Stochastic Simulation of NOM with RePast: A Visualization

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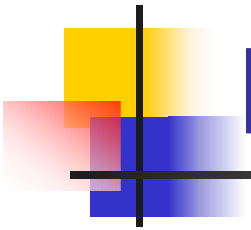
Computer Science and Engineering

Civil and Geological Sciences

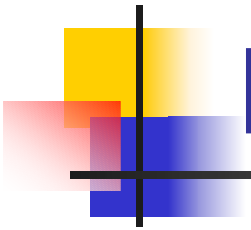
Natural Organic Matter (NOM)

- 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



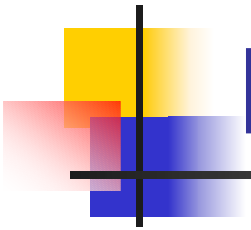
NOMSim

- 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



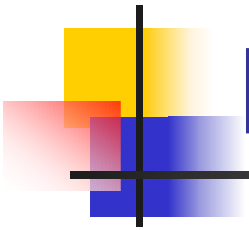
NOM GUI

- 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

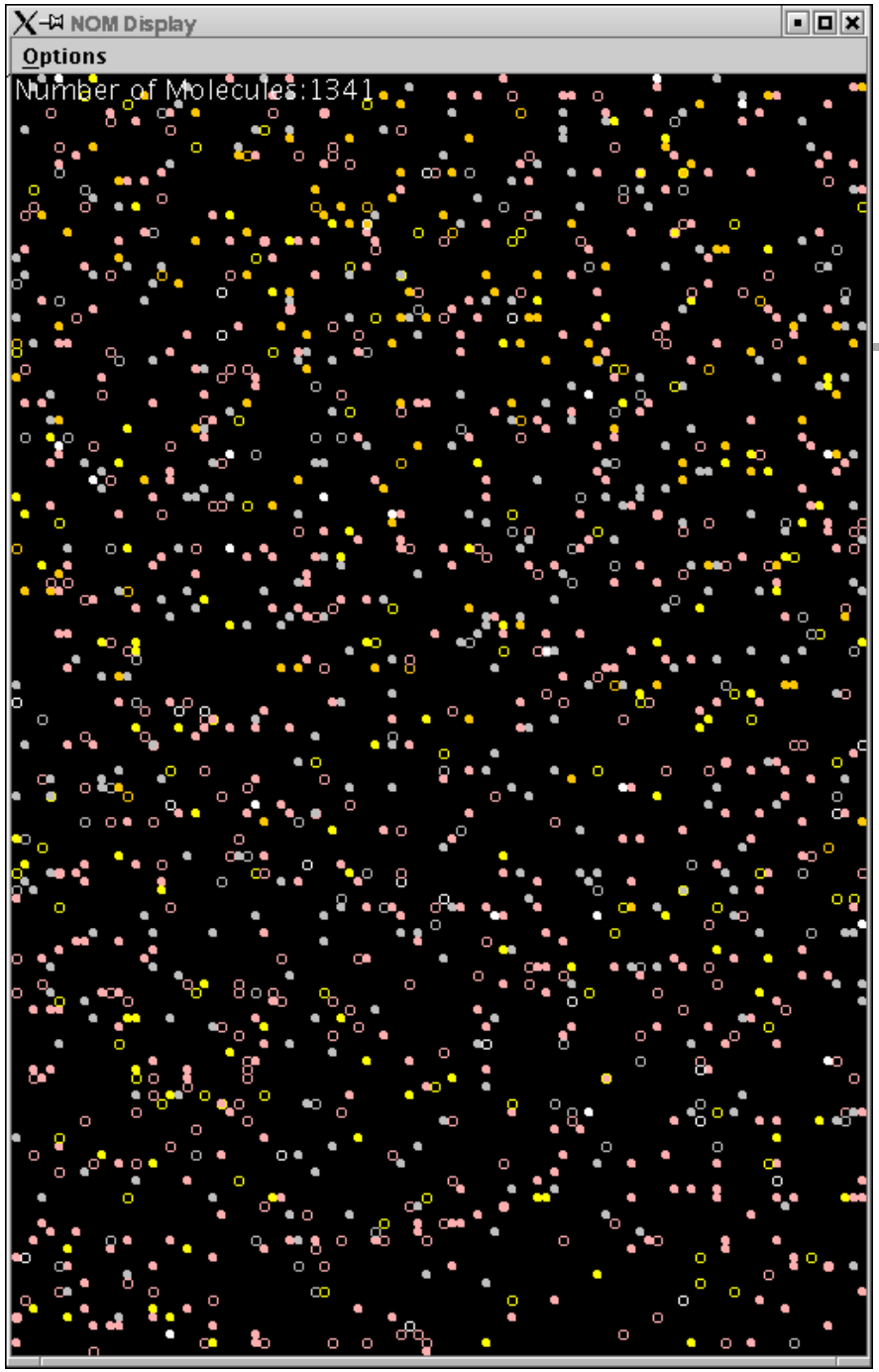


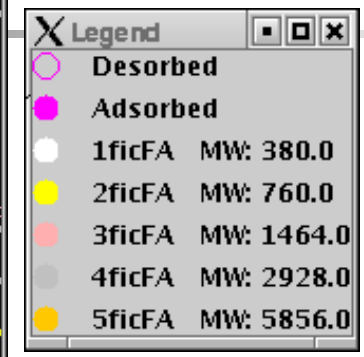
NOM GUI

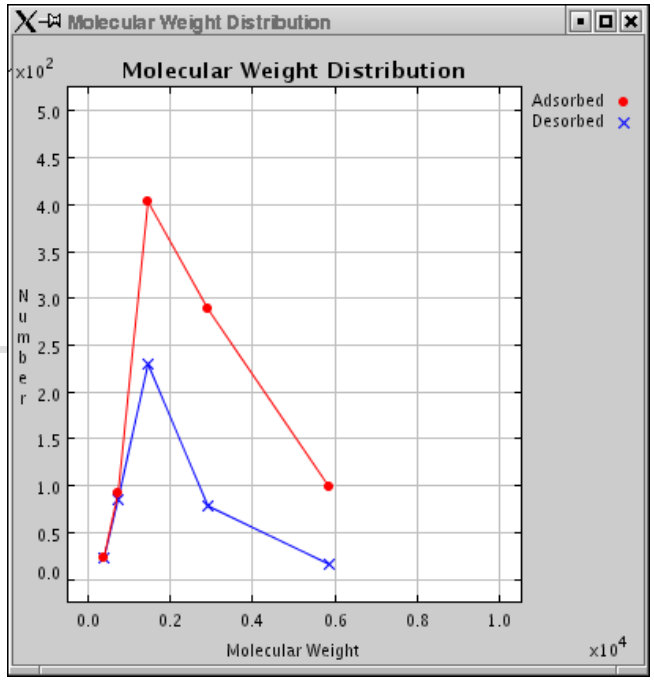
- More Display Components
  - Settings Window
    - Displays user-controllable variables and options
    - Defaults to values specified by the particular simulation
  - Graph Windows
    - Molecular Weight vs. Number of Molecules Adsorbed
    - Input / Output Molecular Weight Distribution
    - Variable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

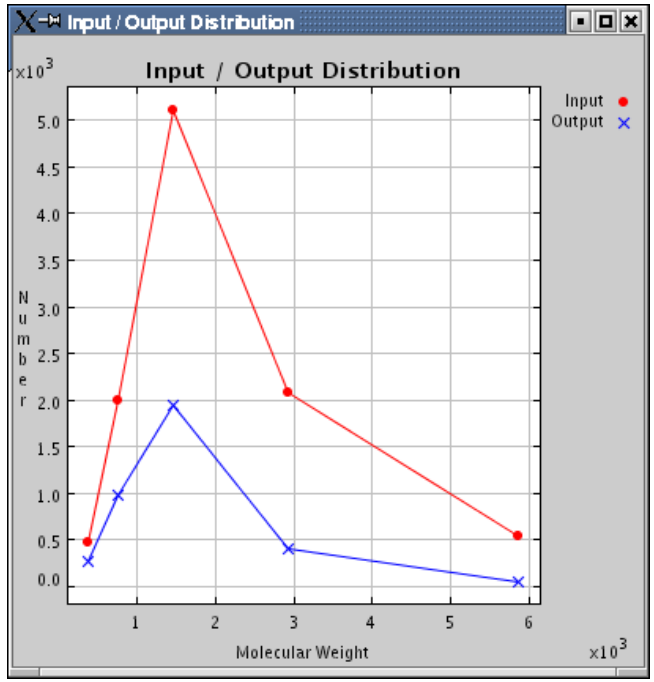
NOM GUI

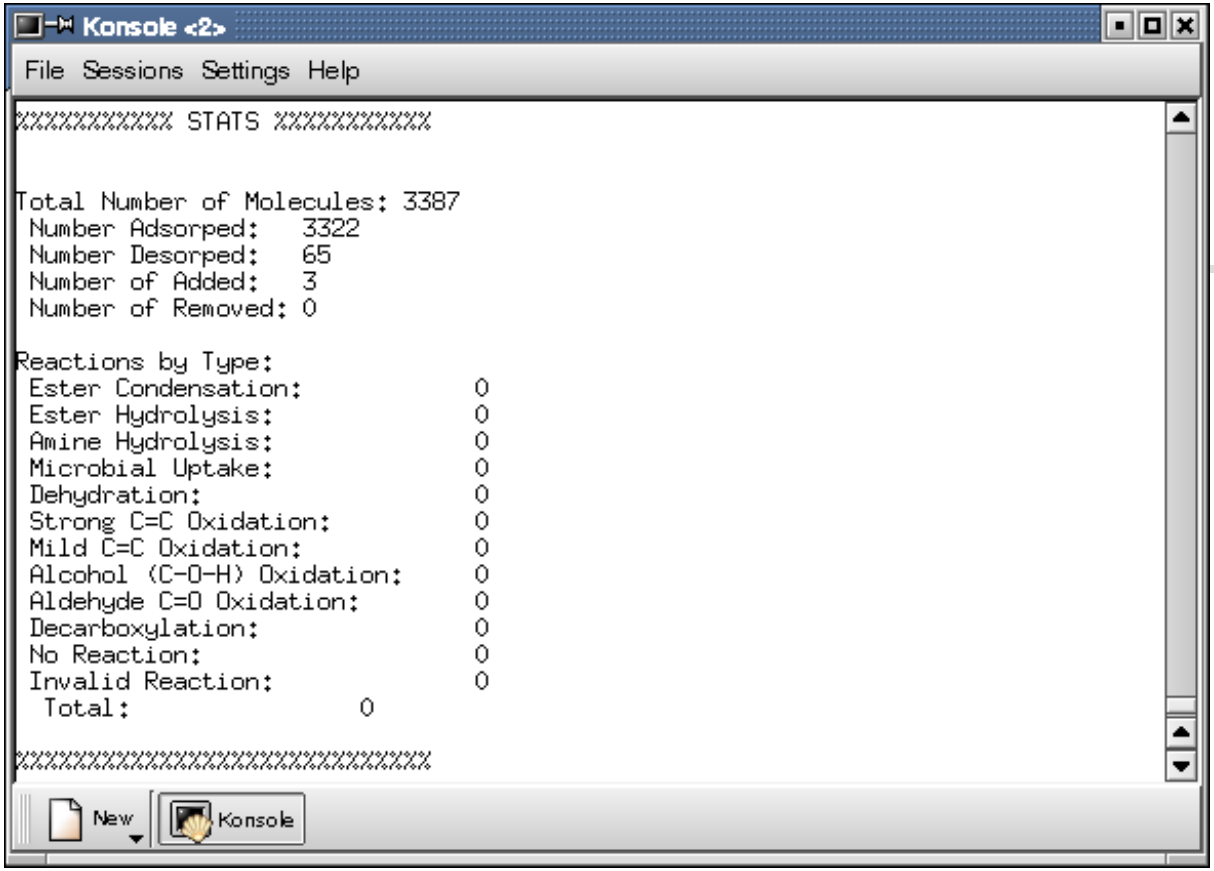
- What you see:
  - Molecules flowing through a system with a defined width
  - Molecules become adsorbed (solid) when they stick to the surface
  - Molecules with a higher molecular weight appear darker and are more likely to stay stuck longer
  - Many reactions take place, which can add or remove molecules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

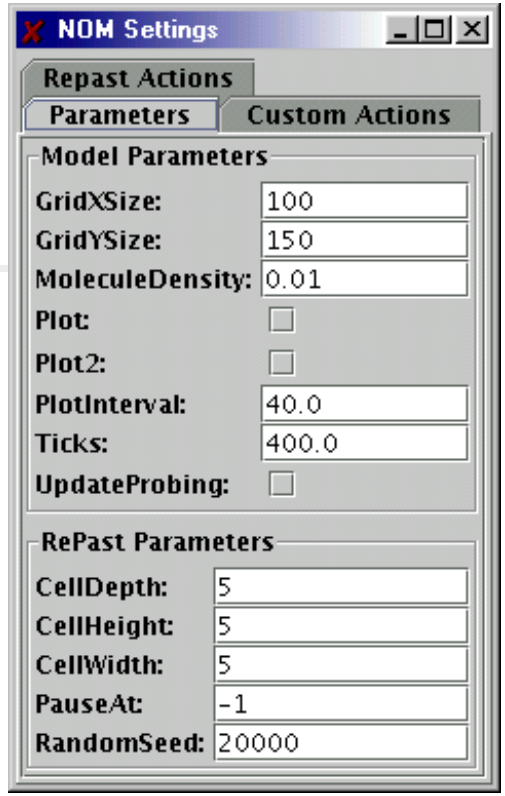

NOM Display
Options
Number of Molecules:1341

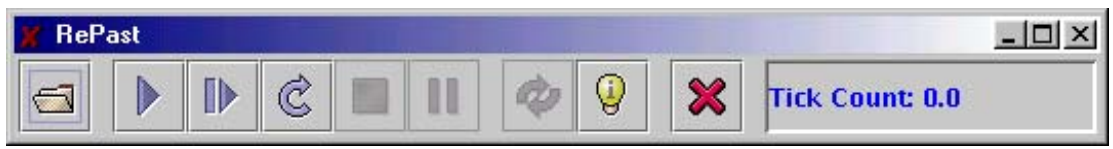

Legend
Desorbed
Adsorbed
1ficFA MW: 380.0
2ficFA MW: 760.0
3ficFA MW: 1464.0
4ficFA MW: 2928.0
5ficFA MW: 5856.0

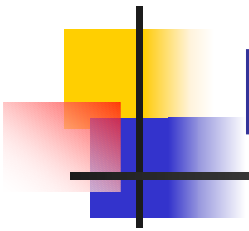

Molecular Weight Distribution
Molecular Weight Distribution
x10^2
Adsorbed
Desorbed
Number
Molecular Weight
x10^4


Input / Output Distribution
Input / Output Distribution
x10^3
Input
Output
Number
Molecular Weight
x10^3


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

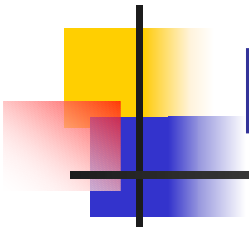

NOM Settings
Repast Actions
Parameters
Custom Actions
Model Parameters
GridXSize: 100
GridYSize: 150
MoleculeDensity: 0.01
Plot:
Plot2:
PlotInterval: 40.0
Ticks: 400.0
UpdateProbing:
RePast Parameters
CellDepth: 5
CellHeight: 5
CellWidth: 5
PauseAt: -1
RandomSeed: 20000


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