Etomica: An API for Molecular Simulation

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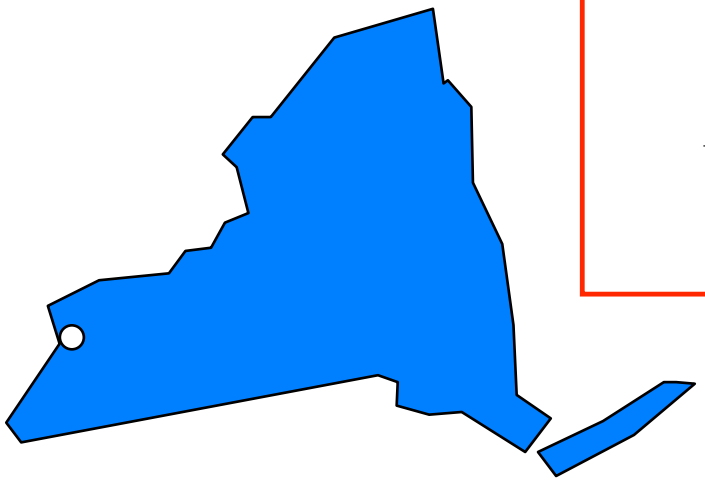

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Outline

- Background
- Design considerations
- Data structures
- Models
- Flow control, actions, and sampling
- Measurements and data processing
- I/O and graphics
- Utilities
- Supporting tools
- Performance
- Some applications

Background

- Fortran-based programmer for 15 years
  - Mostly MC applied to simple fluid and crystalline model systems
- Developed interest in object-oriented programming
  - Took up Java when it emerged in mid-1990's
- Sabbatical at UT-Knoxville/ORNL with PTC
  - 1996-97
- PTC initiated CACHE Molecular Modeling Task Force
  - Wrote successful proposal to develop molecular simulation modules for undergraduate instruction
  - Based in Java for portability, ability to construct browser-based applets
- Initiated molecular simulation API in support of activity

Educational Applications of Etomica

- Summer 1999, 2000
  - Two-week high-school workshop in Computational Chemistry at UB Center for Computational Research
- Fall 2001
  - Freshman/Sophomore honors seminar on molecular simulation
- Spring 2000, 2003
  - CE530 Molecular Simulation
- Summer 2000, 2003, 2004
  - REU students
- Fall 2000, Spring 2004
  - CE 526 Statistical Mechanics
- Spring 2004, 2005
  - Molecular Modeling (senior elective)
- Spring 2005
  - CE 304 Thermodynamics, homework problem

Research Applications of Etomica

- Development of free-energy methods
  - Lennard-Jones, water, simple ionic systems (no Ewald)
- Study of vacancies, defects, miscibility in solids
  - Hard spheres, Lennard-Jones, Valence-force-field models
- Mayer-sampling method for evaluation of virial coefficients
  - Hard spheres, Lennard-Jones, water, alkanes
- Study of vapor-liquid interfacial properties of associating fluids
  - Anisotropic Lennard-Jones, square-well based models

Design Considerations

- Goals
  - Extensible, broadly applicable
  - Computational efficiency
  - Suitable to run interactively or in batch
- Guidelines
  - Highly granular pieces with convenience classes that assemble them
  - Separate components as much as possible
    - Graphics separate from other parts
    - Used objects don't know about user
  - Try to re-use themes that guide design of data and other constructs
    - Parallel hierarchies
    - Event model

Simulation

- Simulation
  - Organizes other elements
  - Common point of reference
  - Independent entity—no simulation knows about or interacts with another Simulation instance
  - No graphical elements
  - Develop new simulations by extending Simulation
    - Assemble simulation in constructor
    - Most fields publicly accessible
    - Reusable in different contexts
  - SimulationContainer gives simulation an interface
    - Graphical elements
    - Remote access as a future consideration
  - Space is assigned to Simulation at construction

Space

- Factory for objects that depend on or define the physical space
  - Vector, Tensor, Orientation, Boundary
- All object methods are implemented in a spatially-independent manner
  - Vector methods defined for vector addition, scalar multiplication, dot product, simple compound operations, etc.
- Easy to convert from simulation in one dimension to another

Data Structures: Atom

- Atom
  - Represents physical atom being simulated
- Contains several fields assigned on construction
  - coord: Coordinate the defines the state of the atom
    - Position, velocity, orientation, spin, etc.
    - Constructed by Space
  - type: AtomType, with information common to multiple atoms
    - Many atoms will reference a single instance of a common AtomType
    - Holds common parameters such as atom mass, size, etc.
    - Holds other information used for operation of simulation
  - seq: AtomSequencer, which is used to place atom in linked list
  - node: AtomTreeNode, which places atom in a tree structure
  - agents[]: Array of objects for anything else
    - Any object can request an instance of its agent be placed in this array for all atoms

Data Structures: AtomFactory

- AtomFactory
  - Builds a molecule according to a specification
  - "Atom" is defined generally
    - "Leaf" atom corresponds to a physical atom
    - Group of atoms, even molecules, are represented by instances of Atom
    - Molecule is represented by a tree structure, using AtomTreeNode
- AtomFactoryMono, AtomFactoryHomo, AtomFactoryHetero
  - Hierarchical: Large molecules built from factories that comprise other factories that build the molecule subunits
- Each factory attaches a unique AtomType to all the Atoms it builds
- Factory has a Conformation that arranges atoms

Data Structures: Phase

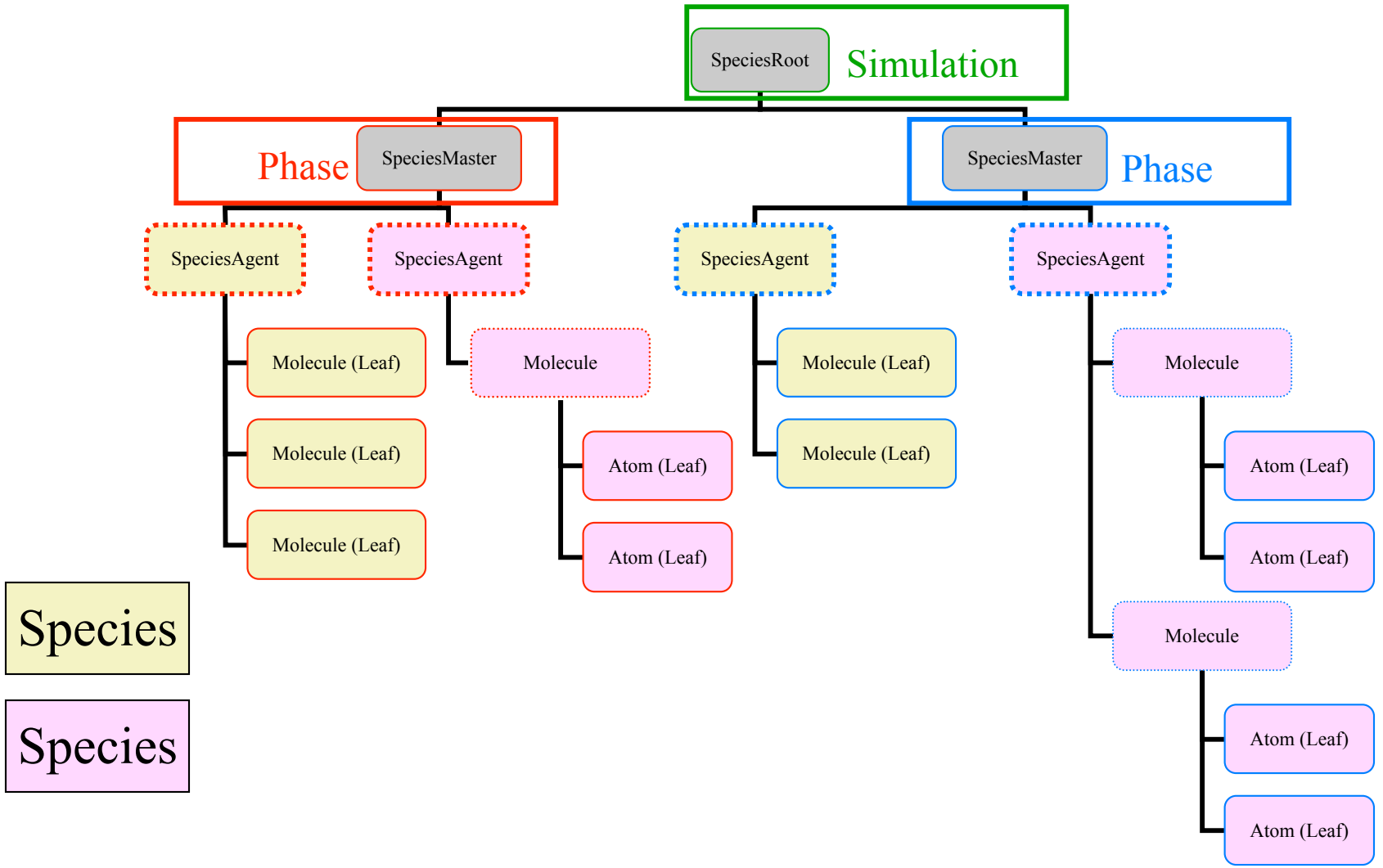
- Phase
  - Collects all atoms that interact with each other
- A single Simulation may employ multiple Phase instances
  - Parallel tempering, Gibbs ensemble
  - No atoms in one Phase interact with atoms in another Phase
  - Phases may interact in more abstract ways (e.g., exchange volume)
- Phase holds a Boundary instance
  - Constructed by Space
  - Implements (or not) periodic boundary conditions
- Phase holds a Lattice, dividing space into cells
  - Useful for neighbor listing, perhaps other things
- Phase holds a Configuration, used to arrange the molecules in a standard way

Data Structures: Species

- Species classes collect information needed to construct and manage molecules
  - AtomFactory
- Extended to make convenience classes
- SpeciesAgent represents Species in each Phase instance
  - extends Atom

Data Structures: Species Hierarchy

- All Atom instances in a Simulation arranged in a hierarchy



Data Structures: AtomsetIterator

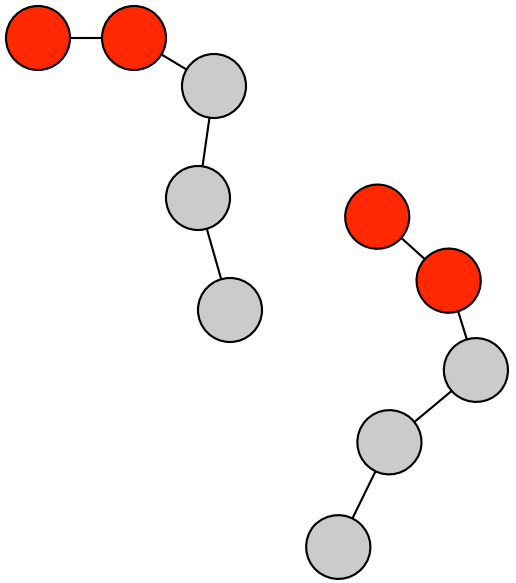
- AtomSet
  - Interface for a set of atoms
    - Atom, AtomPair most often used
- Many types of atom-set iterators
  - Iterate atoms or atom pairs at a particular level in hierarchy
  - Iterate pairs formed with a particular atom
  - Iterate in one or both directions from a given atom
  - Many interfaces defined
    - AtomsetIteratorPhaseDependent
    - AtomsetIteratorBasisDependent
    - AtomsetIteratorDirectable
    - AtomsetIteratorTargetable
    - AtomsetIteratorListDependent
    - etc.

Models: Potential

- Potential
  - Defines manner of interaction of atoms
  - public void energy(AtomSet atoms)
- Subclasses specific to 1-body, 2-body, *etc.* forms
- Interfaces for hard and soft potentials
  - PotentialSoft
    - energy, virial, hypervirial, gradient
  - PotentialHard
    - energy, collisionTime, bump

Models: PotentialGroup

- PotentialGroup
  - Collects several potentials that all interact on a single AtomSet
- 1-body PotentialGroup
  - acts on a single Atom (which typically is a group of atoms)
  - collects intramolecular interactions
- 2-body PotentialGroup
  - acts between two Atom instance
  - collects intermolecular interactions



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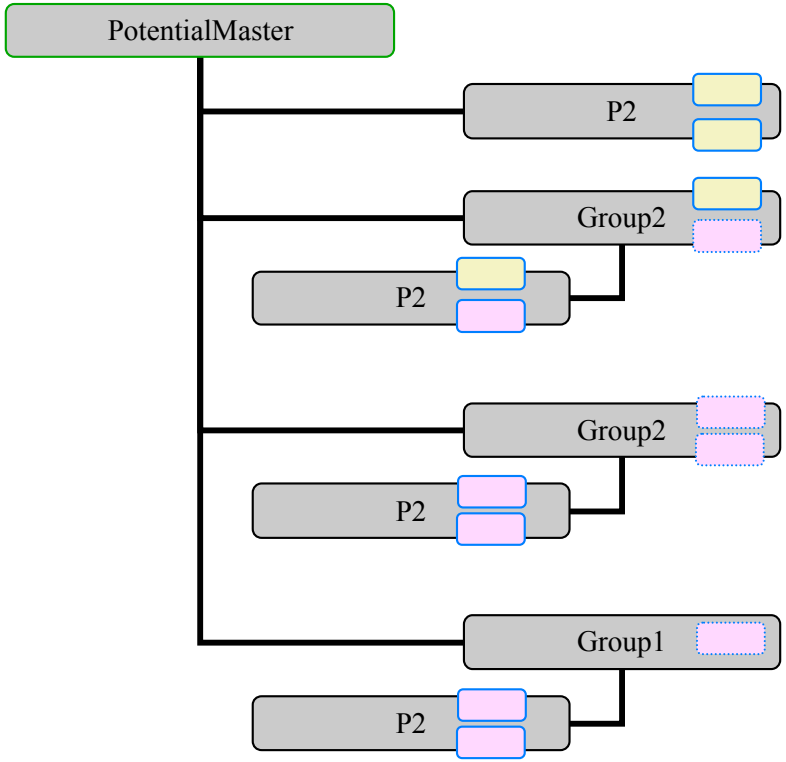
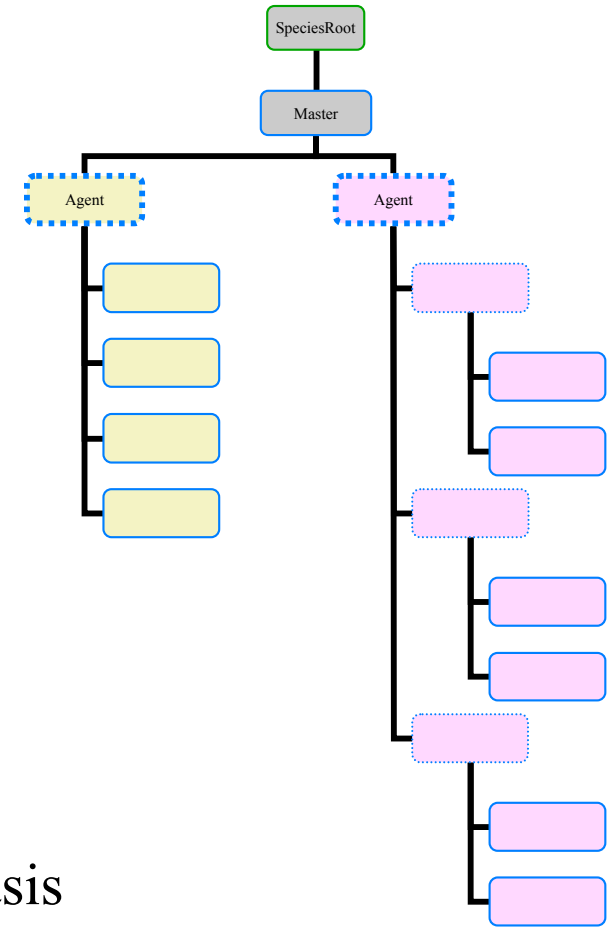
Models: Potential Hierarchy

- Parallels Species hierarchy
  - but not segregated by Phase

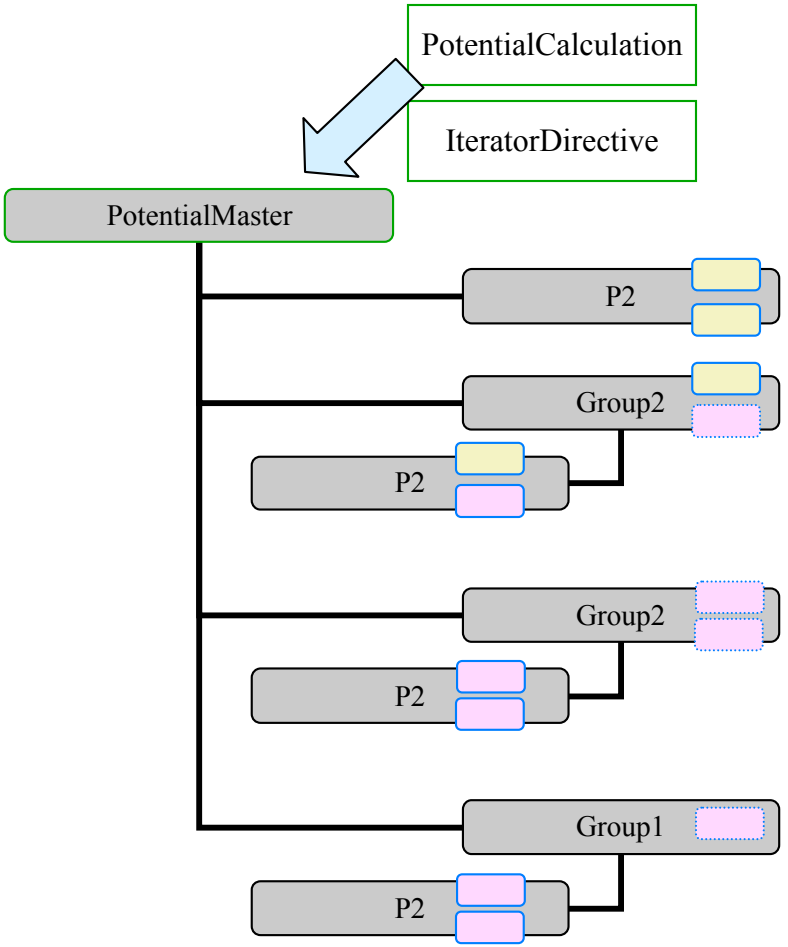




- Each potential iterates over atoms in a basis
  - Iterates form basis for subpotential iteration

Models: PotentialCalculation

- PotentialCalculation
  - Encapsulates the calculation of a property that depends on the potential
  - For example
    - Energy sum
    - Virial sum
    - Collision time
- IteratorDirective
  - Encapsulates specification of atoms to which calculation is applied
  - For example
    - All leaf atom pairs
    - All pairs formed with a specific Atom
    - All child Atoms of a specifc Atom
    - All leaf atoms of a specific Species



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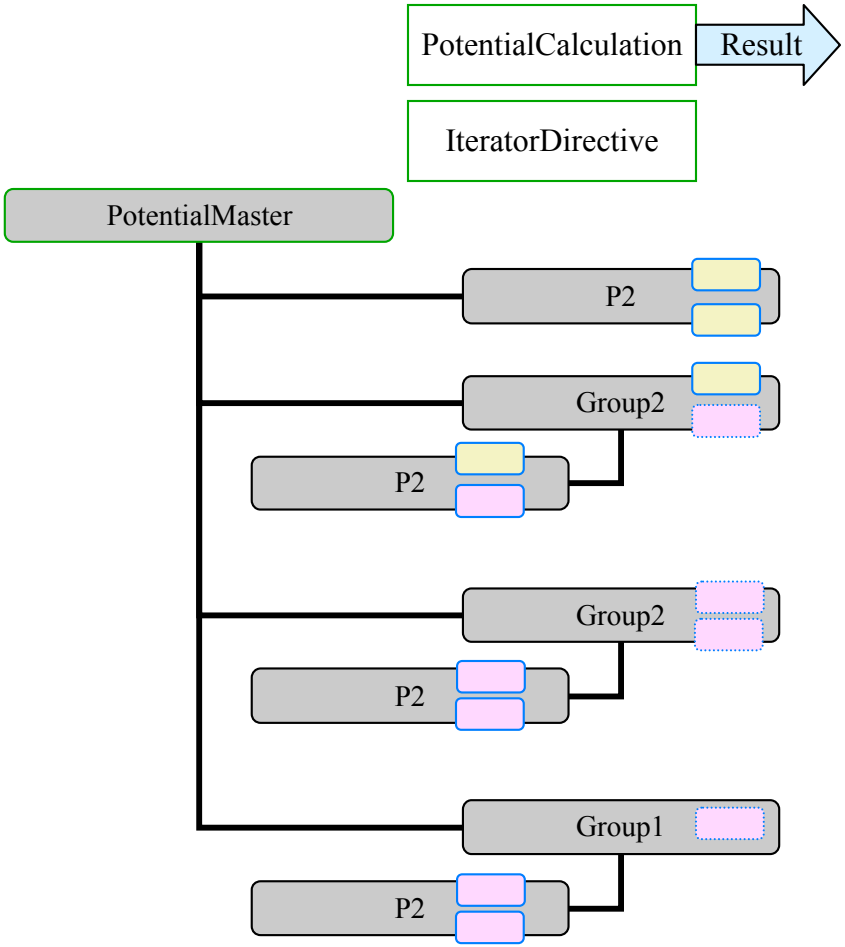


Models: PotentialMaster

- Traversal of hierarchy inefficient for routine application
  - Main role is to define the model
- PotentialMaster subclasses
  - Same interface
  - Permits extension to other iteration schemes
  - PotentialMasterCell
    - Cell-based neighbor iteration
  - PotentialMasterNbr
    - List-based neighbor iteration
- Implement parallel/high-performance schemes by subclassing PotentialMaster

Models: Model

- Model
  - class to simplify specification of model
  - coordinates construction of species and potentials
  - still in development

Flow Control: Action and Activity

- Action
  - interface for abstract, elementary action that does something
  - public void actionPerformed()
  - can be grouped for series implementation
  - for example
    - AtomActionRandomizeVelocity
    - AtomActionTranslateBy
    - IntegratorReset
    - PhaseInflate
- Activity
  - more complex, time-consuming extension of Action
  - can be started, stopped, paused, resumed
  - can be grouped for series or parallel implementation
  - for example
    - ActivityIntegrate
    - EquilibrationProduction

Flow Control: Controller

- Two ways to conduct simulation
  - interactively
  - batch
  - (or hybrid of both)
- Specification of actions must be mutable
  - even while simulation proceeds
- Controller
  - schedules actions to be performed
  - single instance constructed for each Simulation
  - actions/activities can be added to queue
  - urgentAction can be requested for immediate implementation
    - all GUI-driven changes follow this path
  - carefully synchronized

Flow Control: Integrator

- Integrator
  - repeatedly changes configuration to follow a sampling algorithm
  - public void doStep()
  - deploys subclass-specific agent to each atom
  - only one integrator acts on a given phase
  - some integrators act on multiple phases
    - IntegratorGEMC (Gibbs ensemble Monte Carlo)
    - IntegratorPT (Parallel tempering)
- IntegratorMD
  - IntegratorVelocityVerlet
  - IntegratorHard
    - discontinuous molecular dynamics
- IntegratorMC

Flow Control: IntegratorMC

- IntegratorMC
  - Monte Carlo sampling
  - Selects trial move, performs trial, decides acceptance, notifies move and other listeners
- MCMove
  - Performs Monte Carlo trial
  - Reports information needed to determine acceptance
    - $\ln(p_{new}/p_{old})$, $\ln(t_{ij}/t_{ji})$
    - Holds fields needed for evaluation
  - Does appropriate update for acceptance or rejection
  - For example
    - MCMoveAtom
    - MCMoveInsertDelete
    - MCMoveRotateMolecule
    - MCMoveVolume
  - Sampled ensemble is determined by set of MCMoves added to integrator

Flow Control: IntegratorEvent

- IntegratorEvent
  - integrator fires event to registered listeners to notify of progress with simulation
- IntegratorListener
  - IntegratorIntervalListener
    - receives repeated events reporting progress
  - IntegratorNonintervalListener
    - receives only events indicating initialization, start, end, etc.
  - For example
    - objects pushing data measurement and processing
    - cell- and neighborlist-updating

Data Processing: DataSource, DataSink

- DataSource
  - interface for class that can provide data
  - data is generally represented by array of double
  - `public double[] getData();`
  - Meter is a DataSource that acts on a Phase
  - for example
    - MeterDensity, MeterEnergy, MeterRDF, MeterTemperature
    - DataSourceCountCollisions, DataSourceCountTime
- DataSink
  - interface for class that can receive data
  - `public void putData(double[] data);`
  - for example
    - DisplayBox, DataSinkConsole, DataBin
    - DataPipe

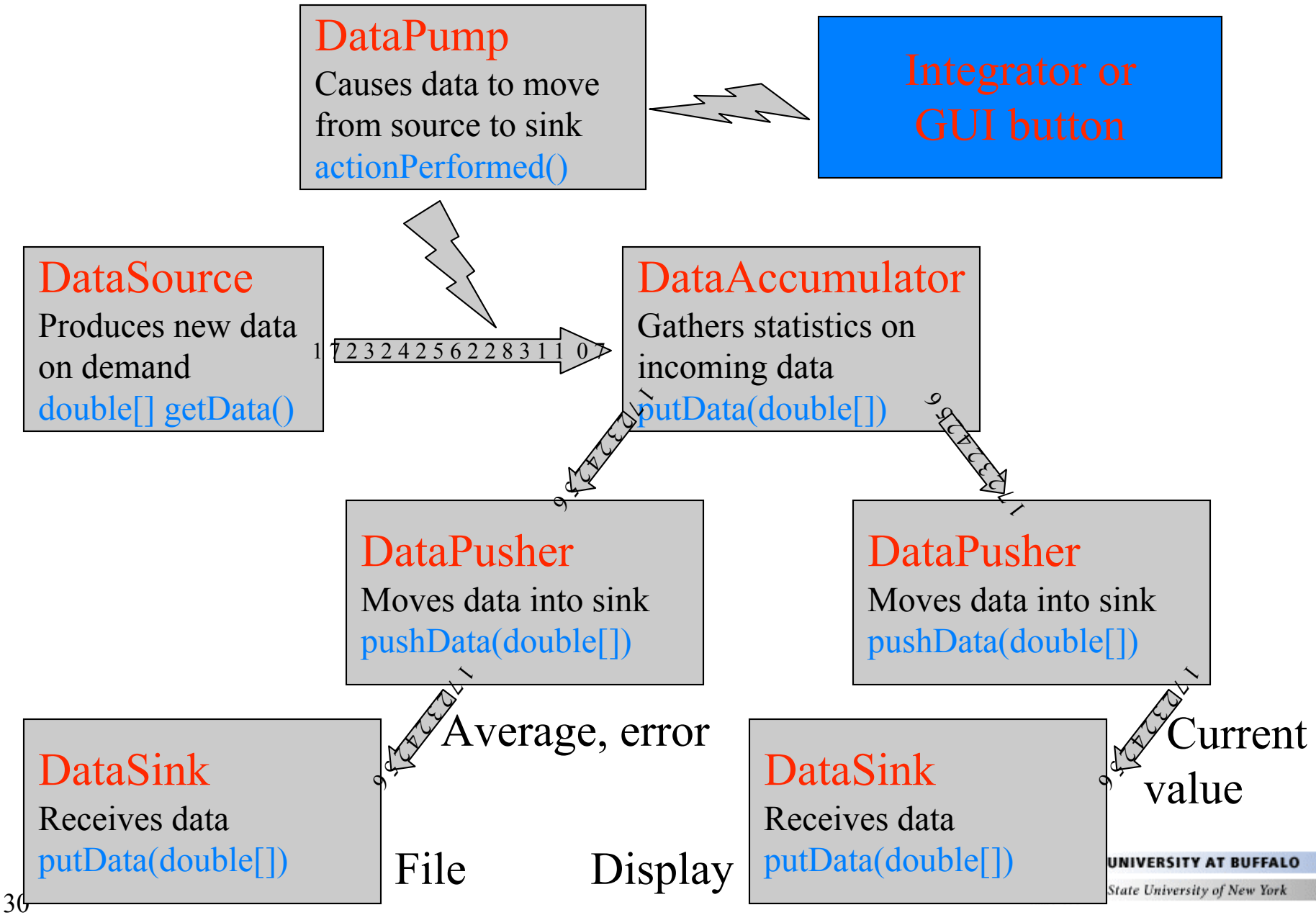
Data Processing: Pipelines

- Data is pushed from a source to a sink
  - It may pass through other elements along the way
  - Each pushes data on to the next element
- DataPusher
  - Holds one or more sinks and pushes data to them on request
  - Has methods to manage data sinks
- DataPipe
  - Abstract, extends DataPusher, implements DataSink
  - Takes data given to it, does something to it, and pushes new data
  - DataAccumulator
    - Collects statistics on data it receives, and pushes it on at intervals
    - *e.g.* AccumulatorAverage, AccumulatorHistory, AccumulatorHistogram
  - DataTranformer
    - Modifies data and immediately pushes it downstream

Data Processing: DataPump

- DataPump
  - Extends DataPusher
  - Holds a DataSource, and moves data from it to the sinks
  - Provides the impetus for moving the data from a source into a pipe
  - Implements Action
    - Typically activated via Integrator IntervalEvent, or GUI action

Data Flows in Etomica



I/O and Graphics: Display

- Display
  - Object to present data in graphical interface
- Boxes, plots, tables, etc.
- All are treated as implementing DataSink
- Logging capabilities still not well developed
- Units
  - Internally, all data are represented in a common unit system
    - picosecond, Angstrom, Dalton
  - Unit classes are defined to handle conversions
  - All I/O and graphics classes hold a Unit instance
  - Classes can declare Dimension for fields so that appropriate units are offered

I/O and Graphics: Device

- Device
  - Widget that allows user to interact with simulation
- Examples
  - DeviceButton
    - Connects to an action, performs action when button is pressed
  - DeviceSlider
    - Changes value of some quantity with movement of a slider
  - DeviceThermoController
    - ComboBox that permits selection from several temperatures
  - DeviceCheckBox
    - Toggles a boolean value using a checkbox
  - DeviceControllerButton
    - Start/stop/pause/resume simulation
- Acts via Controller
  - Invokes urgentAction
  - Controller handles Action request ASAP
    - Pauses current Activity, or finishes current Action
    - then attends to requested Action
  - Prevents collision between user and integrator threads

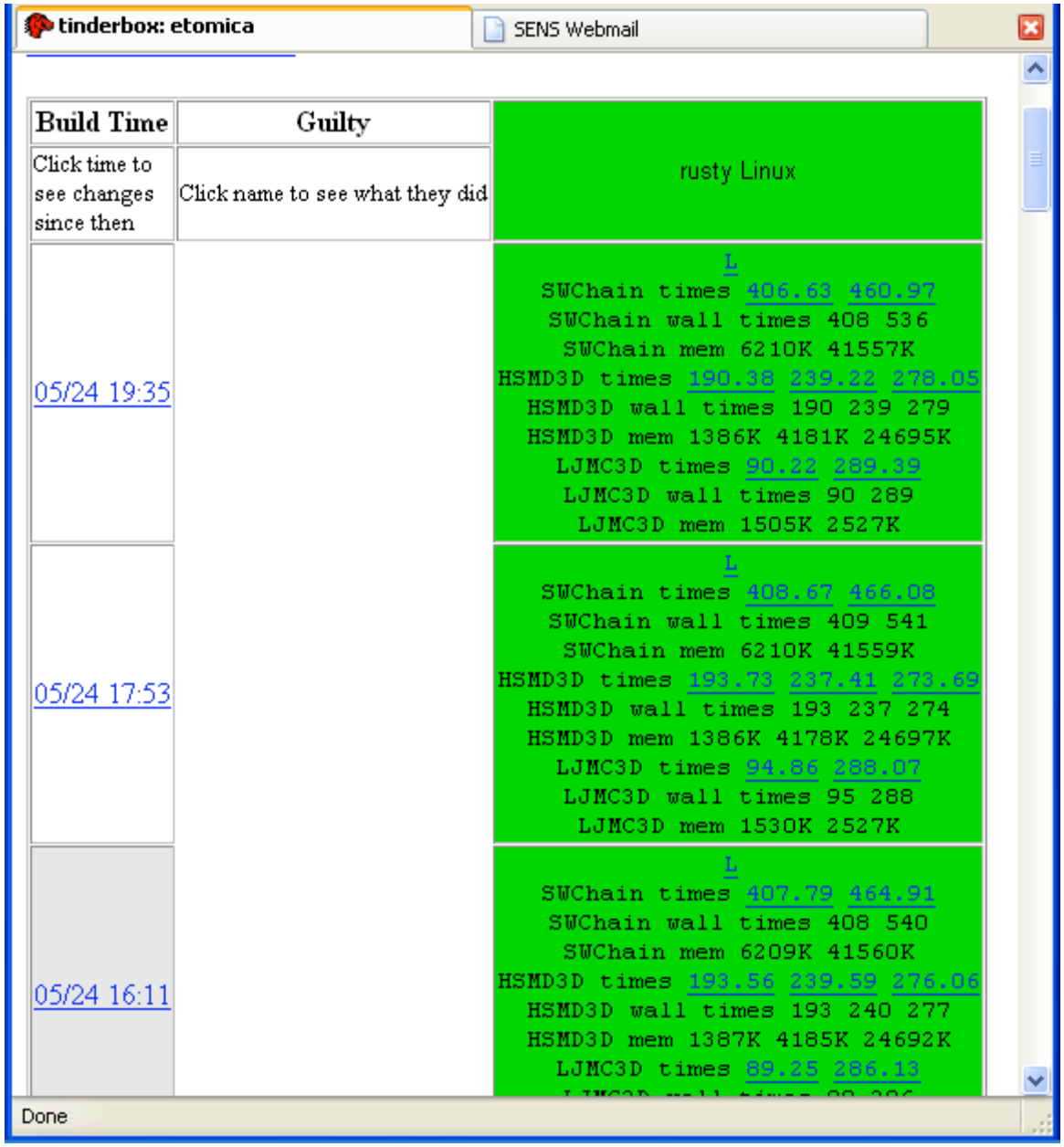
Utilities

- Utility classes developed as needed
  - versatile lattice capabilities
  - Polytope for defining shapes
  - very small set of math classes
    - linear algebra
    - special functions
    - permutations/combinations

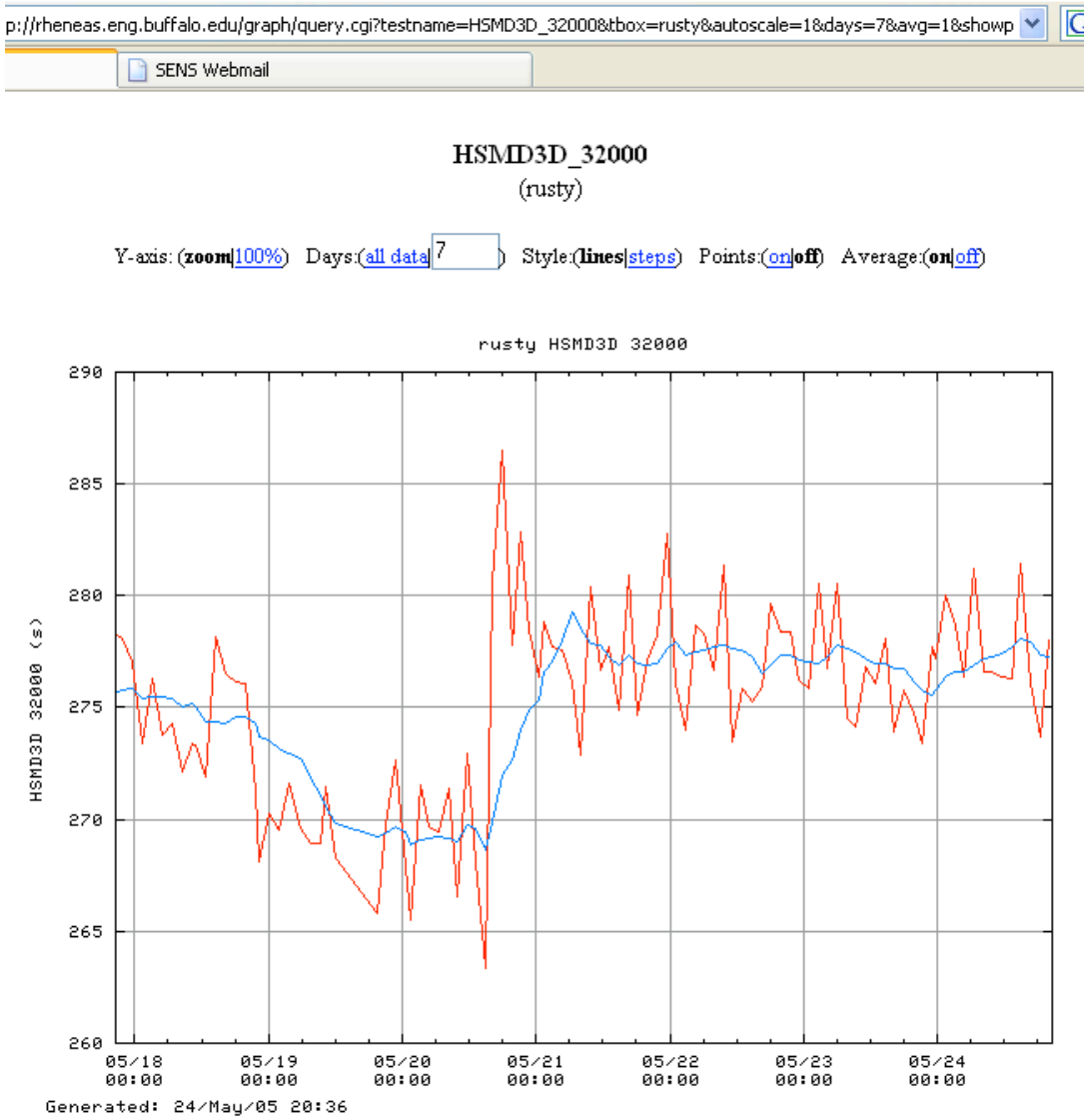
Supporting Tools

- CVS
- JUnit
  - facility for developing unit tests
- javadoc
  - facility to generate hyperlinked documentation from comments
- bugzilla
  - bug tracking
- tinderbox
  - performance tracking

Supporting Tools: Tinderbox



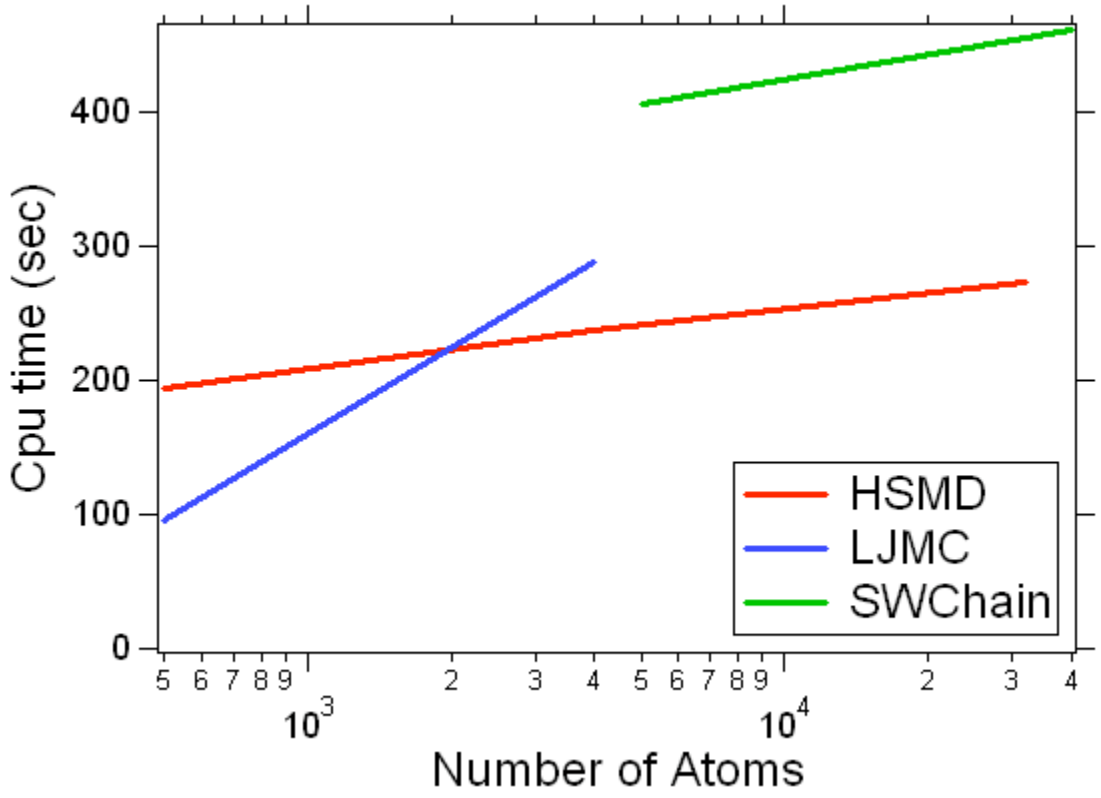
Supporting Tools: Tinderbox



Performance

- Benchmark tests
  - Hard-sphere molecular dynamics
  - Square-well chain molecular dynamics
  - Lennard-Jones Monte Carlo
- Comparison to specialized fortran codes
  - 2- to 4-times slower
- No problem scaling to large systems

Performance: Scaling



Some Applications

- Piston-cylinder MD simulation
- Diffusion through a nanotube: DCVGCMD
- Ising model

Acknowledgements

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