All About Meters and Data

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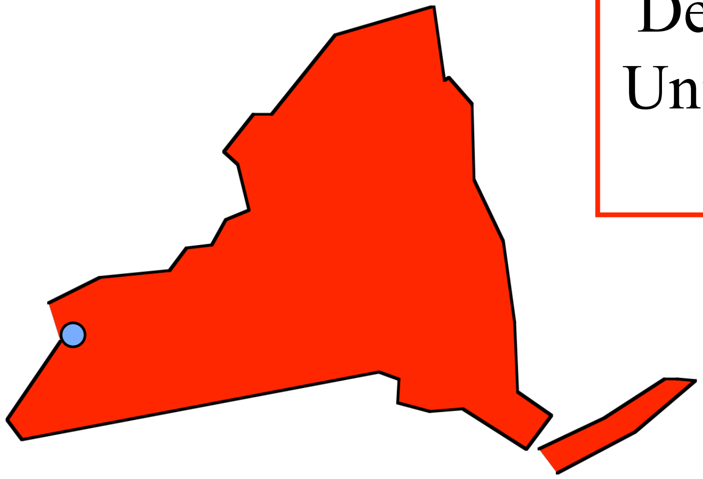

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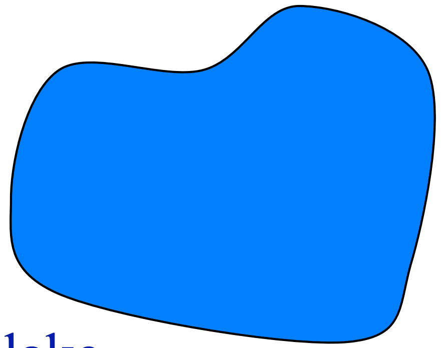
Statistical Mechanical Averages

- Mechanical properties
  - Value can be associated with each configuration
  - Examples
    - Energy
    - Pressure
    - Density
    - Structure
- Entropic properties
  - Value describes not one configuration, but the whole set
  - Examples
    - Entropy (multiplicity)
    - Free energy
    - Chemical potential
- Analogy
  - Average depth of a lake versus the area of the lake



Ensemble Averages

- Consider molecular configurations in proportion to their statistical mechanical weight
  - E.g., Boltzmann distribution

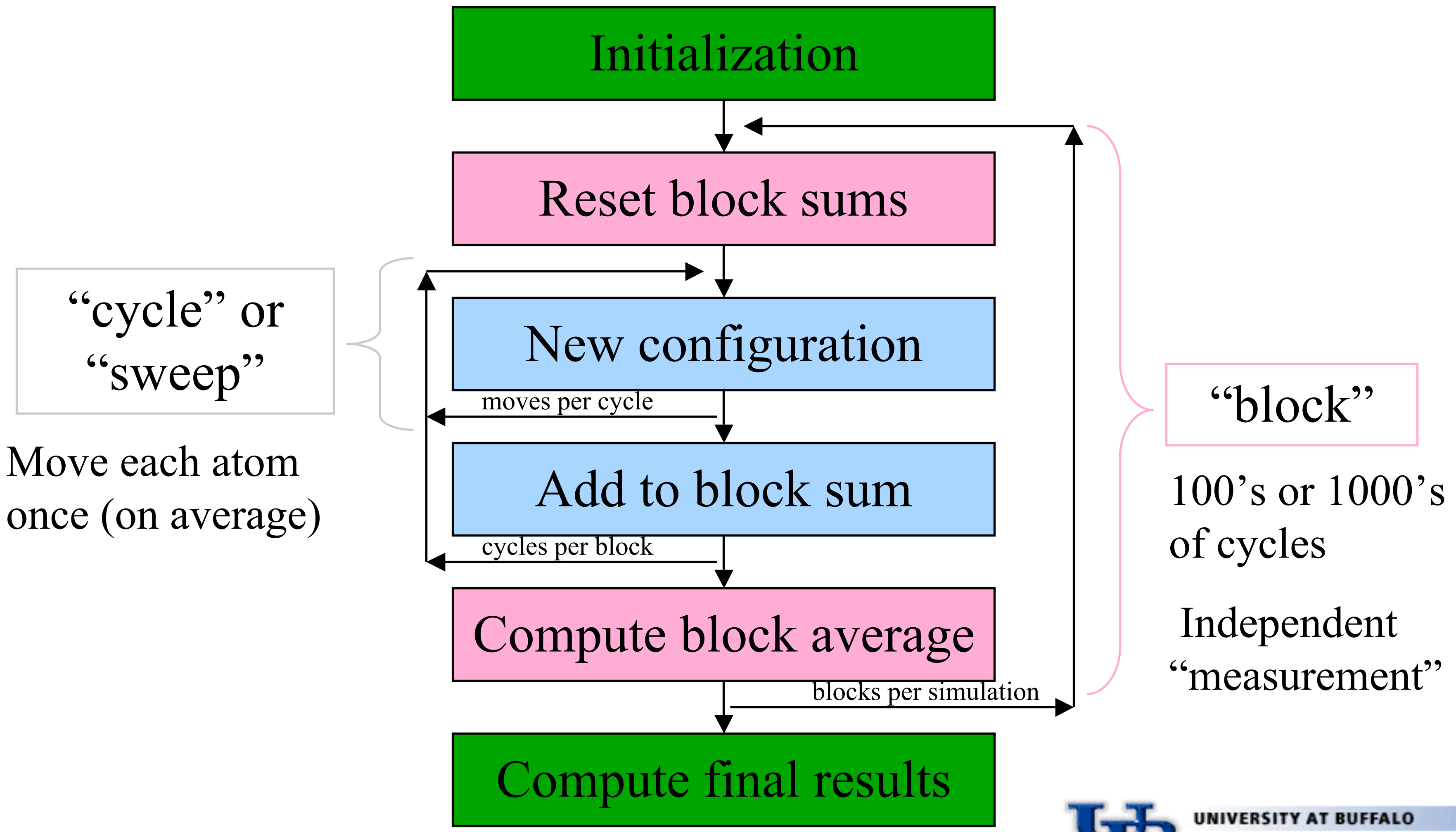
$$\pi_i = \frac{1}{Q} e^{-\beta U_i}$$

- Accumulate average of mechanical property over all configurations
  - E.g., Average internal energy

$$\begin{aligned} U &= \langle U \rangle_\pi \\ &= \int d\mathbf{r}^N U\left(\mathbf{r}^N\right) \pi\left(\mathbf{r}^N\right) \end{aligned}$$

Measurements in Molecular Simulation

- General structure of a simulation



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Measurements in Molecular Simulation

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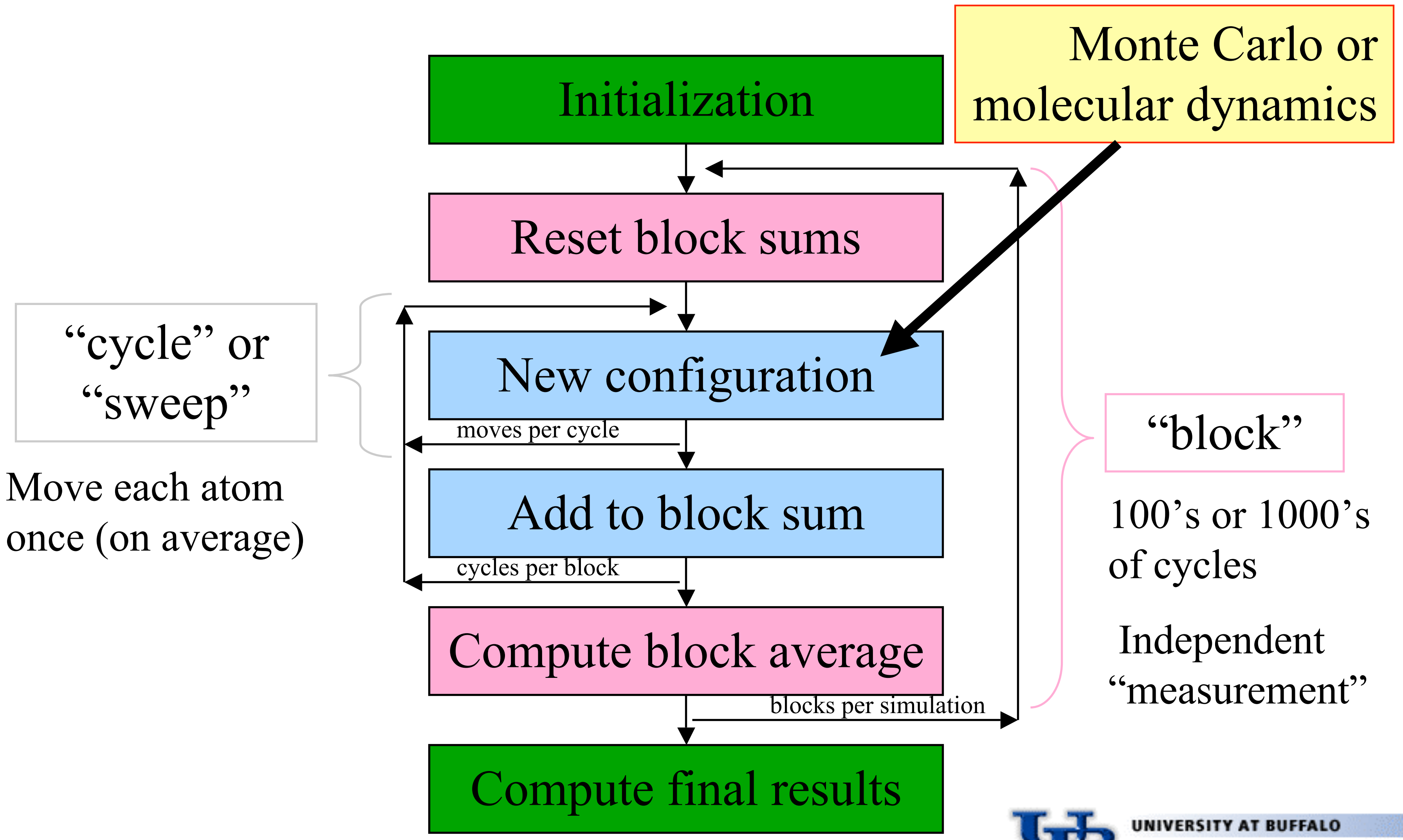
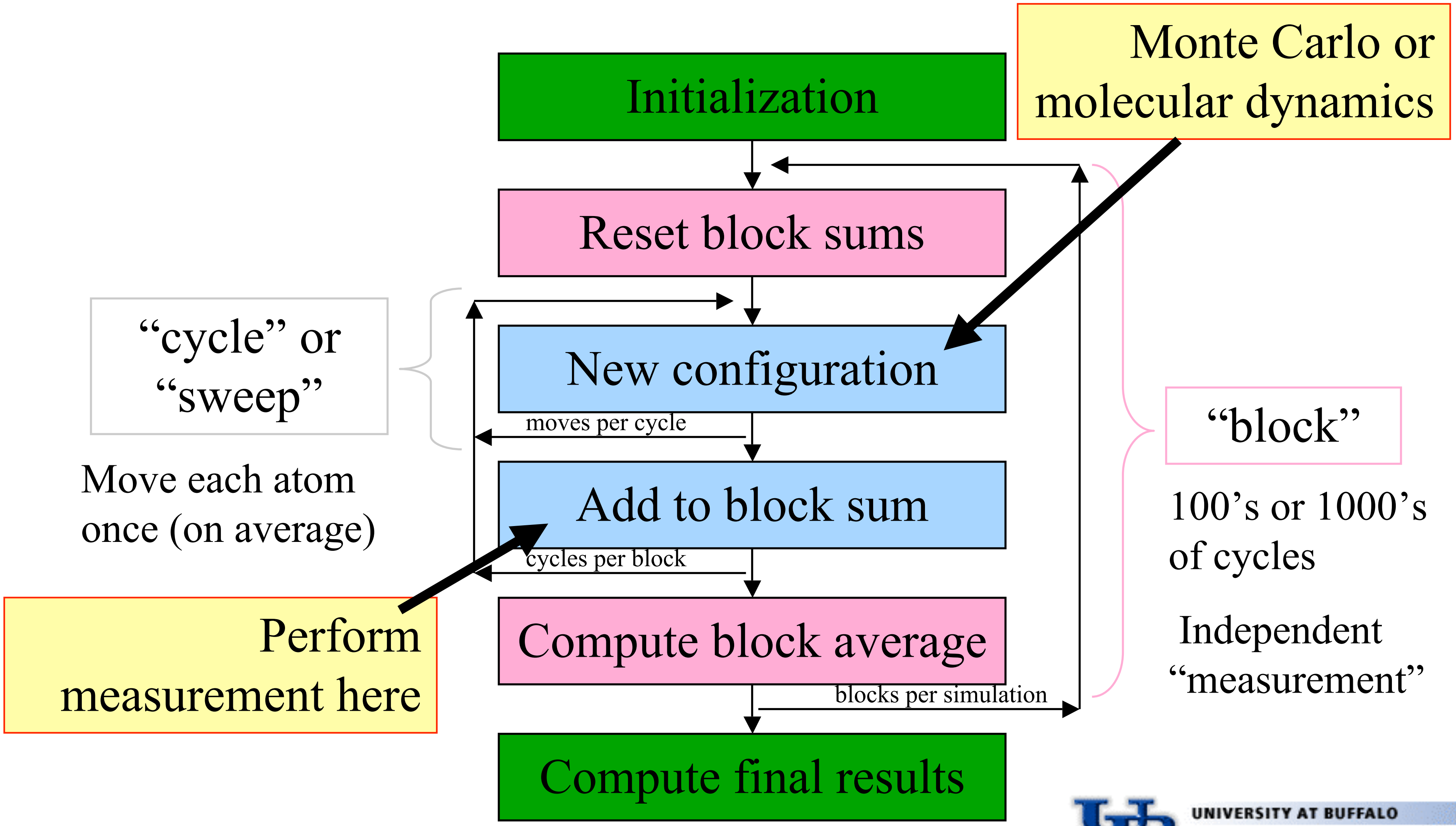


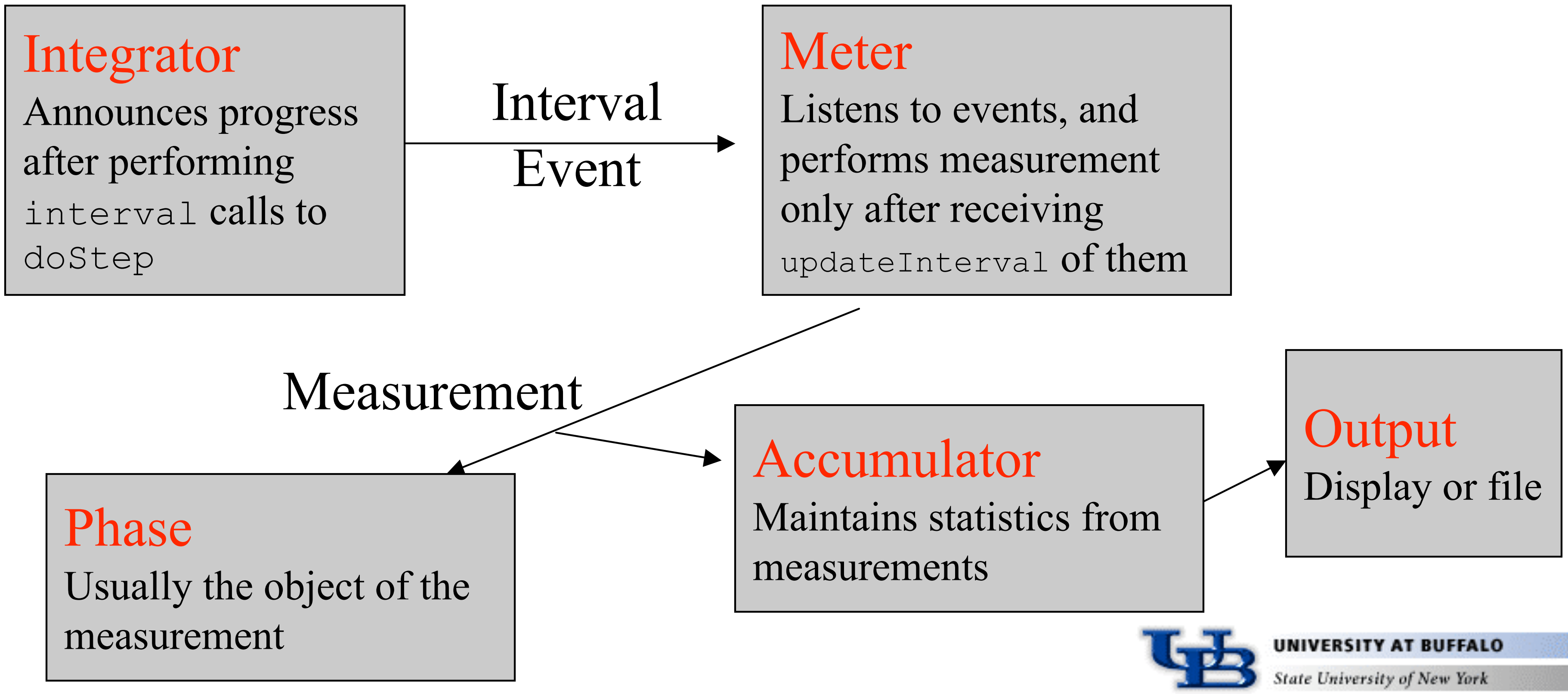
Measurements in Molecular Simulation

- General structure of a simulation

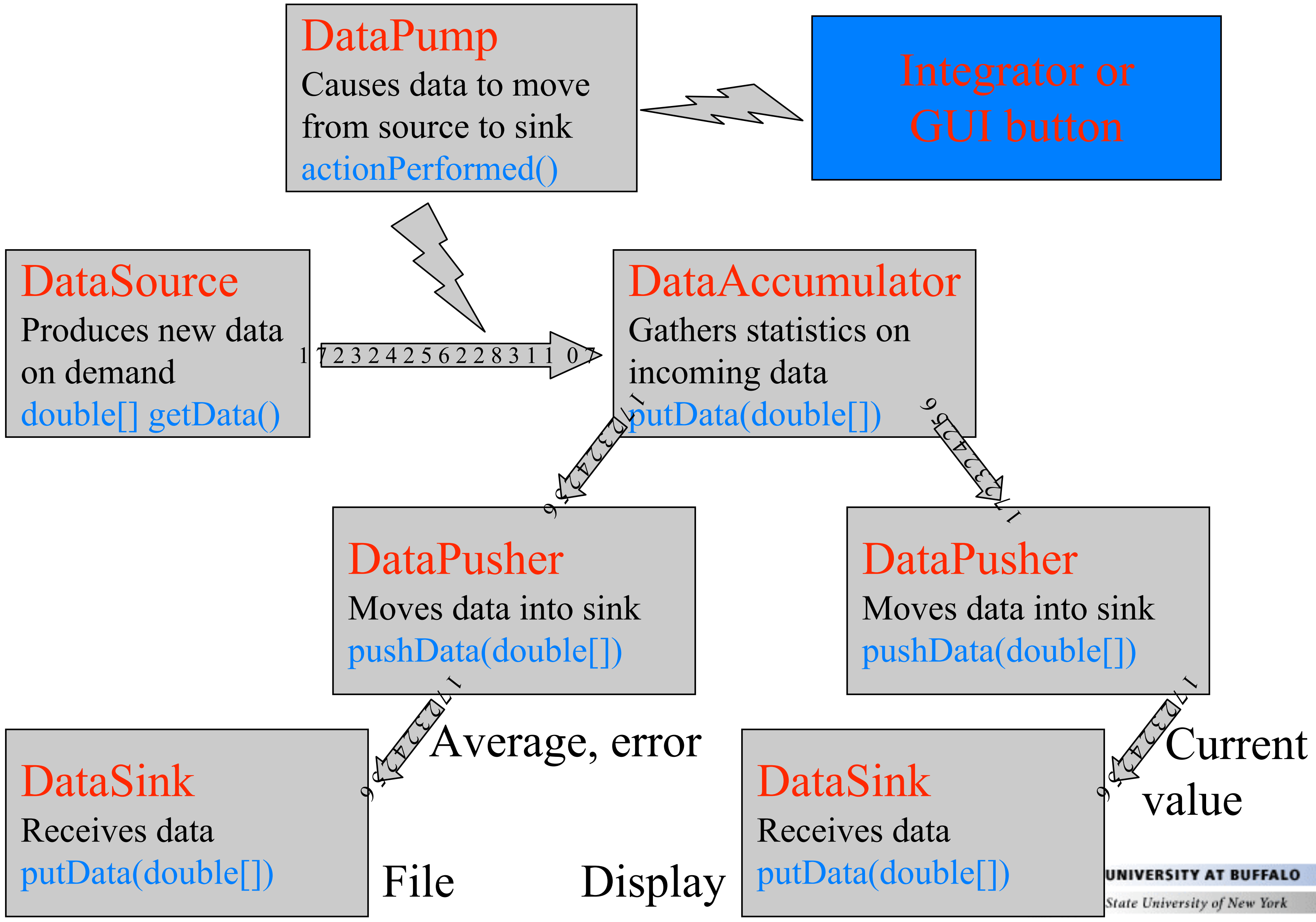


Property Measurement in Etomica

- Meters perform measurements on phases
  - Conducted on Integrator's thread, so system is static while measurement is performed
- Chain of events leading to a measurement


Integrator
Announces progress after performing `interval` calls to `doStep`
Interval Event
Meter
Listens to events, and performs measurement only after receiving `updateInterval` of them
Measurement
Phase
Usually the object of the measurement
Accumulator
Maintains statistics from measurements
Output
Display or file

Data Flows in Etomica



DataSource, DataSink, Meter

- DataSink – Interface for classes that receive data

```
public interface DataSink {
    public abstract void putData(double[] values);
}
```

- DataSource – Interface for classes that provide data

```
public interface DataSource {
    public abstract double[] getData();
}
```

- MeterAbstract – DataSource that acts on a Phase

```
public interface DataSource {
    public abstract double[] getData();
}
```

DataPusher

- Abstract class
- Holds one or more data sinks, and pushes data into them on request
- Has methods to manage data sinks

```
public abstract class DataPusher {

    protected void pushData(double[] data) {
       for(int i=dataSinkList.length-1; i>=0; i--) {
          dataSinkList[i].putData(data);
       }
    }

    public void addDataSink(DataSink dataSink) {
    ...
    }

    public void removeDataSink(DataSink dataSink) {
    ...
    }
}
```

DataPump

- Extends DataPusher
- Holds a DataSource, and moves data from it to the sinks
- Implements action
  - Typically activated via Integrator IntervalEvent, or GUI action

```
public class DataPump {

    public void actionPerformed() {
        pushData(dataSource.getData());
    }
}
```

- IntervalActionAdapter
  - Transmits an Integrator IntervalEvent into an Action

```
public class IntervalActionAdapter {
    public void intervalAction(Integrator.IntervalEvent evt)
{
        if (--iieCount == 0) {
           iieCount = actionInterval;
           action.actionPerformed();
}   }   }
```

DataPipe

- Abstract, extends DataPusher
- Implements DataSink
- Takes data given to it, does something to it, and passes on new data

DataAccumulator

- Abstract, extends DataPipe implements DataSource
- Collects statistics on data given to it
- Passes data down stream only after some interval of data collecting

```
public abstract class DataAccumulator {

    public void putData(double[] newData) {
        if(!active) return;
        addData(newData);
        if (--putCount == 0) {
            putCount = pushInterval;
            pushData(getData());
        }
    }

    public abstract void addData(double[] data);
}
```

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DataAccumulator subclasses

- AccumulatorAverage
  - Generates statistics for average, error, standard deviation, and more

```
public class AccumulatorAverage extends DataAccumulator {

    public void addData(double[] value) {
        for(int i=nDataMinus1; i>=0; i--) {
            double v = value[i];
            mostRecent[i] = v;
            blockSum[i] += v;
            blockSumSq[i] += v*v;
        }
    }
}
```

- AccumulatorHistogram
  - Generates histogram of data given to it
- AccumulatorHistory
  - Records history of data given to it

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            blockSum[i] += v;
            blockSumSq[i] += v*v;
         }
    }
    public double[] getData() {
      ...
}   }
```

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Display

- Abstract class that puts information to screen
- Sometimes implements DataSink
- Example: DisplayBoxesCAE
  - Designed to take data from AccumulatorAverage

```
public class DisplayBoxesCAE extends Display implements DataSink {

    public void setAccumulator(AccumulatorAverage accumulatorAverage) {
        this.accumulatorAverage = accumulatorAverage;
        accumulatorAverage.makeDataPusher(new AccumulatorAverage.Type[] {
                AccumulatorAverage.MOST_RECENT,
                AccumulatorAverage.AVERAGE,
                AccumulatorAverage.ERROR}).addDataSink(this);
    }
    public void putData(double[] data) {
        datumC[0] = data[0];
        currentBox.putData(datumC);
        datumA[0] = data[1];
        averageBox.putData(datumA);
        datumE[0] = data[2];
        errorBox.putData(datumE);
}   }
```

Putting it together

```
import etomica.*;
import etomica.action.*;
import etomica.data.*;
import etomica.graphics.*;
import etomica.integrator.*;
import etomica.potential.P2HardSphere;
import etomica.space2d.Space2D;

public class HSMD2D extends Simulation {

    public ActivityIntegrate activityIntegrate;
    public AccumulatorAverage pressureAverage;

    public HSMD2D() {
         super(new Space2D());

        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});

       //(CONT'D)
```

Putting it together

```
        integrator.addIntervalListener(new PhaseImposePbc(phase));
        phase.speciesMaster.addSpecies(species);
        integrator.addPhase(phase);
        integrator.setIsothermal(true);

        MeterPressureHard meterPressure = new MeterPressureHard(integrator);
        meterPressure.setPhase(phase);
        pressureAverage = new AccumulatorAverage();
        DataPump pressurePump = new DataPump(meterPressure, pressureAverage);
        IntervalActionAdapter pressureAction =
                 new IntervalActionAdapter(pressurePump, integrator);
    }

    /**
     * Demonstrates how this class is implemented.
     */
    public static void main(String[] args) {
        HSMD2D sim = new HSMD2D();
        SimulationGraphic graphic = new SimulationGraphic(sim);
        sim.activityIntegrate.setDoSleep(true);
        DisplayBoxesCAE pressureDisplay = new DisplayBoxesCAE();
        pressureDisplay.setAccumulator(sim.pressureAverage);
        graphic.add(pressureDisplay);
        graphic.makeAndDisplayFrame();
    } //end of main
}
```