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Web-Based Molecular Simulation using Agent-Based Modeling Techniques

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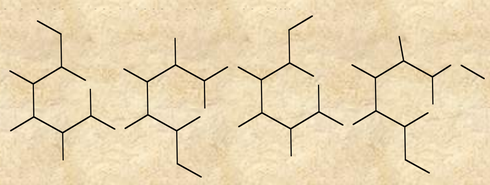

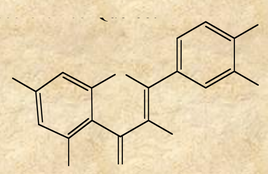

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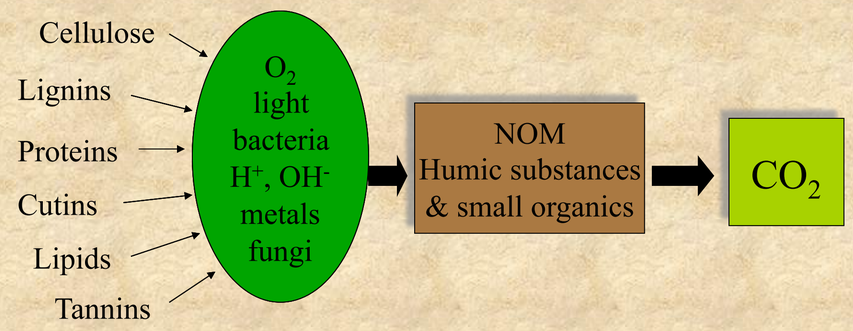
Natural organic matter (NOM), a heterogeneous mixture of molecules, plays a crucial role in the evolution of soils, the transport of pollutants, and the carbon cycle, hence global climate change. The evolution of NOM over time is an important research area in biology, geochemistry, ecology, soil science, and water resources. Due to its complexity and structural heterogeneity, new simulation approaches are needed to help to better understand the structure and evolution of NOM. We present a new stochastic model, implemented using Java/Swarm, which explicitly treats NOM as a large number of discrete heterogeneous molecules. The NOM, micro-organisms, and their environment are taken together as a complex system, and simulated using an agent-based modeling approach. The global properties of NOM evolution over time and space can be studied by simulating the physical and chemical reactions between individual agents with temporal and spatial properties. Unlike the previous stand-alone simulation models, the NOM simulation model serves as an example of E-science, in which we do science on the Web by combining recent information technologies (Java 2 Enterprise Edition, J2EE) with an agent-based computational approach. An intelligent Web-based interface is developed to allow scientists to access the remote simulation model from a standard Web browser. The Web-based interface enables scientists to remotely provide parameters for their simulations, start and stop the simulations, and view the results. The initial users of the NOM simulation model includes a geographically separated group of NSF sponsored scientists from different research areas. An NOM collaboratory is built to promote collaboration among these scientists and allow them to share their data and information across distributed sites. An XML-based Markup Language, NOML, is provided to build the XML-based Web components and facilitate Web services development in the future.

What is Natural Organic Matter (NOM)?

Sources - Plant and animal decay products
Terrestrial - woody and herbaceous plants
Aquatic- algae and macrophytes
Structures - derived from cellulose, lignins, tannins, cutin, proteins, lipids, sugars

Stochastic Synthesis of NOM



What is Natural Organic Matter (NOM)?

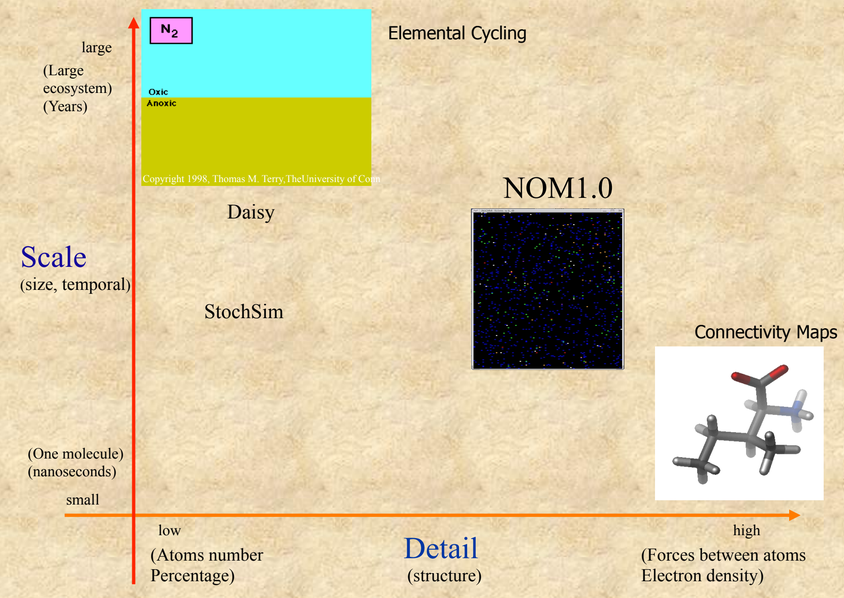
A mixture of degradation and repolymerization products from aquatic and terrestrial organisms which is heterogeneous with respect to structure and reactivity, includes humic substances and smaller molecules.

Stochastic Algorithm: Initialization

- Create initial pseudo-molecules (objects)
  - –Composition (protein, lignin, cellulose, tannin)
  - –Location (top of soil column, stream input)
  - –Input function (batch mode, continuous addition, pulsed addition)
- Create environment
  - –specify pH, light, enzyme activity, bacterial density, humidity, T°, reactive mineral surfaces, flow regime

Goal: A widely available, testable, mechanistic model of NOM evolution in the environment.

Meso-Scale Modeling



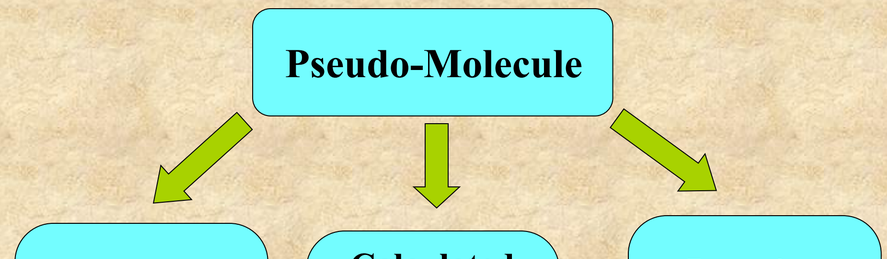
Stochastic Algorithm: Reaction Progress

- Chemical reaction: For each time slice, each pseudo molecule
  - –determine which reaction (if any) occurs
  - –modify structure, reaction probabilities
- Transport: For each time-slice, each pseudo-molecule
  - –Determine mobility
  - –Modify location, reaction probabilities
- Repeat, warehousing 'snapshots' of pseudo-molecules and aggregate statistics

Why Model NOM?

Natural ecosystem functions
Nutrition, buffering, light attenuation
Effects on pollutants
Radionuclides, metals, organics
Water treatment
DBP's, membrane fouling, Fe solubility
Carbon cycling & climate change

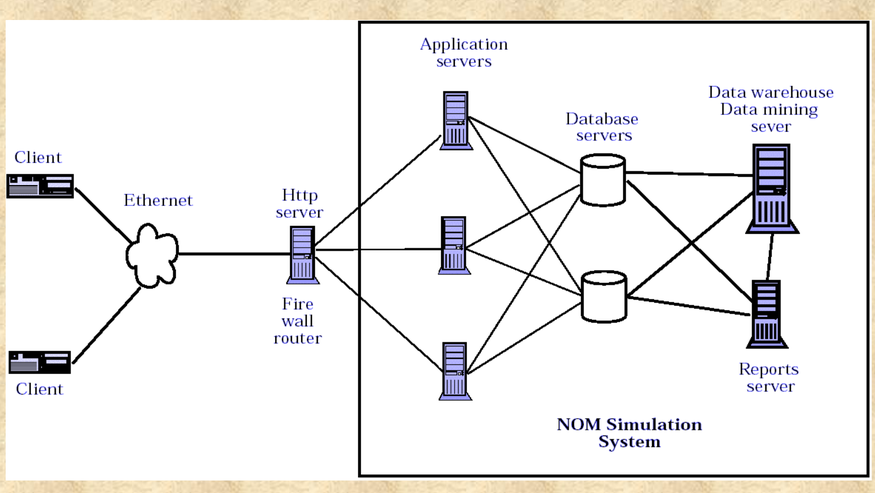
Stochastic synthesis: Data model



Molecules are Agents (Objects)

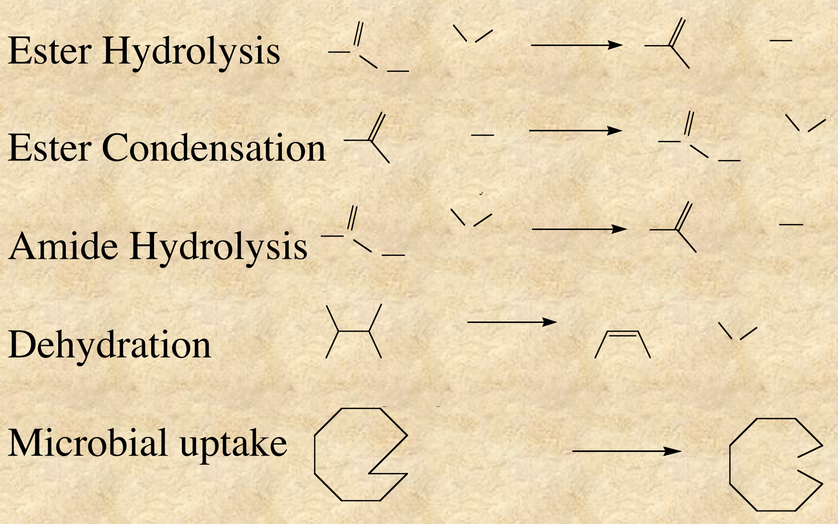
- Heterogeneous properties and behaviors
- Elemental composition
- Molecular weight
- Characteristic functional groups
- Reaction probabilities
  - Molecular structure
  - Environment (pH, light intensity, etc.)
  - Proximity of near molecules
  - State (adsorbed, micellar, etc.)
  - Length of time step, Δt

Web Access to NOM Simulation

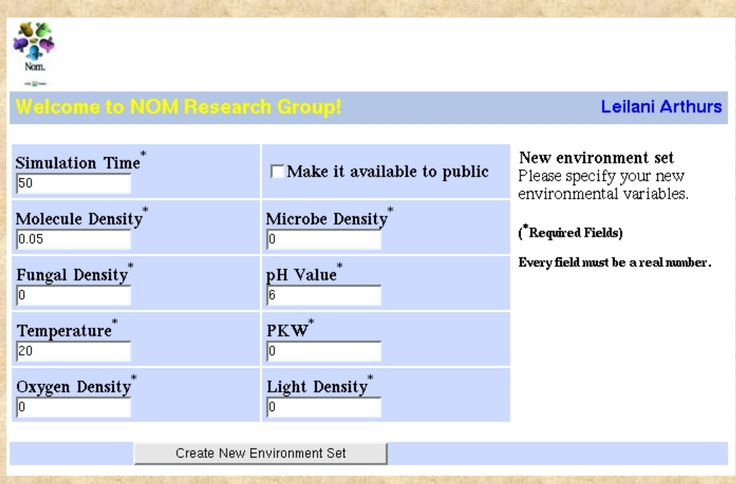


- Implementation
  - **Swarm** toolkit
  - **Java** programming language (JDK 1.4.1_01)
  - **Oracle** RDBMS
- Read simulation parameter from the database (JDBC)
  - Environmental parameters (pH, temperature, light intensity, and so on)
  - Molecule types, and/or molecular weights, and distributions
- User defined time has been separated to a large number of equal size time steps
- Write relevant data into the database every time step (JDBC)
  - Trace the dynamic properties of individuals and the system over time

Model reactions transform structure



Web Browser Setup, Control, and Data Analysis



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