All About Meters

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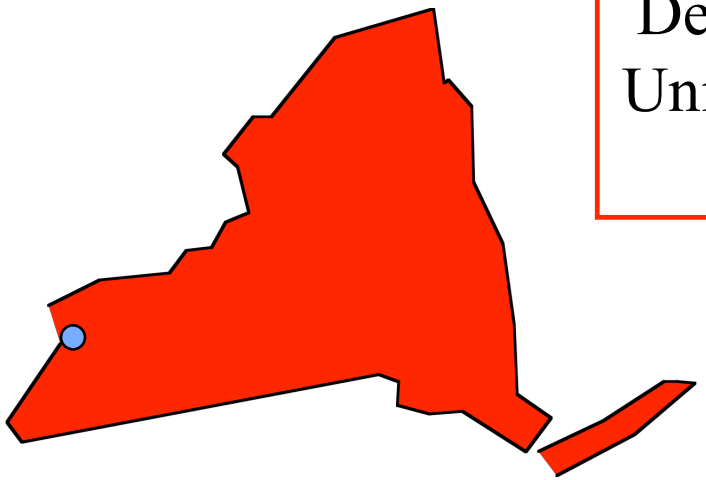

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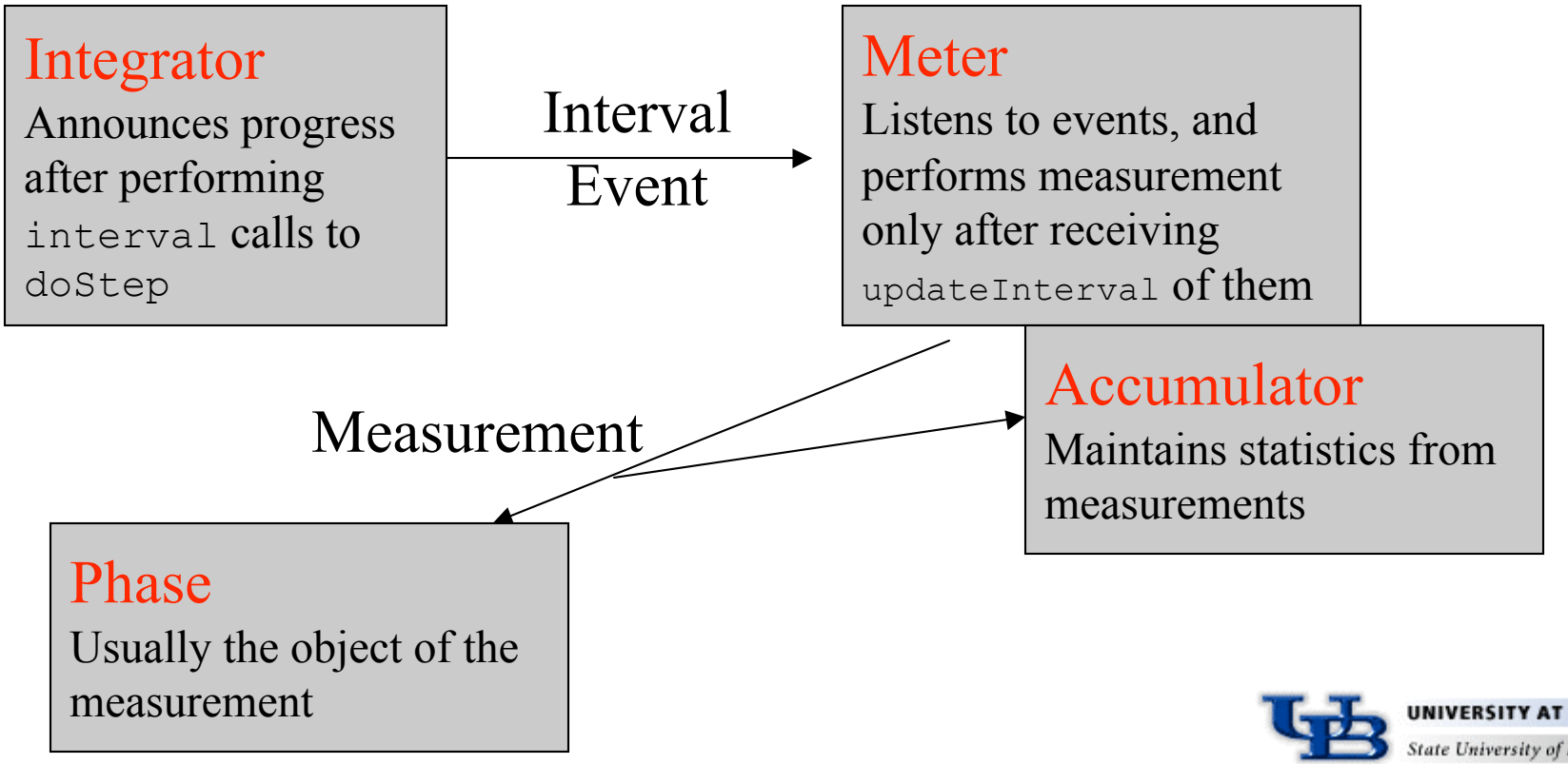
Measurement of Data

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



Relevant Code. Event Firing

- Inside Integrator

```
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
```

Relevant Code. Event Handling

- Inside MeterAbstract

```
public void intervalAction(Integrator.IntervalEvent evt) {
      //meter can be turned off
    if(!active) return;

      //don't act on start, done, initialize events
    if(evt.type() != Integrator.IntervalEvent.INTERVAL) return;

      //go ahead
    if(--iieCount == 0) {
      iieCount = updateInterval;
      updateSums();
    }
}

public abstract void updateSums();
```

- Meters vary in data types they measure
  - `updateSums` defined differently for each kind

Subclasses of MeterAbstract

- Meter
  - Single value is outcome of measurement
  - Measurement is defined in `currentValue` method

```
public void updateSums() {accumulator.add(currentValue());}

public abstract double currentValue();
```

- MeterFunction
  - 1-D array of values (points on a function) is outcome of measurement

```
public void updateSums() {
    double[] values = currentValue();
    for(int i=0; i<nPoints; i++) accumulator[i].add(values[i]); //accumulator for each value
}
public abstract double[] currentValue();
```

- MeterTensor
  - Defined similarly

Accumulator

- MeterAbstract.Accumulator (should make as top-level class)
- Evaluates statistics on data
  - Averages, confidence limits
  - Histograms, history

```
public void add(double value) {
  mostRecent = value; //hold to access most-recent without recalculation
  if(Double.isNaN(value)) return;

  blockSum += value;
  if(--blockCountDown == 0) {//count down to zero to determine completion of block
    blockSum /= blockSize;//compute block average
    sum += blockSum;
    sumSquare += blockSum*blockSum;
    count++;
    if(count > 1) {
      double avg = sum/(double)count;
      error = Math.sqrt((sumSquare/(double)count - avg*avg)/(double)(count-1));
    }
    //reset blocks
    mostRecentBlock = blockSum;
    blockCountDown = blockSize;
    blockSum = 0.0;
  }
  if(histogramming) histogram.addValue(value);
  if(historying) history.addValue(value);
}
```

Accessing Statistics

- Available from the Meter

```
public double average() {
  return (function==null) ? accumulator.average() : function.f(accumulator.average());
}

public double variance() {return accumulator.variance();}

public double error() {
  if(function == null) return accumulator.error();
  else {//have not carefully considered if this is correct
      return Math.abs(function.dfdx(accumulator.average()))*accumulator.error();
  }
}

public double mostRecent() {
  return (function==null) ?
          accumulator.mostRecent() : function.f(accumulator.mostRecent());}

public double mostRecentBlock() {
  return (function==null) ?
          accumulator.mostRecentBlock() : function.f(accumulator.mostRecentBlock());}


public Histogram getHistogram() {return accumulator.histogram();}
```

- Function can be used to modify value…

Function (An aside)

- Interface for a function (transforming a double to a double)

```
package etomica.utility;

public interface Function {
    public double f(double x);
    public double inverse(double f);
    public double dfdx(double x);

     // The function f(x) = 1/x
    public static class Reciprocal implements Function {

        public double f(double x){return 1.0/x;}
        public double dfdx(double x){return -1.0/(x*x);}
        public double inverse(double x){return 1.0/x;}
    }
     // The function f(x) = a*x + b
    public static class Linear implements Function {
        private final double a, b, ra;
        public Linear(double slope, double intercept) {
            this.a = slope;
            this.b = intercept;
            ra = 1.0/a;
        }
        public double f(double x) {return a*x + b;}
        public double inverse(double f) {return ra*(f-b);}
        public double dfdx(double x) {return a;}
    }
          //etc.
}
```

Accessing Any Statistic

- Sometimes need to specify desired statistic at run time
- `value(MeterAbstract.DataType type)` method permits this
- Inside Meter…

```
public double value(MeterAbstract.ValueType type) {
    if(type==MeterAbstract.AVERAGE || type == null) return average();
    else if(type==MeterAbstract.MOST_RECENT) return mostRecent();
    else if(type==MeterAbstract.CURRENT) return currentValue();
    else if(type==MeterAbstract.MOST_RECENT_BLOCK) return mostRecentBlock();
    else if(type==MeterAbstract.ERROR) return error();
    else if(type==MeterAbstract.VARIANCE) return variance();
    else return Double.NaN;
}
```

- Method often applied by Display objects
  - Inside DisplayBox…

```
public void doUpdate() {
  if(source == null) return;
  value.setText(format(unit.fromSim(source.value(whichValue)),precision));
}
```

- Used particularly by Etomica GUI…(demo)

Typed (Enumerated) Constants 1.

- Some methods are meant to accept only a limited set of values for their arguments
  - VERTICAL/HORIZONTAL
  - NORTH/EAST/SOUTH/WEST
  - CURRENT, AVERAGE, ERROR, VARIANCE, MOST_RECENT
- One strategy is to key each value to a static integer constant
  - public static final HORIZONTAL = 0; etc.
  - public void setOrientation(int k) {…}
- Disadvantages
  - Method will accept any integer
  - No way to access full set of acceptable values at runtime
- Alternative approach is provided by Typed Constants
  - Define a type for each set of values
  - Create unique instances of only acceptable values
  - Key actions to equality with unique instances
  - Disadvantage: won't work in `case` statement

Typed (Enumerated) Constants 2.

- Inside etomica.Constants…

```
public static abstract class TypedConstant implements java.io.Serializable {
   private final String label;
   protected TypedConstant(String s) {label = s;} //constructor accessible only to subclasses
   public String toString() {return label;}
   public abstract TypedConstant[] choices();
}
/**
 * Typed constant for specifying HORIZONTAL/VERTICAL alignment.
 */
public static class Alignment extends TypedConstant {
  private Alignment(String label) {super(label);} //cannot instantiate externally
  public static final Alignment[] CHOICES = new Alignment[] {
      new Alignment("Horizontal"), //these are the only instances that will ever be made
      new Alignment("Vertical")};
  public final TypedConstant[] choices() {return CHOICES;}
}
public static final Alignment HORIZONTAL = Alignment.CHOICES[0];
public static final Alignment VERTICAL = Alignment.CHOICES[1];
```

- Access
  - Constants.HORIZONTAL
  - Constants.VERTICAL
  - Constants.Alignment.CHOICES or *instance*.choices()

DatumSource/DataSource Interfaces

- Data might be displayed from sources other than Meter
  - E.g., Controller that integrates over a range of conditions
  - Interface lets displays operate with other sources

```
public interface DataSource {
  public double[] values(ValueType type);
   //Returns a label used to describe the data when presented
  public String getLabel();
   //Returns the physical dimensions (e.g., length) of the data
  public etomica.units.Dimension getDimension();
  //Type class used to indicate to the data source which data is requested
  public static abstract class ValueType extends Constants.TypedConstant {
     protected ValueType(String label) {super(label);}
  }
  // Interface for a data source that has associated "x" values
  public interface X extends DataSource {
    public double[] xValues();
    public String getXLabel();
    public etomica.units.Dimension getXDimension();
  }
  // Indicates an object that uses a DataSource.  Useful mainly to the Mediator
  public interface User {
    public void setDataSource(DataSource source);
    public DataSource getDataSource();
  }
  public interface MultiUser {…
  public interface Wrapper {…
}//end of DataSource
```

- DatumSource defined similarly to yield a single value

History and Histogram

- Accumulator can provide other information
  - Histogram of values passed to it via the `add` method
  - History of those values
    - Development needed here to make History treat long-period data in different ways
      - Cycle back to beginning (current functionality)
      - Coarse-grain
      - Expand window with addition of new data
- Functionality initiated only if directed via
  - `setHistogramming(true);` or
  - `setHistorying(true)`
- History/Histogram obtained from meter (get methods)
  - Objects obtained this way implement DataSource interface

MeterGroup

- Some properties are best calculated all together, but a function isn't appropriate
  - E.g., species mole fractions
- MeterGroup acts like a set of independent meters
  - `public Meter[] allMeters()` method gives array of pseudo-meters that each act as stand-alone meters would
  - Internally, calculations for each pseudo-meter are performed together
- For example, see `MeterDimerFraction` class defined as part of the `KineticsModule` simulation
- MeterMultiFunction (sort of) acts similarly for a group of MeterFunctions

Miscellany

- MeterCollisional
  - Interface that defines method to be called every time IntegratorHard processes a collision
  - Meter acts on data generated by these calls
- MeterProfile
  - Wraps a meter that implements Meter.Atomic, which guarantees that property can be measured separately for each atom
  - Profile keeps track of values as a function of linear position in the simulation volume
- MeterDatumSourceWrapper
  - Wraps a non-Meter DatumSource to add Meter-like functionality, such as historying or histogramming