



Stochastic Simulation of NOM with RePast: A Visualization

Ryan Kennedy, Xiaorong Xiang,
Leilani Arthurs, Patricia A. Maurice,
Yingping Huang, Gregory R. Madey
Computer Science and Engineering
Civil and Geological Sciences



Natural Organic Matter (NOM)

- Heterogeneous mixture of organic molecules
- Slow and difficult to study in nature
- Complex and very large scale
- Traditional methods are very tough to apply to NOM studies



NOMSim

- Web-based Collaboratory
- Scientists can submit, run, and observe custom simulations
- Simulation algorithm written in Java, utilizing RePast modeling toolkit
- A GUI allows scientists to more easily observe trends and patterns



NOM GUI

- Molecules move about a Multi2DGrid and are displayed via a Multi2DDisplay
- Display extends SimModelImpl
- Molecules enter through the top and leave through the bottom
- Molecules are bounded in the x-direction



NOM GUI

- Display Components:
 - Main Window
 - Displays molecules that move and react according to given methods
 - Displays number of molecules in system
 - Updates every timestep
 - Legend
 - Displays color key for molecules and the molecular weight it represents



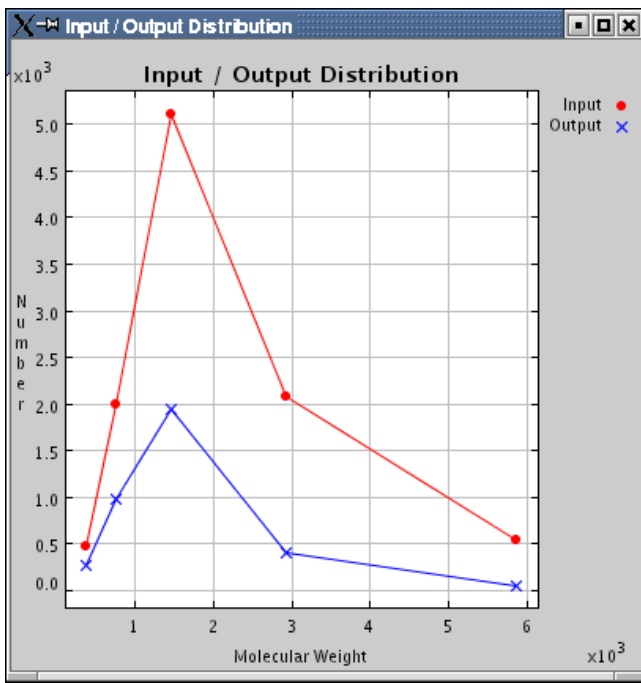
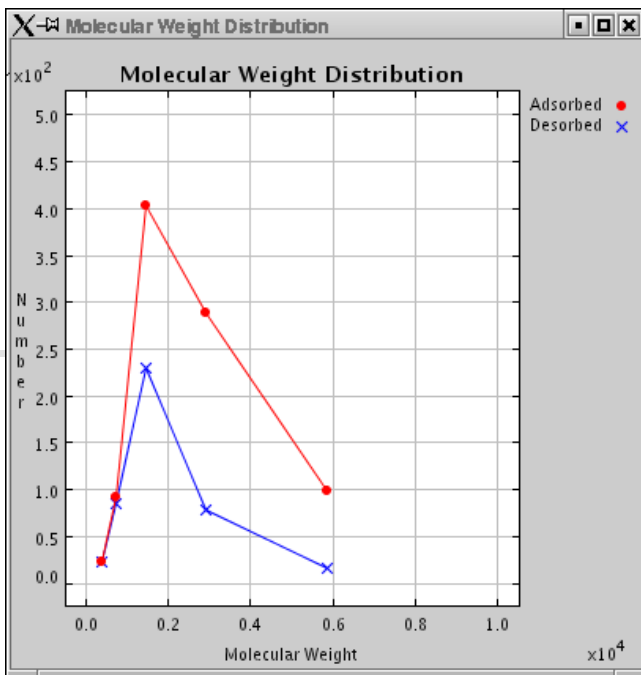
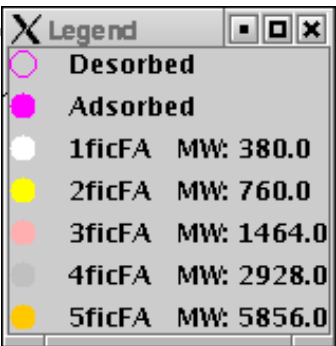
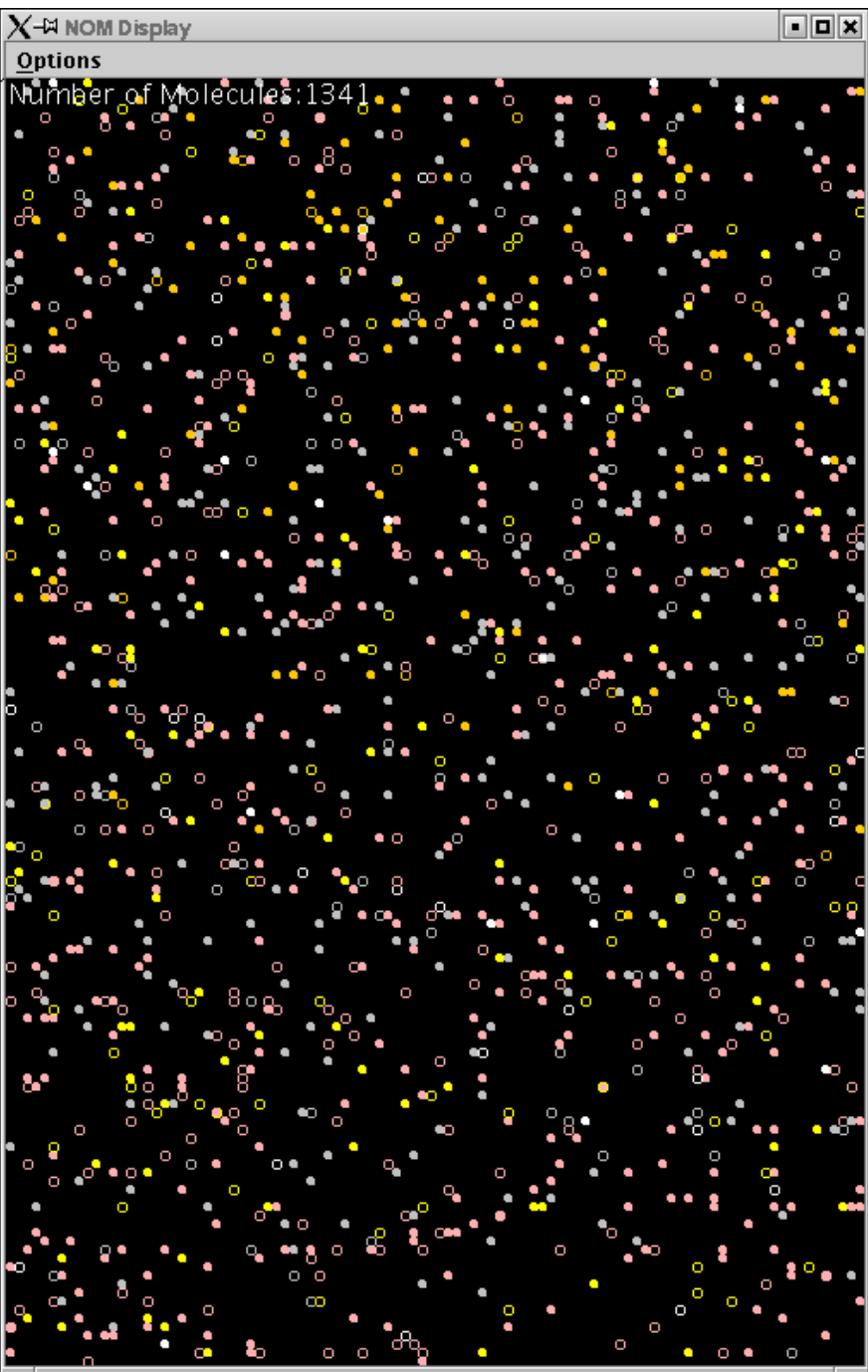
NOM GUI

- More Display Components
 - Settings Window
 - Displays user-controllable variables and options
 - Defaults to values specified by the particular simulation
 - Graph Windows
 - Molecular Weight vs. Number of Molecules Adsorbed
 - Input / Output Molecular Weight Distribution
 - Variable update frequency



NOM GUI

- What you see:
 - Molecules flowing through a system with a defined width
 - Molecules become adsorbed (solid) when they stick to the surface
 - Molecules with a higher molecular weight appear darker and are more likely to stay stuck longer
 - Many reactions take place, which can add or remove molecules (only results of a reaction are displayed)



Konsole <2>

File Sessions Settings Help

```

////////////////////// STATS ////////////////////////
Total Number of Molecules: 3387
Number Adsorped: 3322
Number Desorped: 65
Number of Added: 3
Number of Removed: 0

Reactions by Type:
Ester Condensation: 0
Ester Hydrolysis: 0
Amine Hydrolysis: 0
Microbial Uptake: 0
Dehydration: 0
Strong C=C Oxidation: 0
Mild C=C Oxidation: 0
Alcohol (C-O-H) Oxidation: 0
Aldehyde C=O Oxidation: 0
Decarboxylation: 0
No Reaction: 0
Invalid Reaction: 0
Total: 0

```

//////////////////////

New Konsole

NOM Settings

Repast Actions

Parameters Custom Actions

Model Parameters

GridXSize: 100

GridYSize: 150

MoleculeDensity: 0.01

Plot:

Plot2:

PlotInterval: 40.0

Ticks: 400.0

UpdateProbing:

RePast Parameters

CellDepth: 5










CellHeight: 5

CellWidth: 5

PauseAt: -1

RandomSeed: 20000

RePast

Tick Count: 0.0



RePast Information

- <http://repast.sourceforge.net>
 - API Documentation
 - Demo Programs
 - FAQ
 - How-To Documents



Future Additions

- Better coloring mechanism
- Web-based movie generation
- Batch simulations
- Multiple heterogeneous molecules per grid square, up to a specified maximum total molecular weight for each grid square