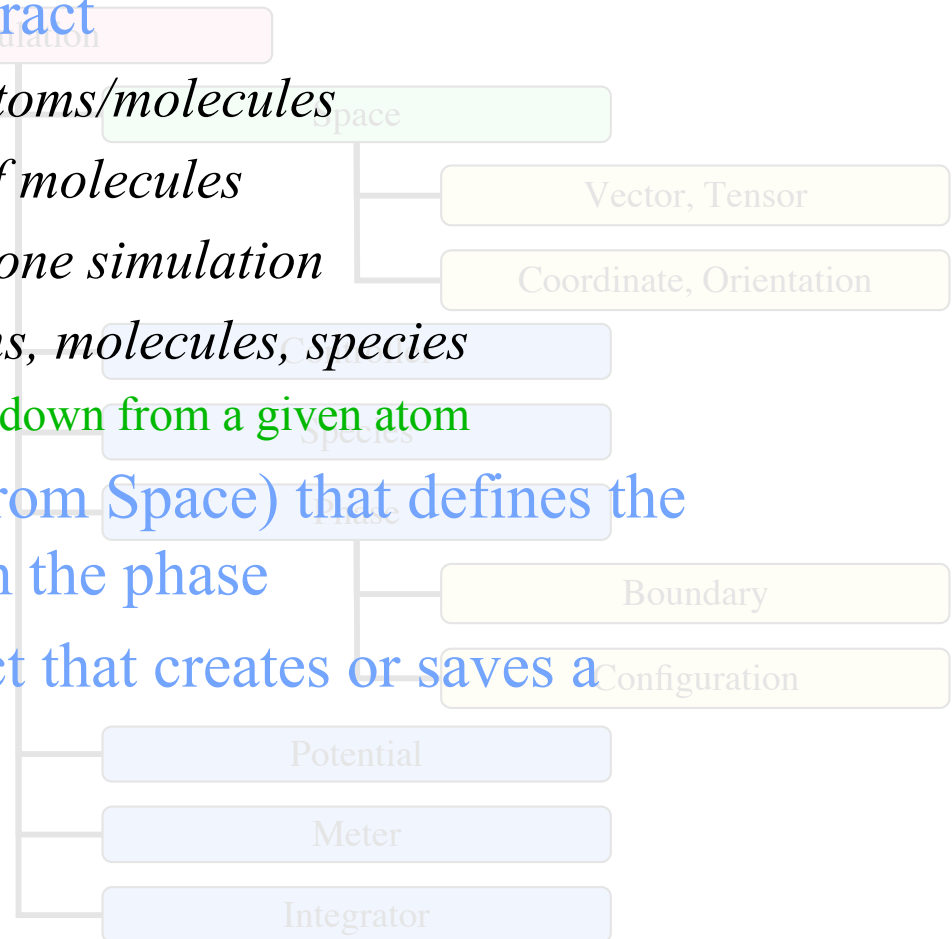
Simulation Elements: Phase

○ Collects molecules that interact

- holds root of hierarchy of atoms/molecules
- handles addition/removal of molecules
- multiple phases possible in one simulation
- sets up base lists of all atoms, molecules, species
defines which atoms are up or down from a given atom

○ Holds a Boundary object (from Space) that defines the boundary conditions used in the phase

○ Houses Configuration object that creates or saves a configuration of molecules



Simulation Elements: Meter

○ Measurement of simulation property

- *Configurational property in a phase*

Display potential energy

Device kinetic energy

density

structure

- *Each phase has by default kinetic and potential energy meters*

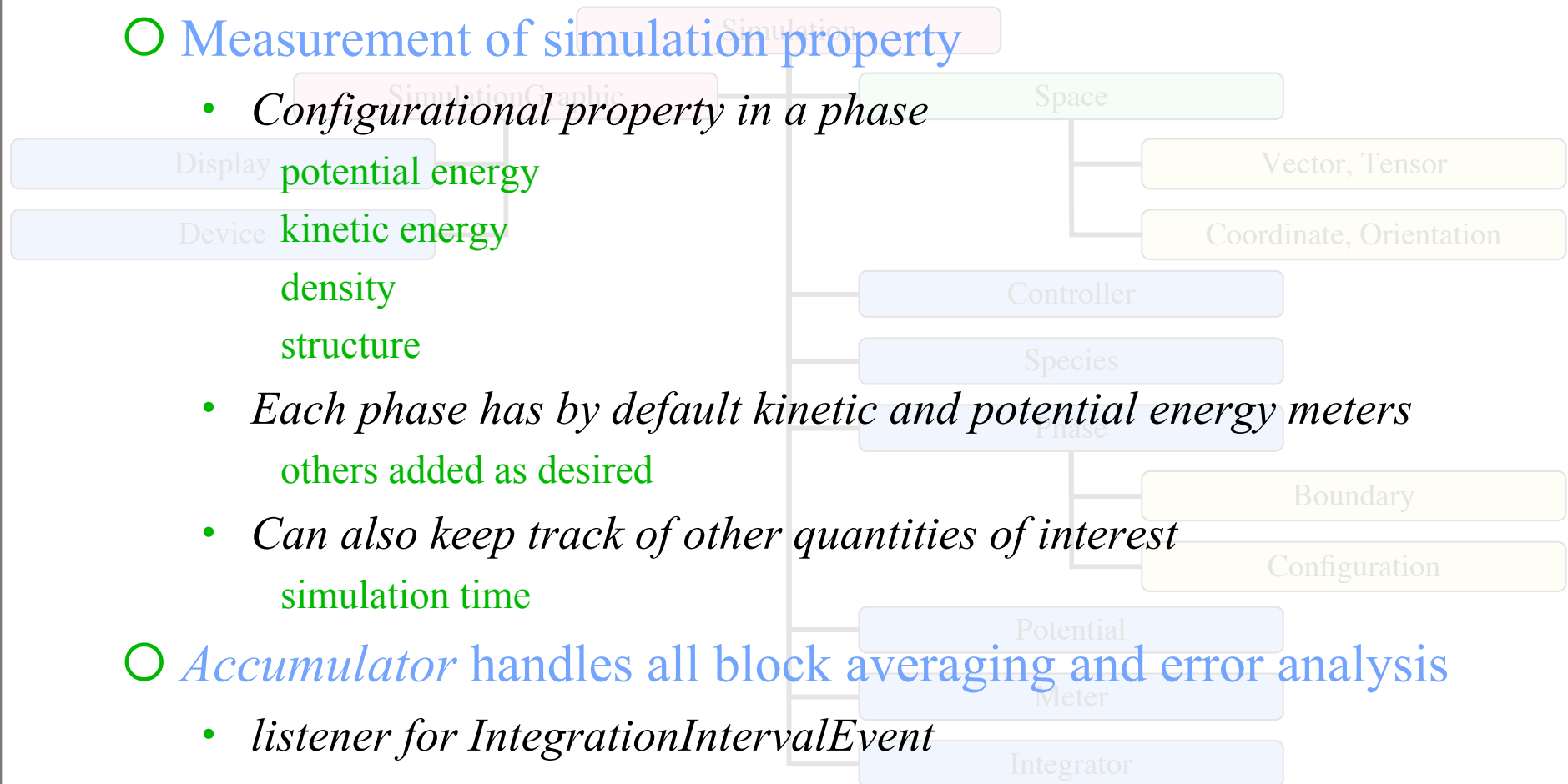
others added as desired

- *Can also keep track of other quantities of interest*

simulation time

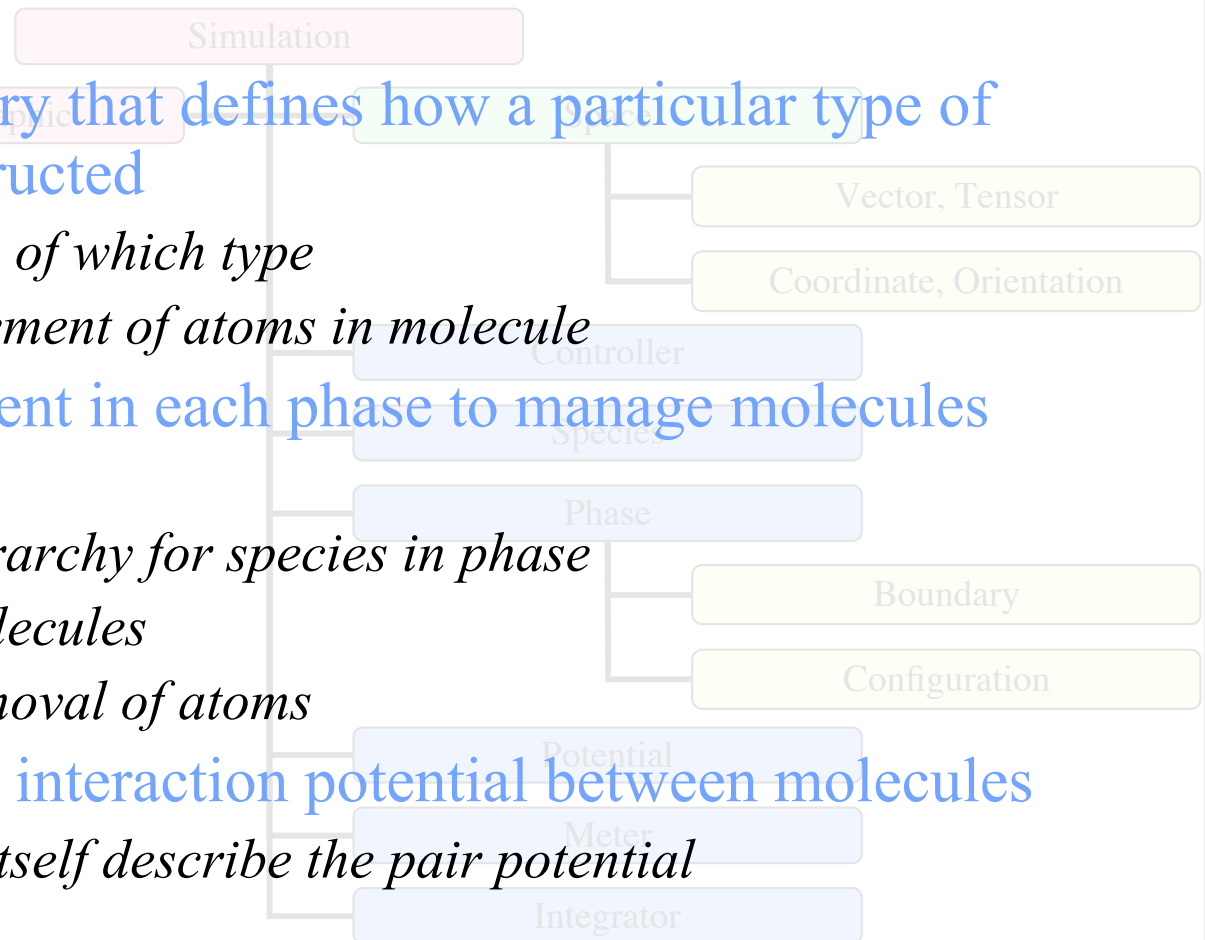
○ Accumulator handles all block averaging and error analysis

- *listener for IntegrationIntervalEvent*



Simulation Elements: Species

- Holds AtomFactory that defines how a particular type of molecule is constructed
 - *how many atoms of which type*
 - *nominal arrangement of atoms in molecule*
- Places SpeciesAgent in each phase to manage molecules there
 - *root of atom hierarchy for species in phase*
 - *looping over molecules*
 - *addition and removal of atoms*
- Basis for defining interaction potential between molecules
 - *but does not by itself describe the pair potential*



Simulation Elements: Potential

○ Defines interaction between atoms (and thereby molecules)

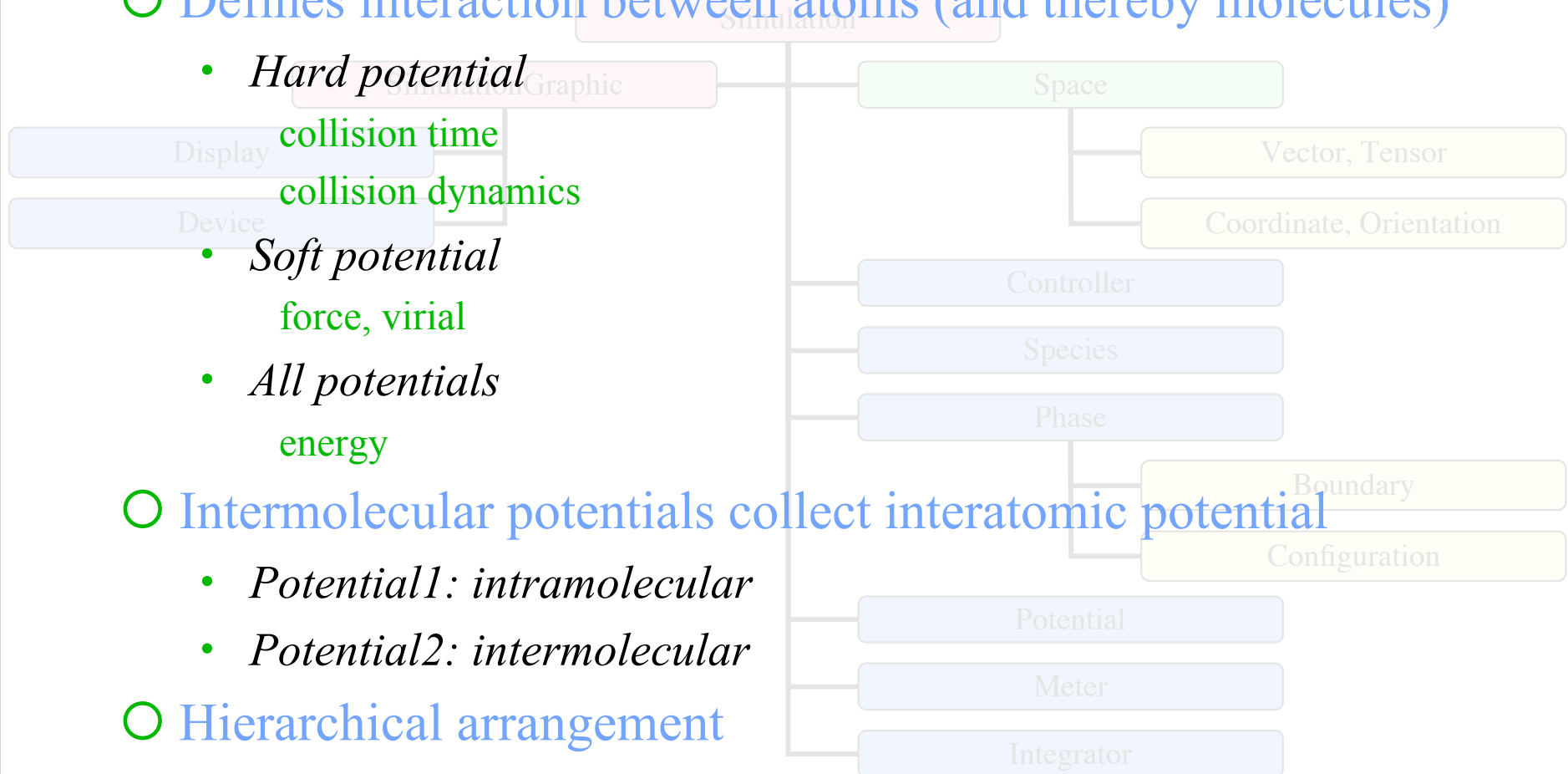
- *Hard potential*
collision time
collision dynamics
- *Soft potential*
force, virial
- *All potentials*
energy

○ Intermolecular potentials collect interatomic potential

- *Potential1: intramolecular*
- *Potential2: intermolecular*

○ Hierarchical arrangement

- *More later*



Simulation Elements: Display

- Presents information from the simulation

- *display of configuration for animation*

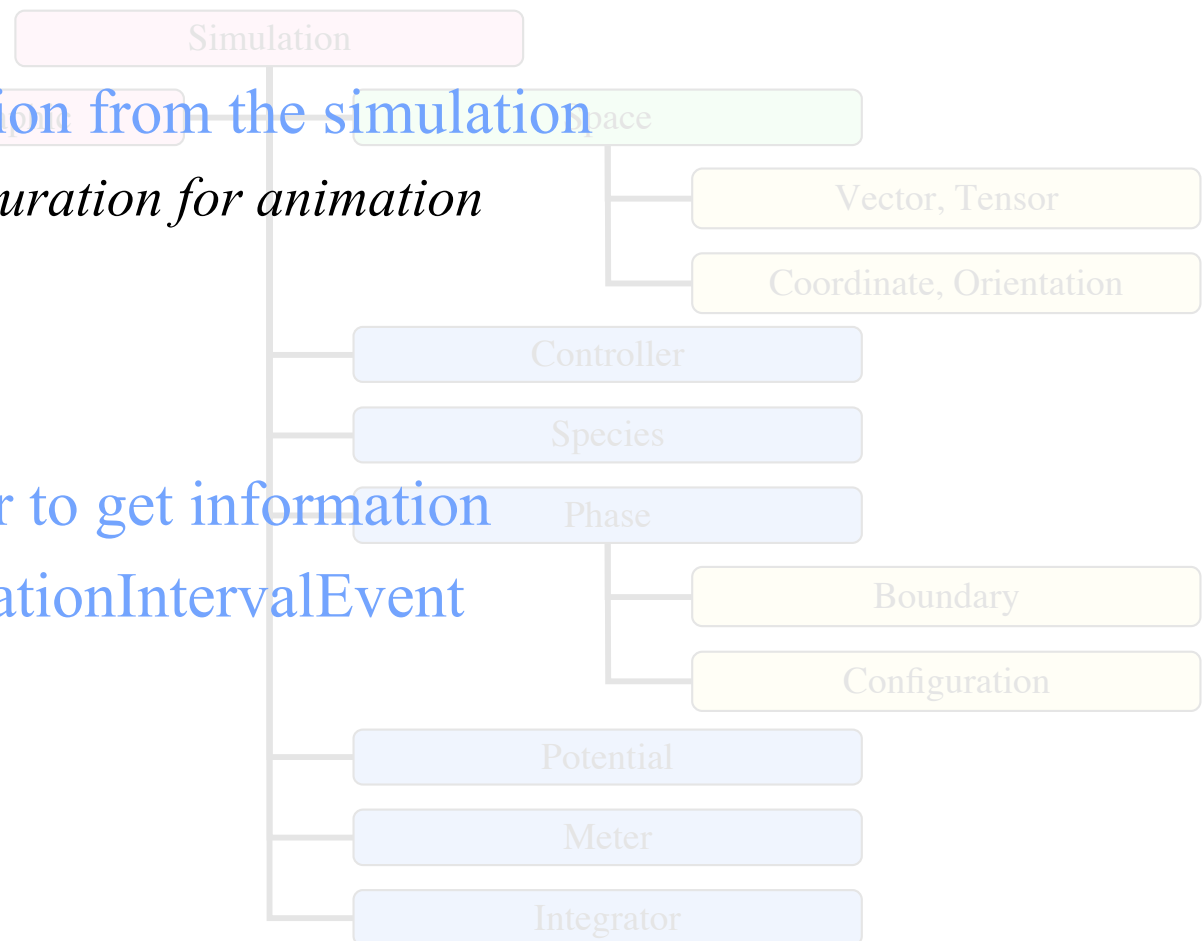
- *display of data*

- table

- graph

- Connects to Meter to get information

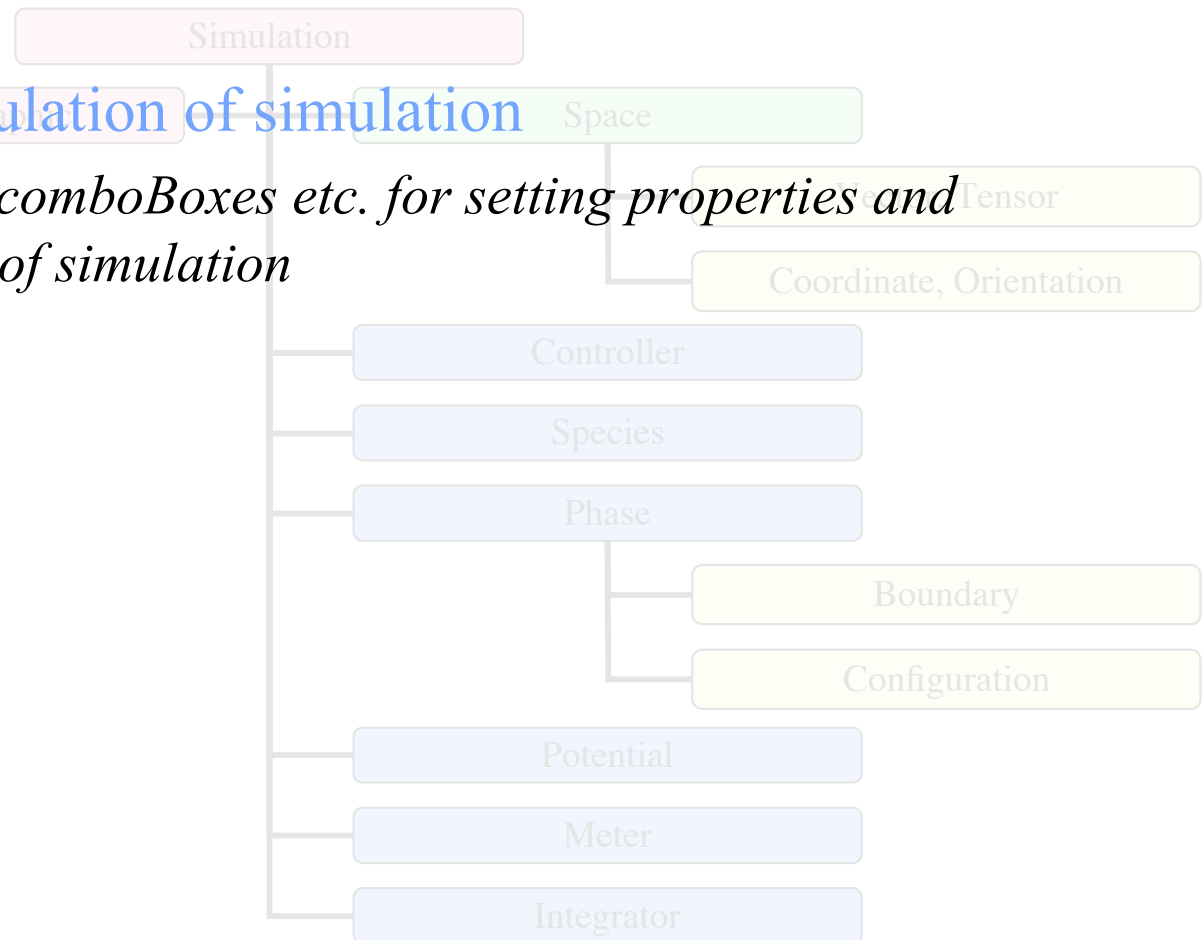
- Listener of IntegrationIntervalEvent



Simulation Elements: Device

○ Interactive manipulation of simulation

• sliders, buttons, comboBoxes etc. for setting properties and affecting course of simulation



Putting It Together

```
//import classes from library
import etomica.*;
import etomica.graphics.*;
import etomica.action.PhaseImposePbc;
import etomica.action.activity.ActivityIntegrate;
import etomica.graphics.SimulationGraphic;
import etomica.integrator.IntegratorHard;
import etomica.potential.P2HardSphere;
import etomica.space2d.Space2D;

public class MySimulation extends Simulation {
```

Continued...

Save this code in a
file named
MySimulation.java

Putting It Together

```

public class MySimulation extends Simulation {

    public ActivityIntegrate activityIntegrate;

    //Constructor
    public MySimulation(Space2D space) {
        super(space);
        //Instantiate classes
        IntegratorHard integrator = new IntegratorHard(potentialMaster);
        integrator.setIsothermal(false);
        activityIntegrate = new ActivityIntegrate(integrator);
        getController().addAction(activityIntegrate);
        SpeciesSpheresMono species = new SpeciesSpheresMono(this);
        species.setNMolecules(64);
        Phase phase = new Phase(space);
        P2HardSphere potential = new P2HardSphere(space);
        potentialMaster.setSpecies(potential,
                                   new Species[]{species,species});

    //Tie elements together
        integrator.addIntervalListener(new PhaseImposePbc(phase));
        phase.speciesMaster.addSpecies(species);
        integrator.addPhase(phase);
    } //end of constructor

```

Save this code in a
file named
MySimulation..java

Continued...

Putting It Together

```
}//end of constructor

/**
 * Demonstrates how this class is implemented.
 */
public static void main(String[] args) {
    MySimulation sim = new MySimulation(new Space2D());
    SimulationGraphic graphic = new SimulationGraphic(sim);
    sim.activityIntegrate.setDoSleep(true);
    graphic.makeAndDisplayFrame();
} //end of main
} //End of MySimulation class
```

Save this code in a
file named
MySimulation..java

Running It: Application

- If needed, obtain the java runtime for your platform from Sun
- Get the etomica class library archive, etomica.jar. Place it in the same directory as your source file
- Compile your source
 - `javac -classpath etomica.jar MySimulation.java`
creates *MySimulation.class*
- Run as an application
 - `java -cp etomica.jar;. MySimulation`

Running It: Applet

- Add an Applet inner class to your source

```

} //End of main
public static class Applet extends javax.swing.JApplet {
    public void init() {
        MySimulation sim = new MySimulation(new Space2D());
        SimulationGraphic graphic = new SimulationGraphic(sim);
        getContentPane().add(graphic.panel());
    }
} //end of Applet
} //End of MySimulation class

```

- Compile to create MySimulation.class, as for application

- Create an html file, named (for example) Applet.html

```

<HTML>
<HEAD> <TITLE>Applet HTML</TITLE> </HEAD>
<BODY bgcolor="#ffffff">
<APPLET CODE= "MySimulation$Applet.class" archive= "etomica.jar"
    WIDTH=640 HEIGHT=350></APPLET>
</BODY>
</HTML>

```

- Run applet, either

- *Using appletviewer at command line: appletviewer Applet.html*
- *Or using your web browser, pointed at Applet.html on your machine*
- *Or deploy to a web server for the rest of the world to enjoy!*

Extend Your Application

- Examine the specification of the classes in the API.
- Consider some modifications
 - *Change the number of atoms*
 - *Add a meter for the temperature*
 - *Add a meter for the radial distribution function*
 - *Add a device to change the temperature*
 - *Add a device to change the density*
- Try them out!