Etomica: An API for Molecular Simulation

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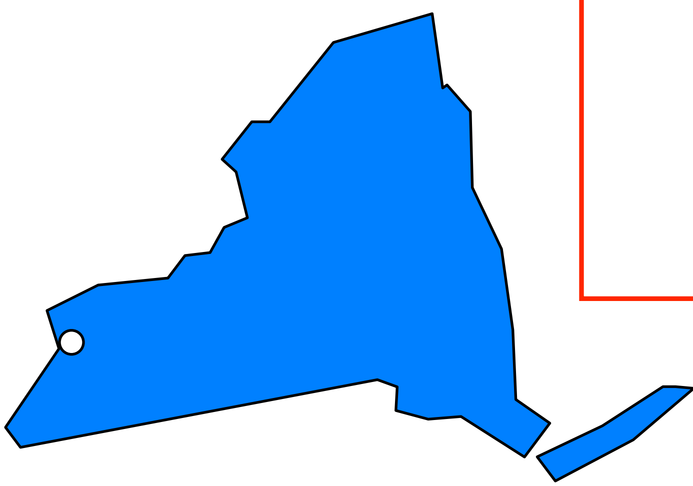

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Object-Oriented Programming

- 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
    - presents a good vehicle for teaching
- It's fun!

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.
  - you define types (classes) as needed to solve your problems
  - types differ in the data they hold and the actions they can perform on it
  - every object is an "instance of a class"
- 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
  - different classes can inherit the same interface, but implement it differently to produce different behaviors

Makeup of an Object

- Fields
  - primitive types (integer, float, double, boolean, etc.)
  - handles to other objects
    - complex objects are composed from simpler objects (composition)
  - Fields are usually not part of the interface
    - "private"
- Methods
  - "subroutines and functions"
  - may take arguments and return values
  - have complete access to all fields of object
  - methods are defined to set and get field values

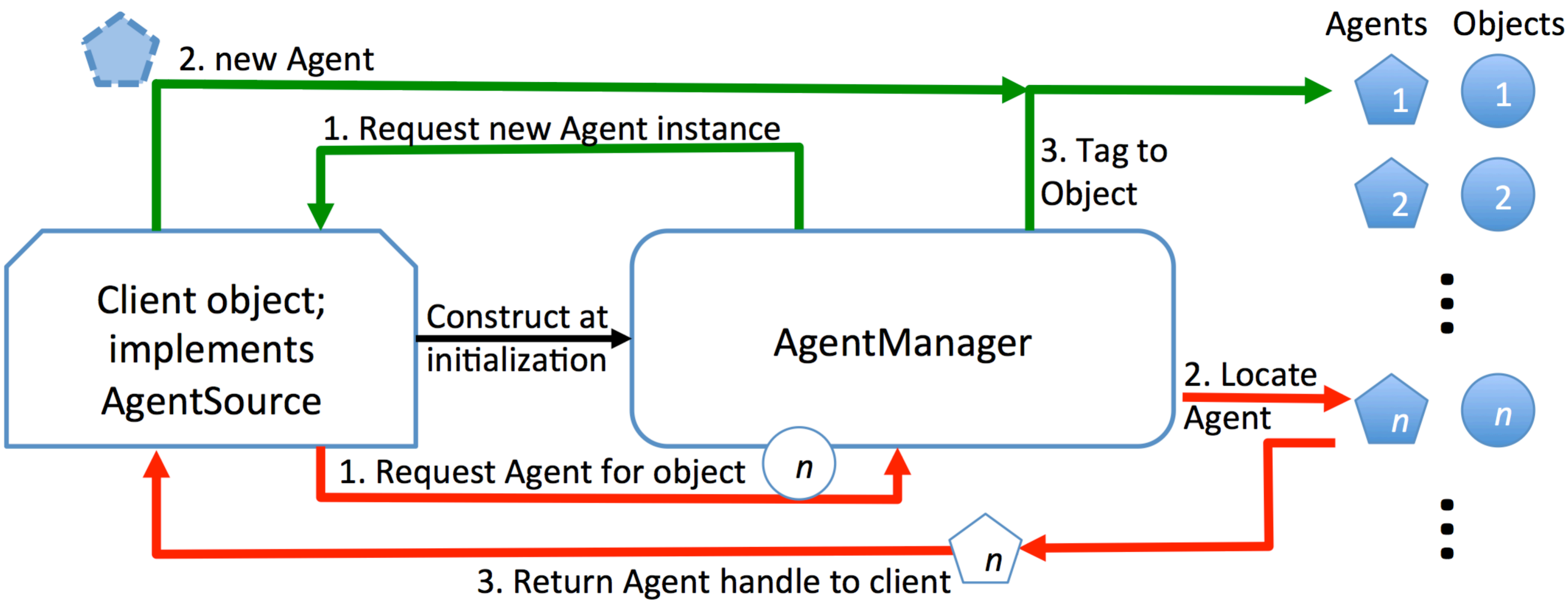
Detailed Look: Molecule and Atom

- Atom methods
  - Vector getPosition()
    - Returns an object that represents the atom's coordinate
  - AtomType getType()
    - Returns an object that specifies important parametric features of the atoms, such as its size, shape, mass, and how it is drawn
  - int getIndex()
    - Returns an integer used to store the Atom instance in an array
- Molecule methods
  - AtomList getChildList()
  - Species getType()
  - int getIndex()
- Click here for the complete API specification

Design Considerations

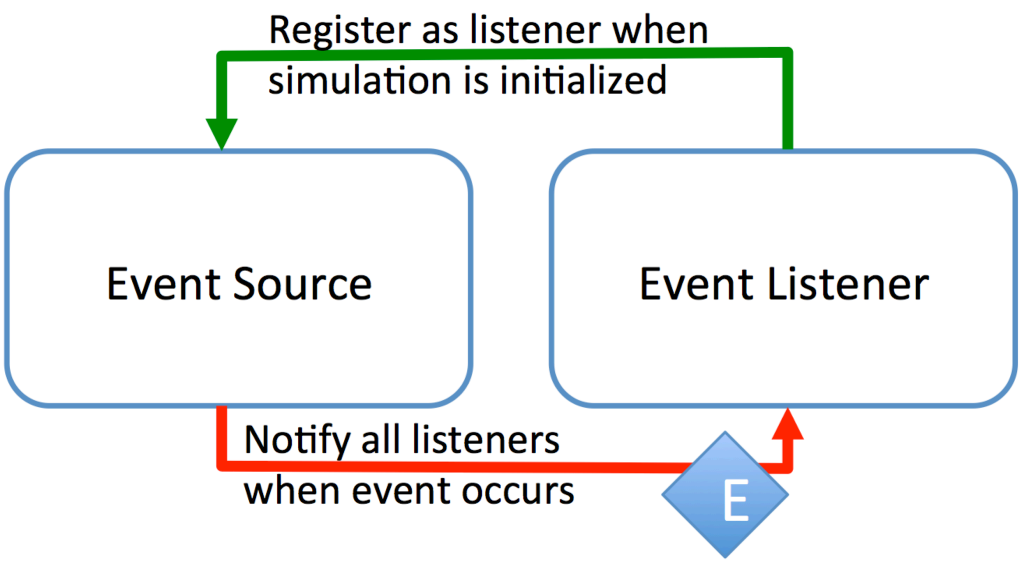
- Goals
  - Extensible, broadly applicable
  - Computational efficiency
  - Suitable to run interactively or in batch
- Guidelines
  - Highly granular pieces with convenience classes that assemble them
  - Separate components as much as possible
    - Graphics separate from other parts
    - Used objects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

Agent Model



2. new Agent
1. Request new Agent instance
3. Tag to Object
Agents
Objects
1
1
2
2
n
n
Client object; implements AgentSource
Construct at initialization
AgentManager
2. Locate Agent
1. Request Agent for object
n
n
3. Return Agent handle to client

Event Model


Register as listener when
simulation is initialized
Event Source
Event Listener
Notify all listeners
when event occurs
E

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

Vector

- Defines Cartesian vector and operations performed on it
- Some methods
  - double squared()
  - double dot(Vector v)
  - void E(Vector v)
  - void PE(Vector v)
  - void Ea1Tv1(double a, Vector v)
  - Vector Mv1Squared(Vector y)
  - void normalize()
  - Etc.
- Different implementations done for different dimensions

Data Structures: Atom

- Atom
  - Represents physical atom being simulated
- Some Important fields
  - position
    - class that holds and manipulates position vectors
  - type
    - class that specifies important parametric features of the atoms, such as its size, shape, mass, and how it is drawn
  - index
    - an integer used to store the Atom instance in an array

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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: Box

- Box
  - Collects all atoms that interact with each other
- A single Simulation may employ multiple Box instances
  - Parallel tempering, Gibbs ensemble
  - No atoms in one Box interact with atoms in another Box
- Box holds a Boundary instance
  - Constructed by Space
  - Implements (or not) periodic boundary conditions
- Manages addition/removal of molecules
- Additional information associated with Box via BoxAgentManager

Data Structures: Species

- Species classes collect information needed to construct and manage molecules
- Subclasses defined for specific molecules
- Serves as a "molecule type" for doing potential calculations

Data Structures: AtomsetIterator

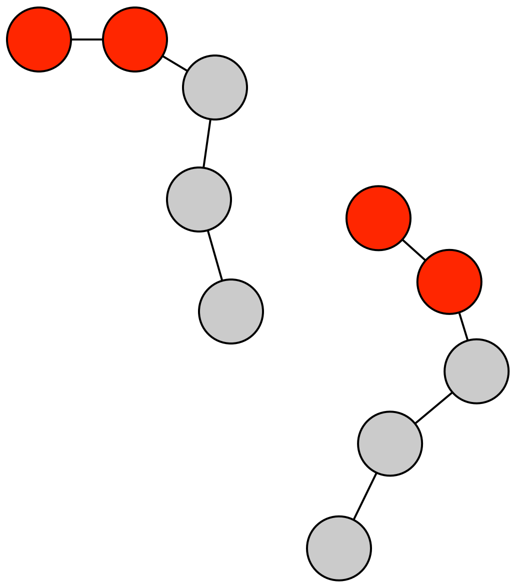
- AtomSet
  - Interface for a set of atoms
    - Atom, AtomPair most often used
- Many types of atom-set iterators
  - Iterate atoms or atom pairs at a particular level in hierarchy
  - Iterate pairs formed with a particular atom
  - Iterate in one or both directions from a given atom
  - Many interfaces 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
- PotentialMaster class collects potentials and manages iterators

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



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 box
  - some integrators act on multiple boxes
    - 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

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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 Box
  - 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

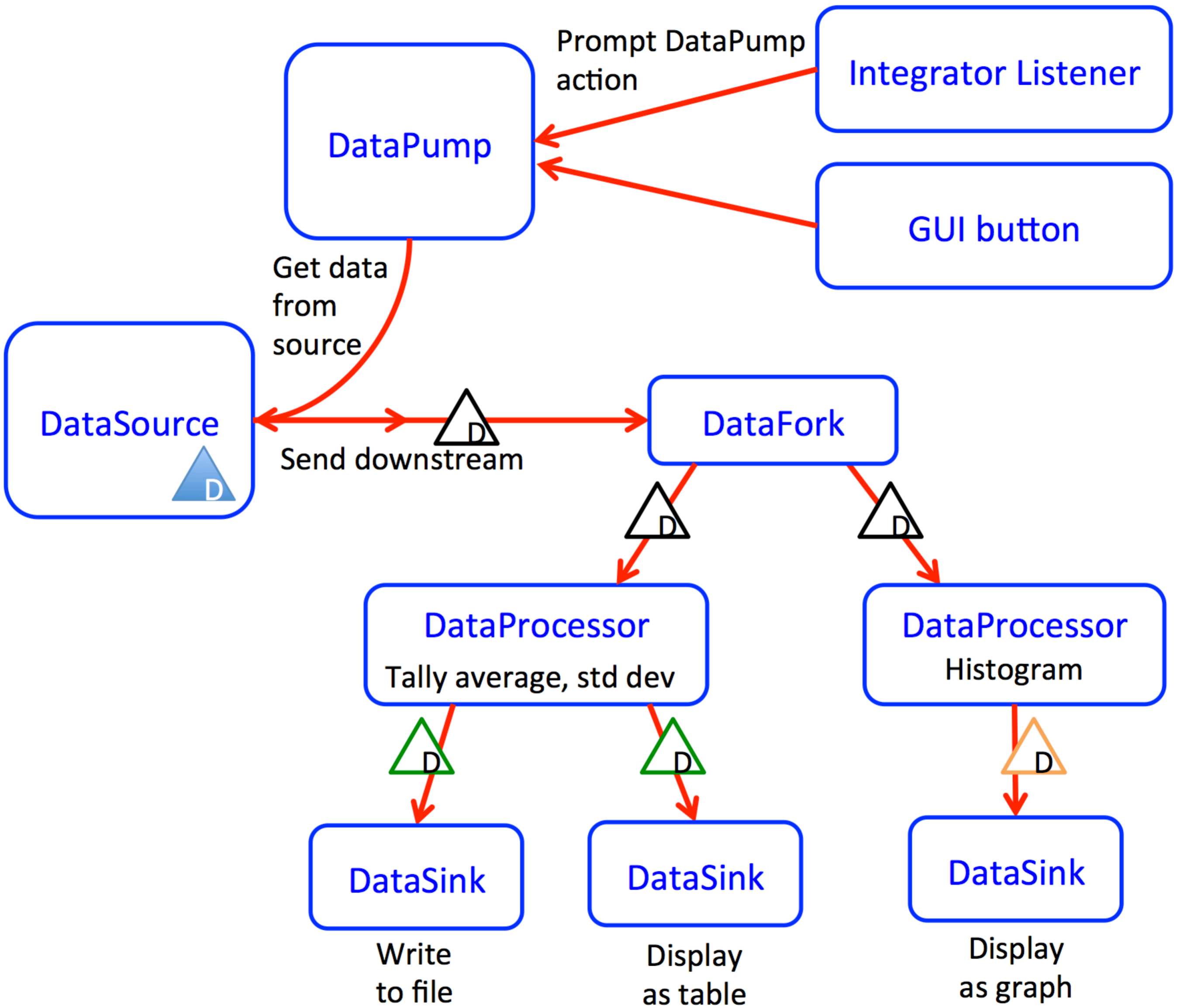
Data Processing: Pipelines

- 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
- DataPipe
  - Abstract, 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
  - DataTransformer
    - Modifies data and immediately pushes it downstream

Data Processing: DataPump

- DataPump
  - Extends DataProcessor
  - 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

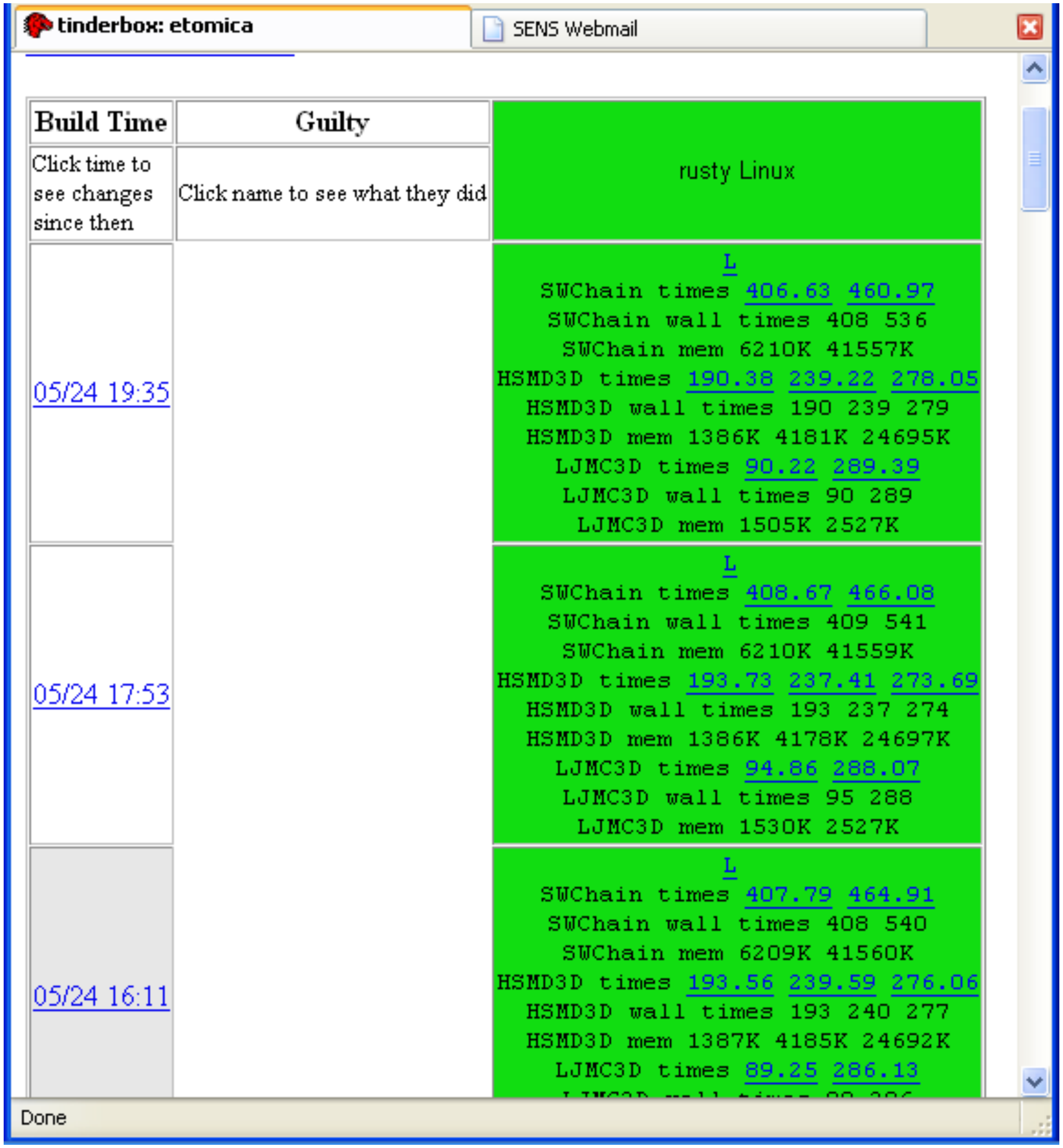
Utilities

- 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



Build Time Click time to see changes since then	Guilty Click name to see what they did	rusty Linux
05/24 19:35		L SWChain times 406.63 460.97 SWChain wall times 408 536 SWChain mem 6210K 41557K HSMD3D times 190.38 239.22 278.05 HSMD3D wall times 190 239 279 HSMD3D mem 1386K 4181K 24695K LJMC3D times 90.22 289.39 LJMC3D wall times 90 289 LJMC3D mem 1505K 2527K
05/24 17:53		L SWChain times 408.67 466.08 SWChain wall times 409 541 SWChain mem 6210K 41559K HSMD3D times 193.73 237.41 273.69 HSMD3D wall times 193 237 274 HSMD3D mem 1386K 4178K 24697K LJMC3D times 94.86 288.07 LJMC3D wall times 95 288 LJMC3D mem 1530K 2527K
05/24 16:11		L SWChain times 407.79 464.91 SWChain wall times 408 540 SWChain mem 6209K 41560K HSMD3D times 193.56 239.59 276.06 HSMD3D wall times 193 240 277 HSMD3D mem 1387K 4185K 24692K LJMC3D times 89.25 286.13

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Supporting Tools: Tinderbox

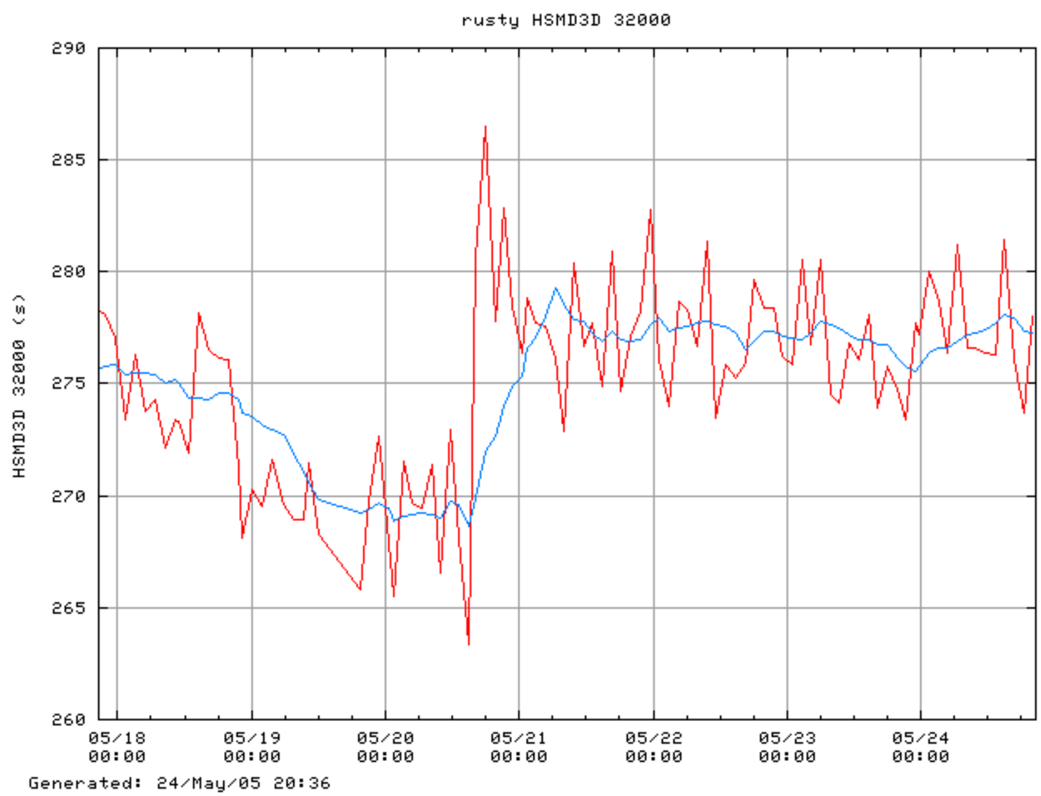
p://rheneas.eng.buffalo.edu/graph/query.cgi?testname=HSMD3D_32000&tbox=rusty&autoscale=1&days=7&avg=1&showp

SENS Webmail

HSMD3D_32000

(rusty)

Y-axis: (**zoom**|100%) Days:(all data| 7) Style:(**lines**|steps) Points:(on|**off**) Average:(**on**|off)



- Other rusty tests: (startup, xulwinopen, pageload, show all tests) Graph size: 1.0
- Show the raw data for this plot

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