Agent-Based Simulation of Biocomplexity: Interactions of Natural Organic Matter, Mineral Surfaces, and Microorganisms

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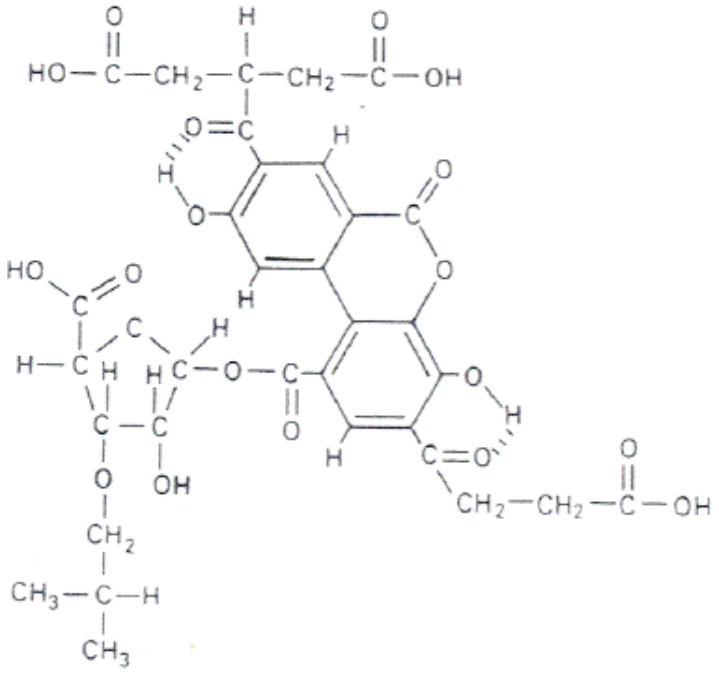
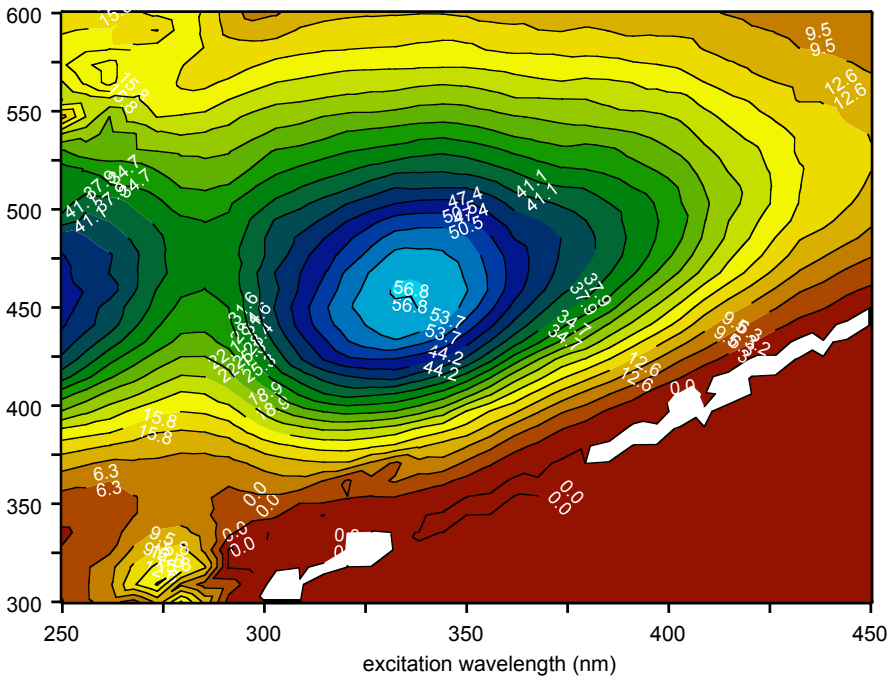
Natural Organic Matter

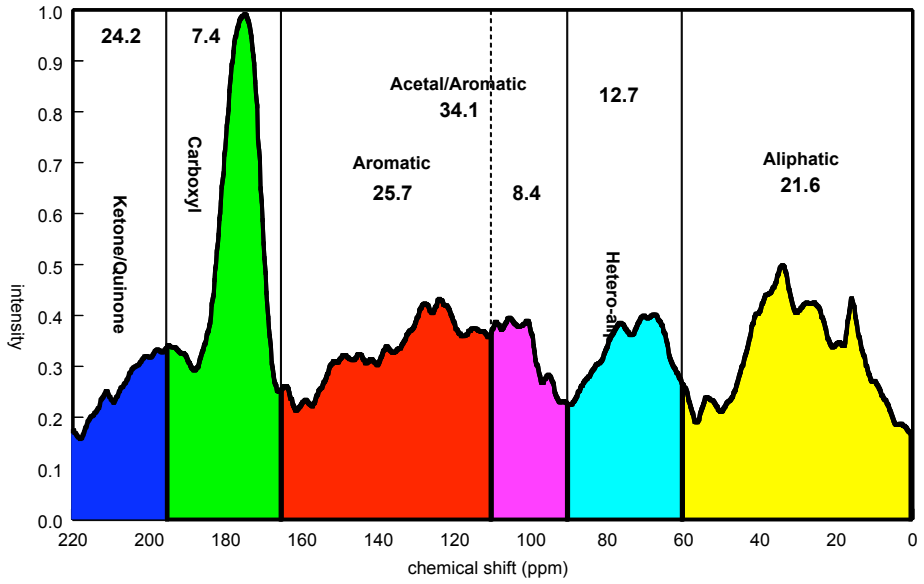
- Forms primarily from the breakdown of organic debris
- Consists of a complex mixture of heterogeneous molecules that varies spatially and temporally
- Is ubiquitous in aquatic and terrestrial environments
- Serves as a primary C source to ecosystems
- Binds metals, radionuclides, organic pollutants and helps to control their mobilities
- Acts as a natural 'sunblock' in surface waters
- Defies simple analysis and deterministic, *ab-initio* modeling because of complex, variable structure.

NOM has complex, variable structure



NOM model (Leenheer)



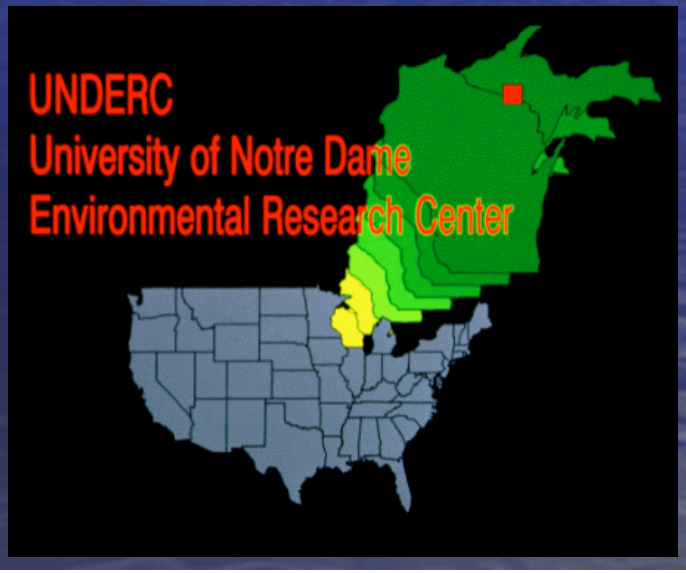


Fluorescence EEM, NMR spectra

Forest Service Bog (FSB) [DOC] 7 MW 2200

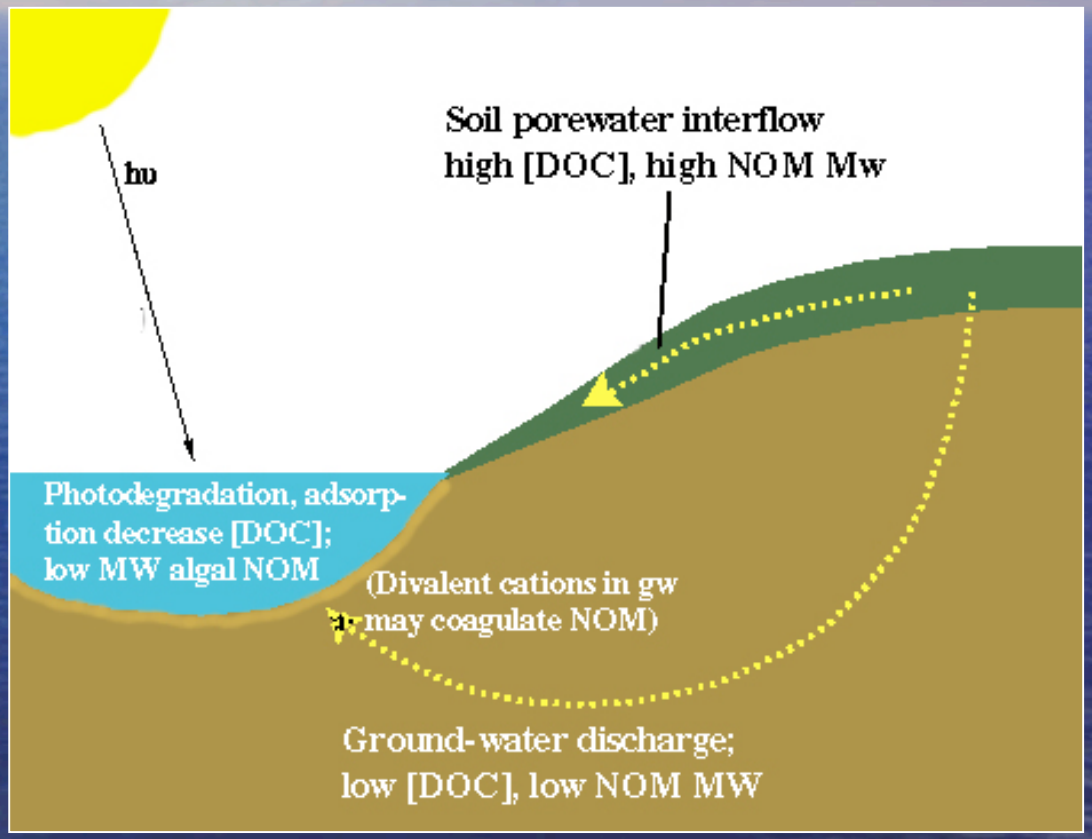
Twomile Creek (TMC) [DOC]
17 MW 1500

Nelson Creek (NLC)[DOC] 79 MW 900



Many processes affect NOM properties

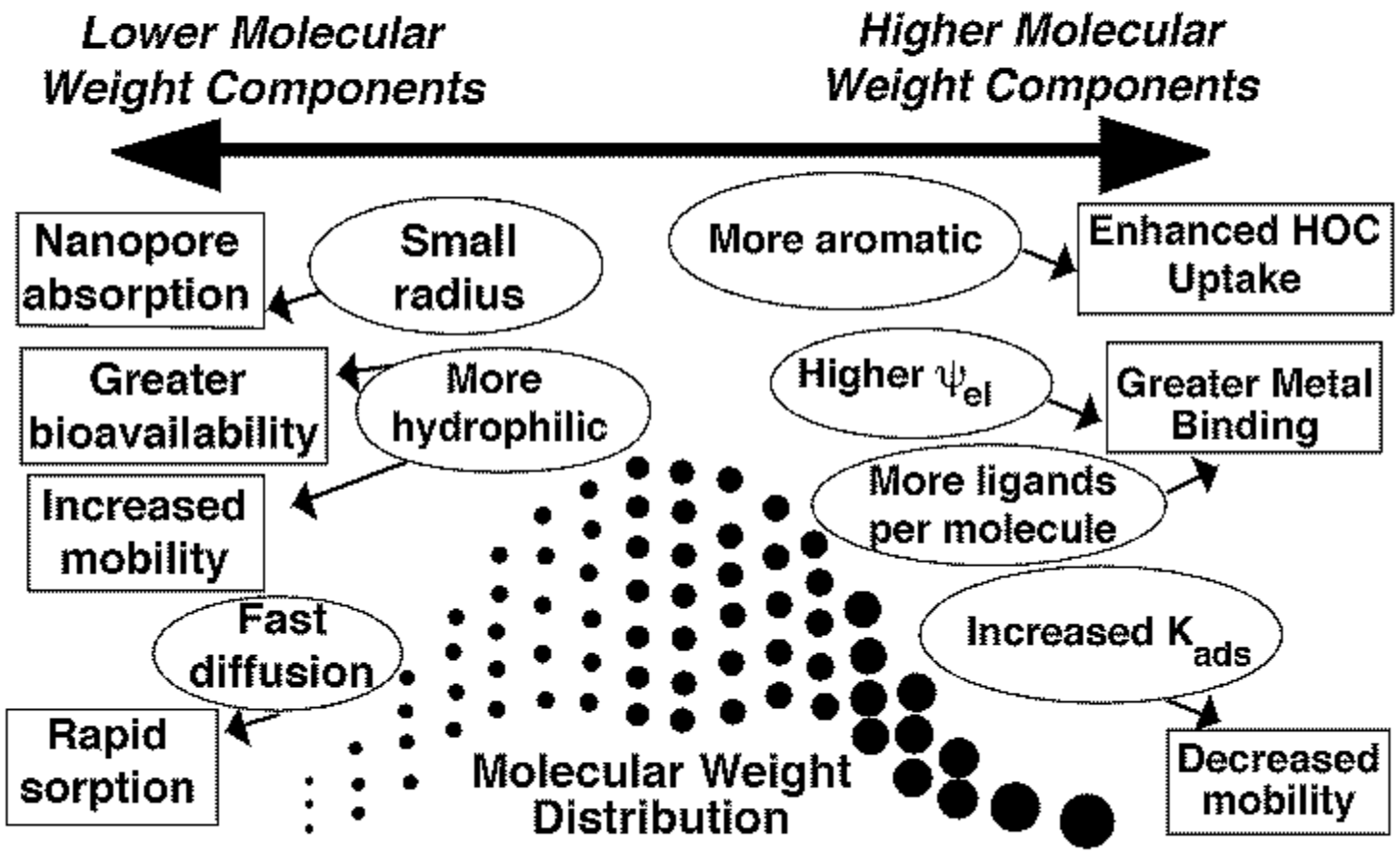
- Adsorption
- Photodegrad-ation
- Coagulation
- Biodegradation
- Primary production



This complexity lends itself well to 'biocomplexity' modeling, agent-based models.

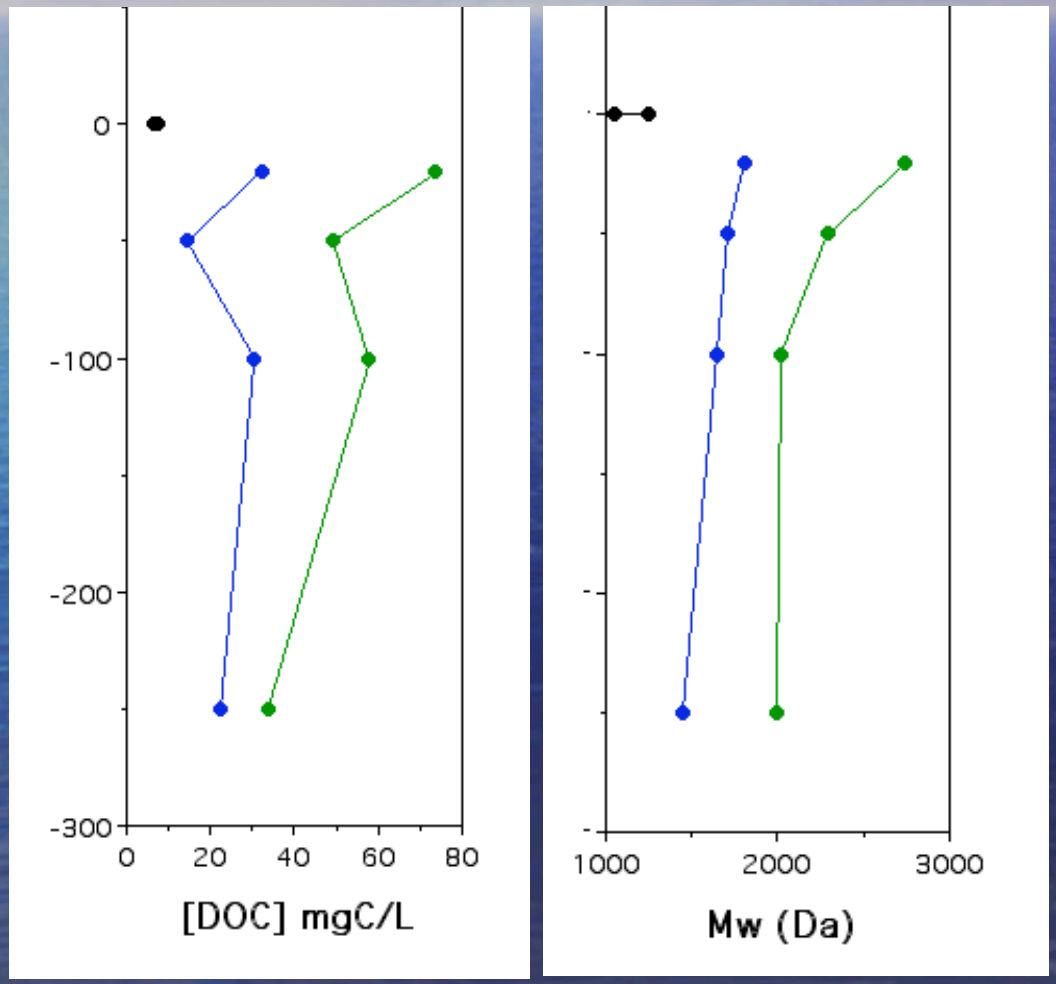
- System heterogeneity controls reactivity
- High degree of spatiotemporal variability
- Complex and cooperative interactions between different components and processes
- Need for scaling between laboratory and field experiments
- Two approaches being used in this model:
  - Composition-based modeling
  - Molecular weight (Mw)-based modeling

Effects of Molecular Weight on NOM Properties and Reactivity

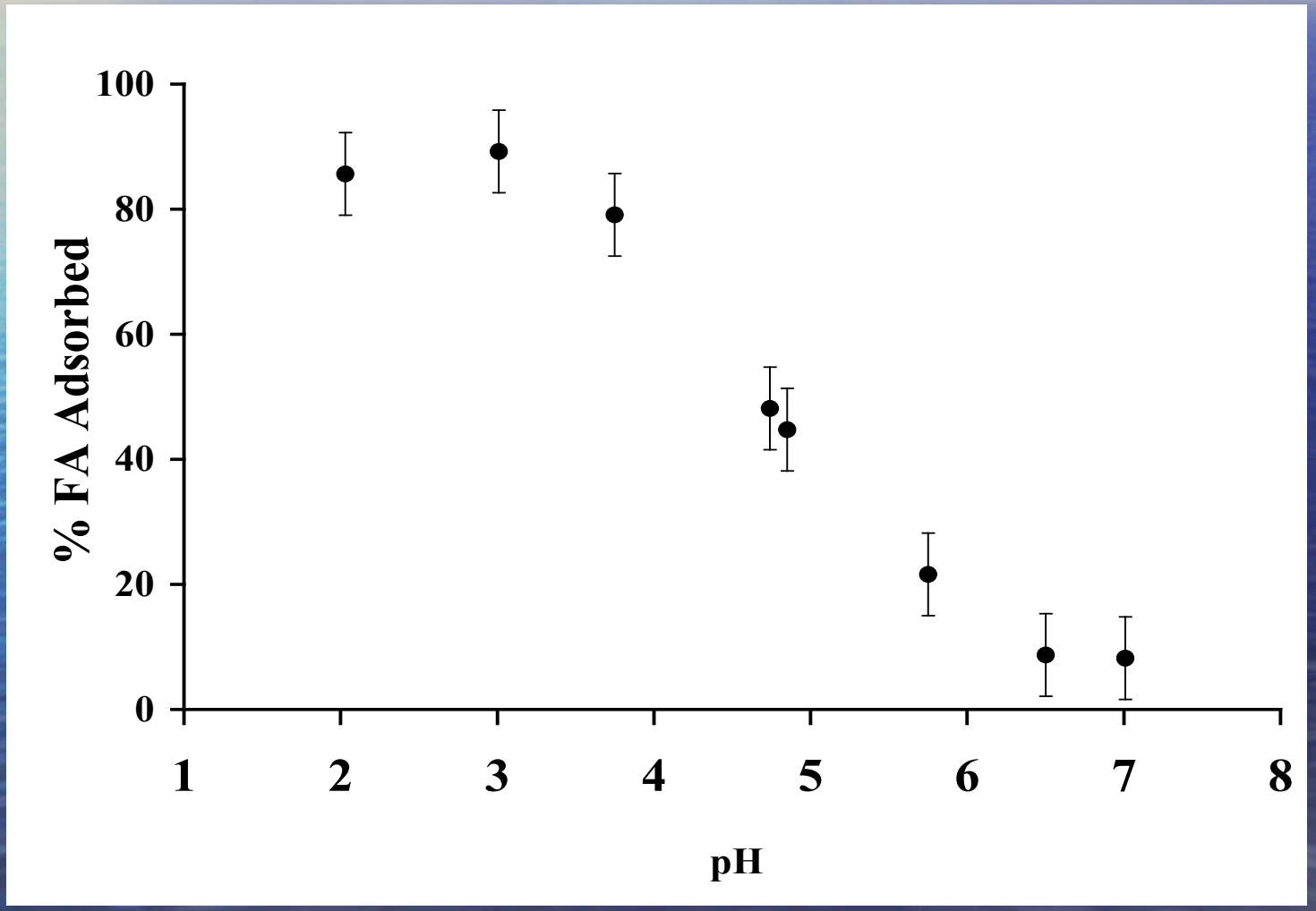


NOM concentration, Mw generally decrease from soils into ground water

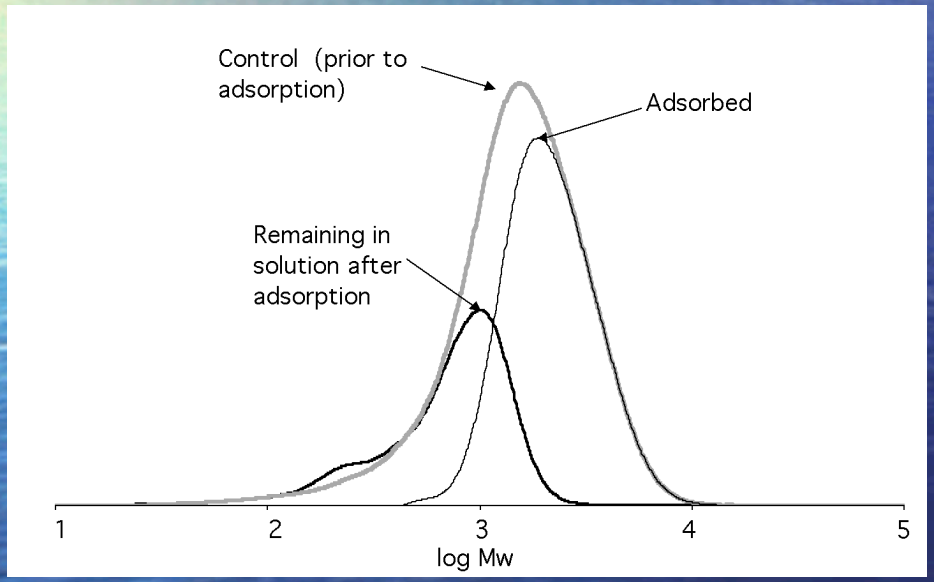
depth below land surface

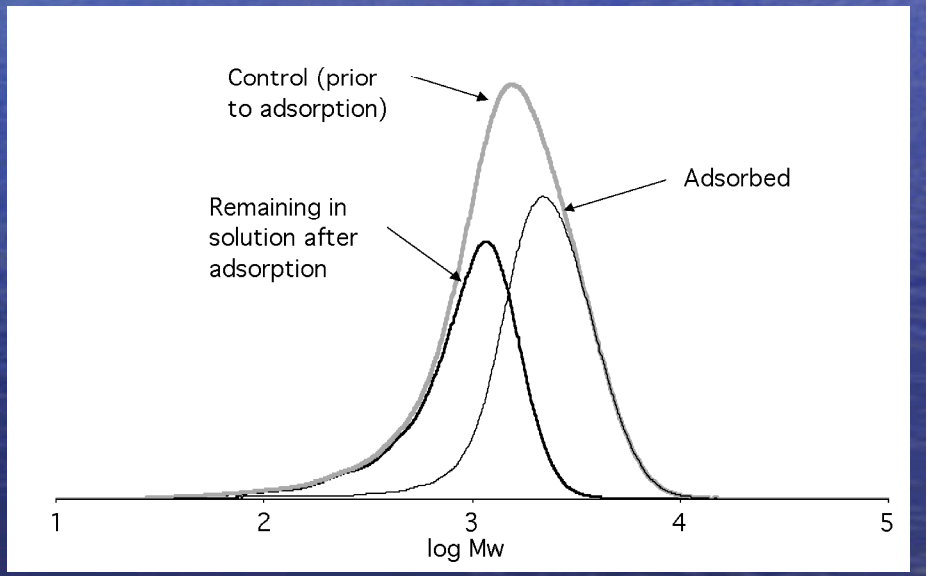


NOM adsorption to minerals and bacteria decreases with increasing pH



Adsorption fractionates NOM
Preferential adsorption of high Mw components





Decreased % sorption---->

Challenges for Research into Biocomplexity

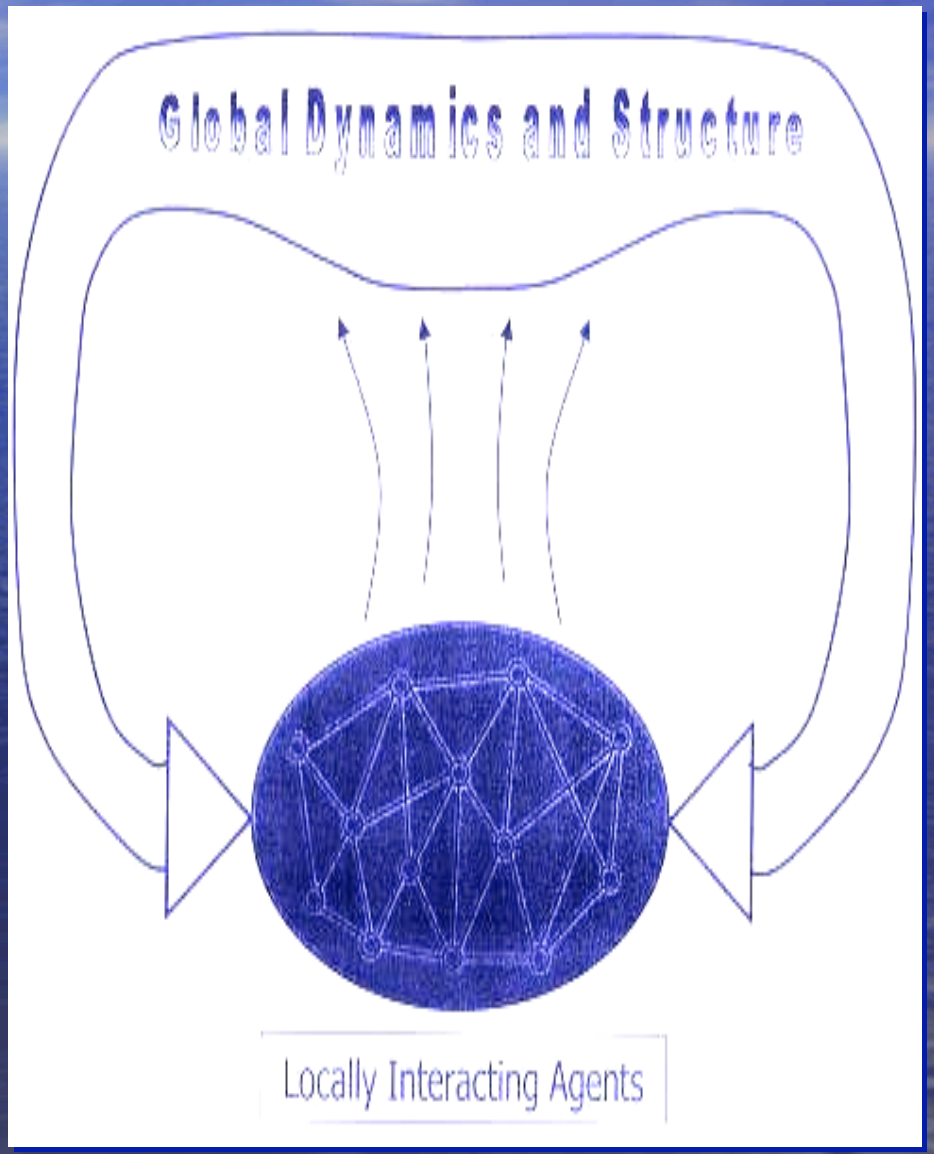
- Heterogeneity of system components
  - Component identities only partially known
  - Often cannot assume homogeneity, averages, aggregate values, or simple distributions; cannot ignore individual differences
- Complex interactions between components
  - Processes and signaling pathways only partially known
  - Often cannot assume a well mixed solution, spatial independence
- Complex interactions with environment
  - Dynamic coupling/feedback between components and system
  - Phenomena at different system levels
- Limitations of
  - Equation-based modeling
  - Reductionism (complexity —> emergence —> scaling problems)
  - Sensitive dependence to initial conditions

New Computer Capabilities —> New Methods for Science

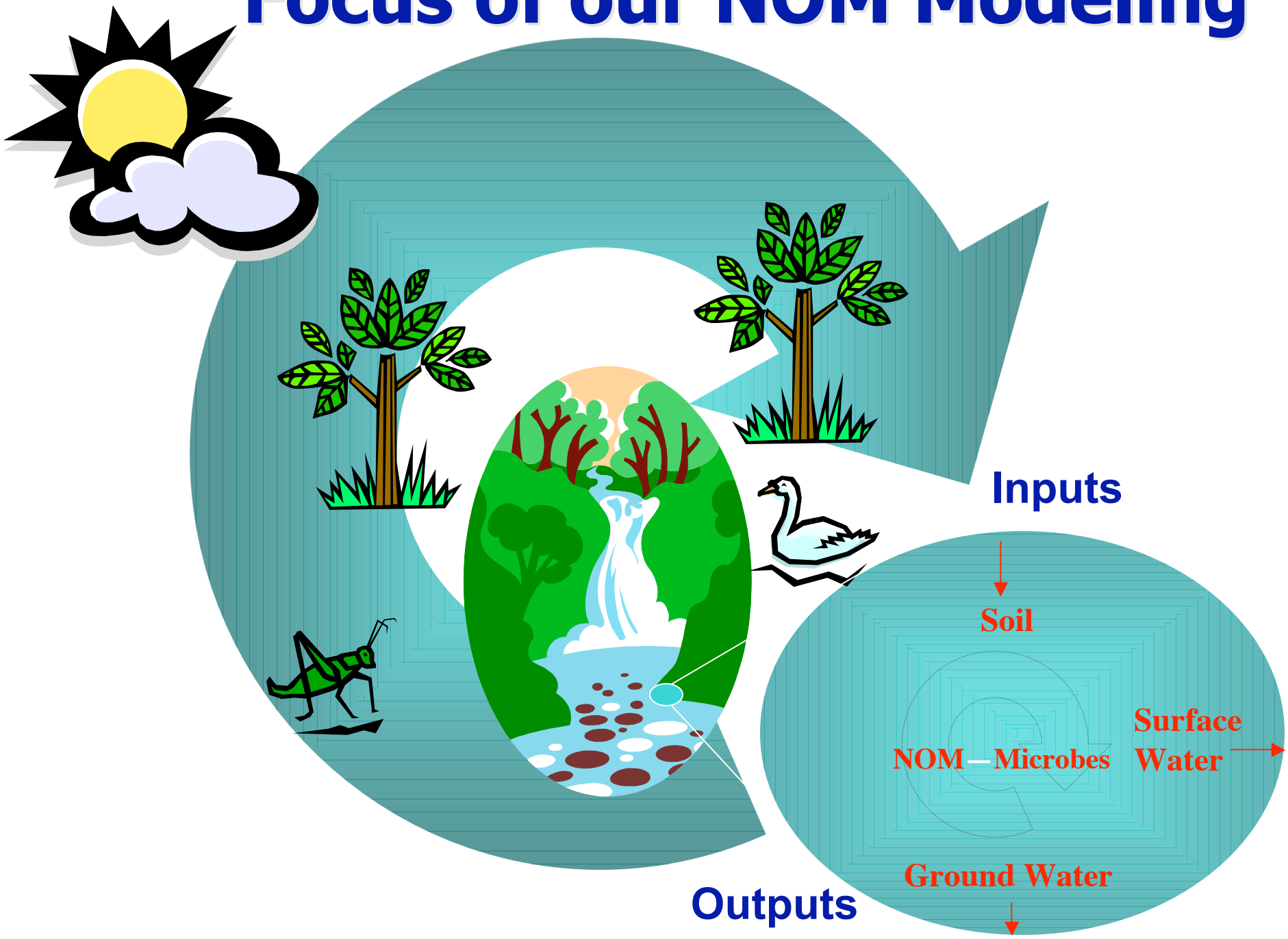
- Faster/cheaper/more CPUs —>
  Individual-based/Agent-based Modeling
  - Stochastic modeling
  - Discrete event simulation
- Bigger/cheaper/more Disk Drives —>
  Data warehouses/Data mining
  - Sensor nets
  - High dimensional, merged data sets
  - Data from simulations
  - Computer-assisted discovery

Agent-based Modeling and Simulation

- Individual-based modeling (IBM)
- Discrete event simulation
- Stochastic birth-death models (SBD)
- Cellular automata (CA)
- Artificial Life (AL)



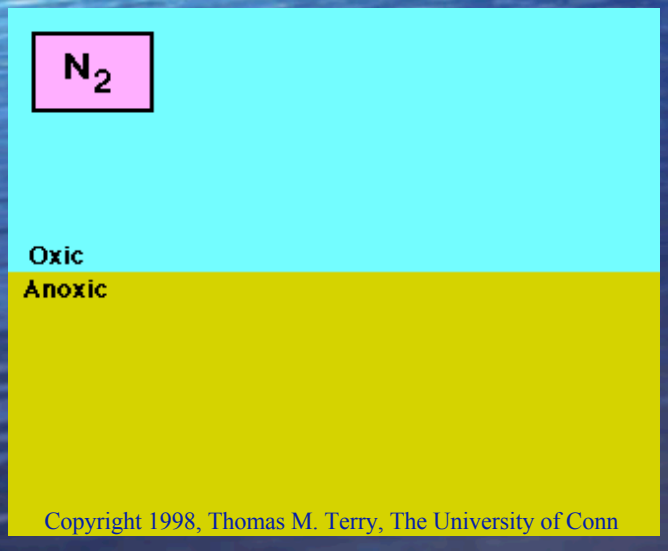
Focus of our NOM Modeling



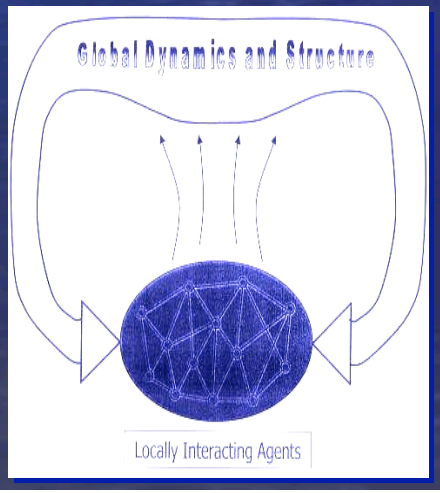
Background

- Prior modeling work often too simplistic to represent NOM heterogeneity and its complex behaviors in ecosystems (e.g., carbon cycling models, nitrogen cycling models)
- Prior modeling work often too compute-intensive to be useful for large-scale environmental simulations (e.g., molecular models employing connectivity maps or electron densities)
- Hence, a **Middle Computational Approach** is taken …

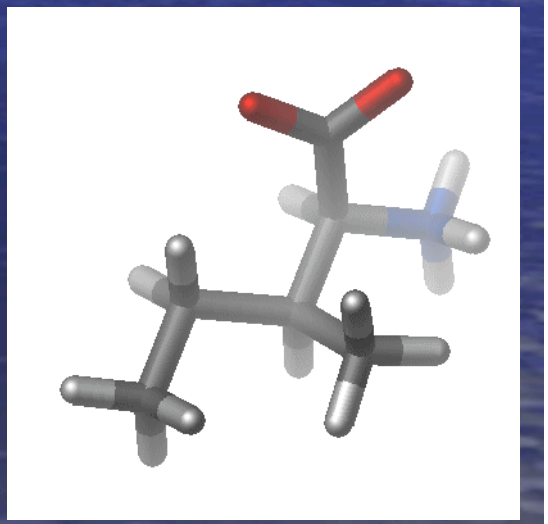
Elemental Cycling



Agent-based Approach



Connectivity Maps



Modeling

- Molecules and microbes are objects
- Molecules and microbes have attributes
  - Heterogeneous, distributions
  - Currently 1,000 objects, testing 10,000 and more
- Molecules have behaviors (reactions)
  - Molecules in simulation are a representative sample of the larger population
  - Behaviors are stochastically determined
  - Dependent on the:
    - Attributes (intrinsic parameters)
    - Reaction rates
    - Environment (extrinsic parameters)

Modeling (cont)

- Objects of interest
  - Macromolecular precursors
    - Polysaccharides
    - Proteins
    - Polynucleotide, tannin, lignin, polyterpene, cutin
  - Smaller molecules
    - Phospholipids
    - Sugars
    - Amino acids
    - Flavonoids
    - Quinones
  - Microbes

Modeling (cont)

- Attributes
  - More specific than "percent carbon" but less detailed than a molecular connectivity map
  - Elemental composition
    - Number of **C, H, O, N, S** and **P** atoms in molecule
  - Functional group counts
    - Double-bonds
    - Ring structures
    - Phenyl groups
    - Alcohols
    - Phenols, ethers, esters, ketones, aldehydes, acids, aryl acids, amines, amides, thioethers, thiols, phosphoesters, phosphates
  - The time the molecule entered the system
  - Precursor type of molecule

Modeling (cont)

- Behaviors (reactions and processes)
  - Physical reactions
    - Adsorption to mineral surfaces
      - Initial adsorption
      - Surface migration to high-energy sites
      - Hemi-micelle formation at high coverage (cooperative, hydrophobicity dependent)
    - Aggregation/micelle formation (e.g., metal cation-induced aggregation) - flocs
    - Transport downstream (surface water)
    - Transport through porous media
    - Volatilization

Modeling (cont)

- Behaviors (reactions and processes)
  - Chemical reactions
    - Abiotic bulk reactions
      - Hydrolysis
      - Hydration
      - Ester condensation
      - Thermal decarboxylation
    - Abiotic surface reactions
    - Direct photochemical reactions
    - Indirect photochemical reactions
    - Extracellular enzyme reactions on large molecules
      - Bacteria
      - Fungi
      - Algae
    - Microbial uptake by small molecules

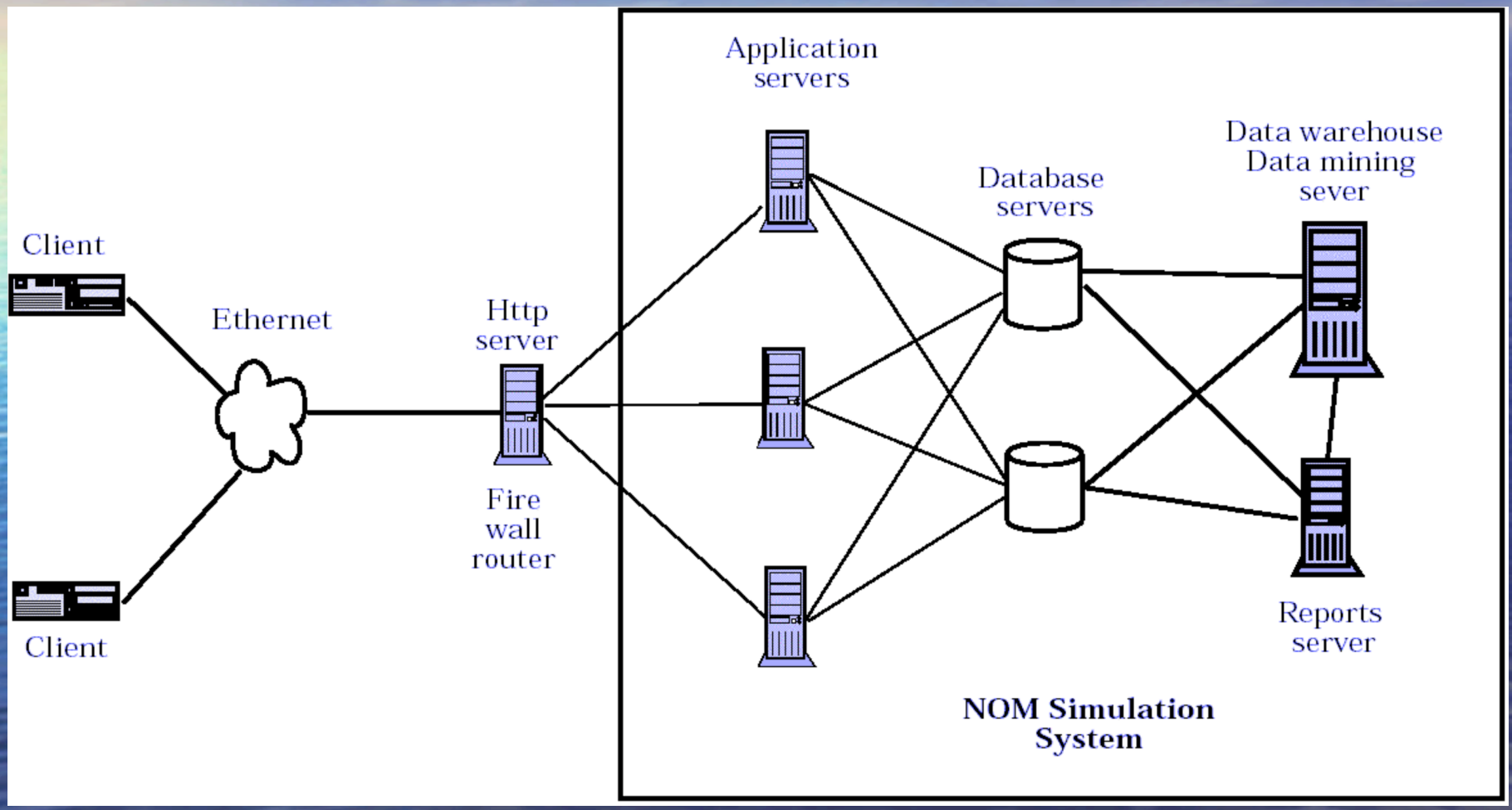
Modeling (cont)

- Environmental parameters
  - Temperature
  - pH
  - Light intensity
  - Metal concentrations (e.g., Al and Fe)
  - Bacterial activity
  - Water flow rate/pressure gradient
- Environment: 2D Grid, mineral surfaces, soil pores
- Simulation parameters: run time, data collection

NOM 1.0

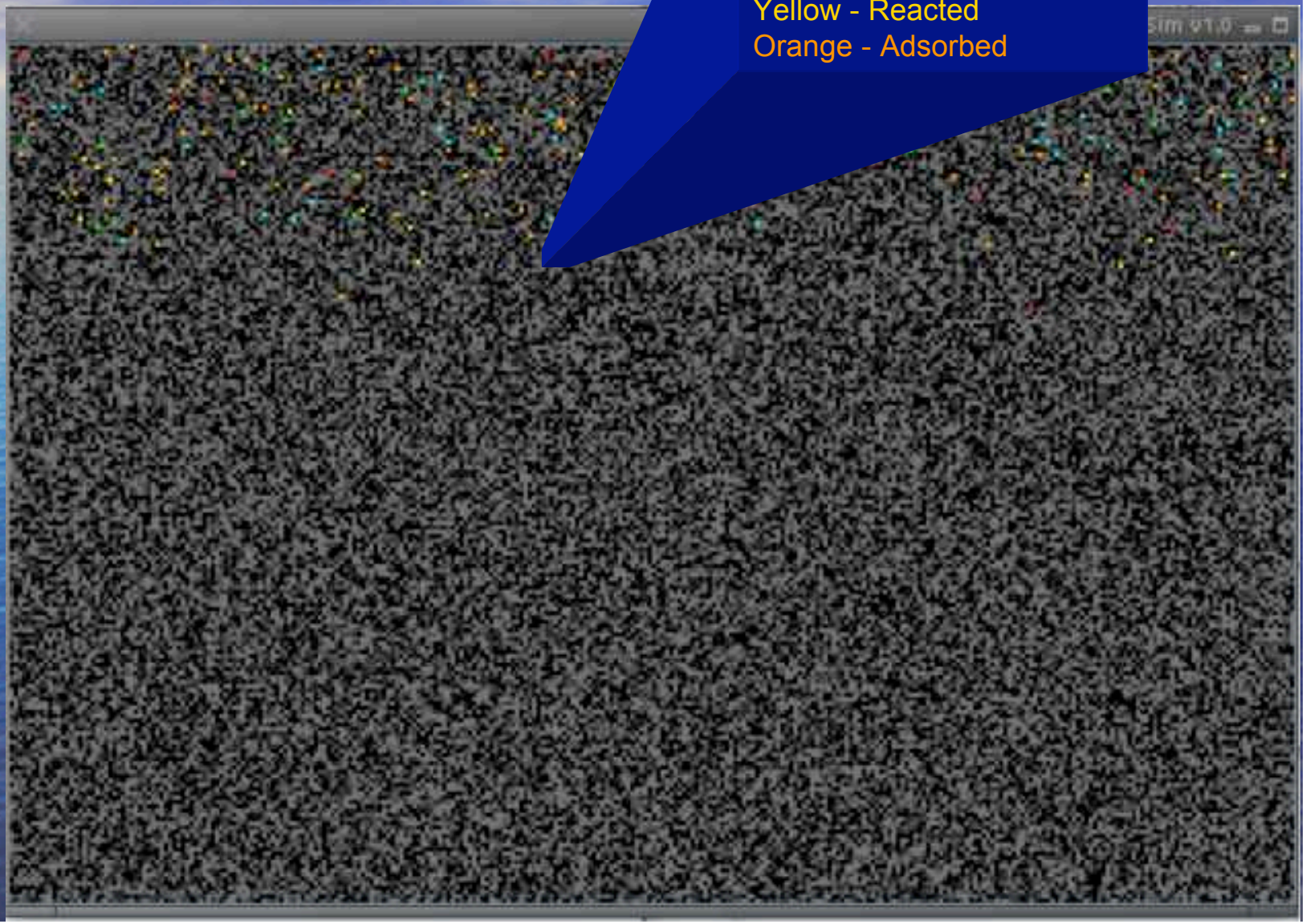
- Visualization
  - Simulation and Animation of Molecules
- Web-Based Access
  - Standard Browser Interface
    - HTML Forms / JSP
    - Java Servlets
    - JDBC - Oracle Database
    - Oracle Forms and Reports
  - Shared Data and Simulations
  - Collaboration Support: Web-board, Chat, mail server, file upload/download

Web Access to NOM Simulation

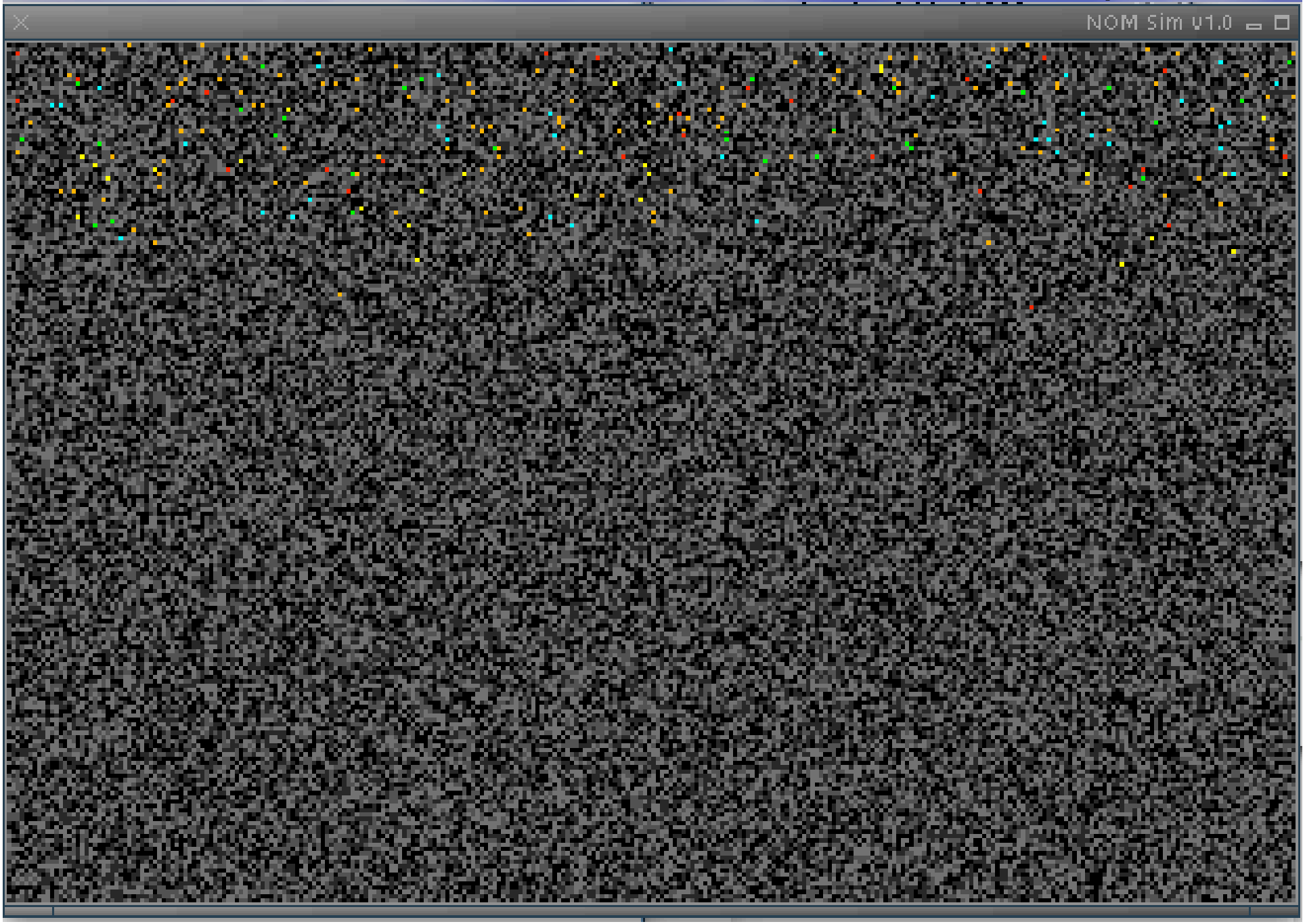


Visualization

Black - No Adsorption
Grays - Levels of Adsorption
Red - Lignins
Green - Cellulose
Blue - Proteins
Yellow - Reacted
Orange - Adsorbed



Visualization - NOM molecules in solution and adsorption



Web Browser Setup

Welcome to NOM Research Group! **Leilani Arthurs**

Simulation Time* 50	☐ **Make it available to public**
Molecule Density* 0.05	**Microbe Density*** 0
Fungal Density* 0	**pH Value*** 6
Temperature* 20	**PKW*** 0
Oxygen Density* 0	**Light Density*** 0

New environment set
Please specify your new environmental variables.

(*Required Fields)

Every field must be a real number.

Create New Environment Set

Welcome to NOM Research Group! Leilani Arthurs

Introduction | Environment | **Molecules** | Summary

NOM Simulator: Molecules

Below are all available molecule types, please choose the molecule types and specify the percentage of each. You can click **here** to create a new molecule type.

Available molecule types:

Choose it	Molecule type	What is it?	Percentage	Edit or Delete
☐	Cellulose			edit | delete
☐	Lignin			edit | delete
☐	Protein			edit | delete
☐	NoFA			edit | delete
☑	1ficFA		5	edit | delete
☑	2ficFA		20	edit | delete
☑	3ficFA		50	edit | delete
☑	4ficFA		20	edit | delete
☑	5ficFA		5	edit | delete

< Back | step 3 of 4 | Next >

Welcome to NOM Research Group!

Leilani Arthurs

(*Required fields)

Molecule Name*
3ficFA

☐ Make it available to public

Atoms of the molecule
Each field must be a non-negative integer.
Default value is 0.

(Atom) C	(Atom) H	(Atom) N
66	64	0

(Atom) O	(Atom) S	(Atom) P
38	0	0

Functional groups of the molecule
Each field must be a non-negative integer.**Default value is 0.**

DoubleBond	Rings	Phenyl	Alcohols	Phenols
0	0	0	0	0

Ethers	Esters	Ketones	Aldehydes	Acids
0	0	0	0	0

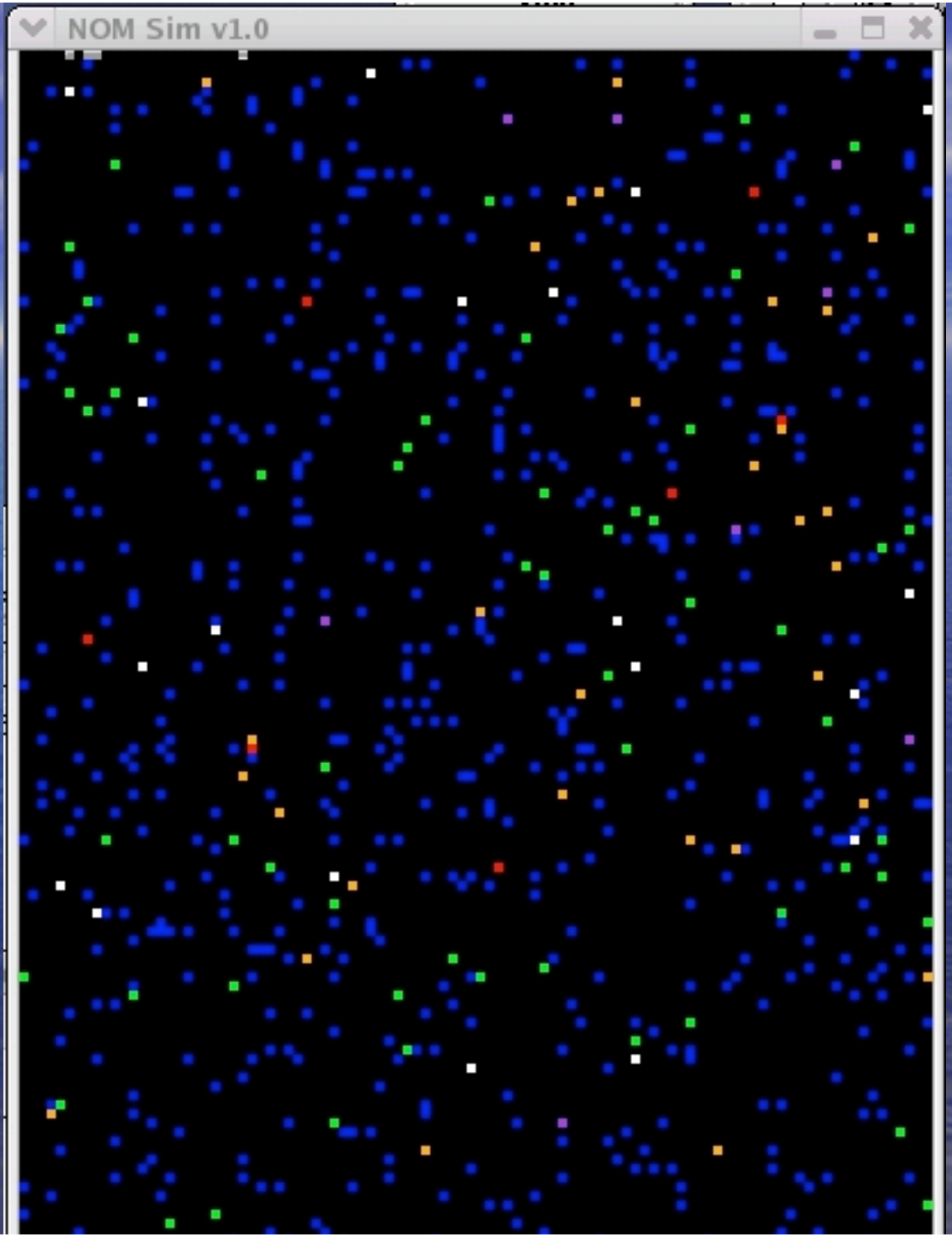
Arylacids	Amines	RingN	Amides	Thioethers
0	0	0	0	0

Thiols	Phosphoesters	HPhosphoesters	Phosphates
0	0	0	0

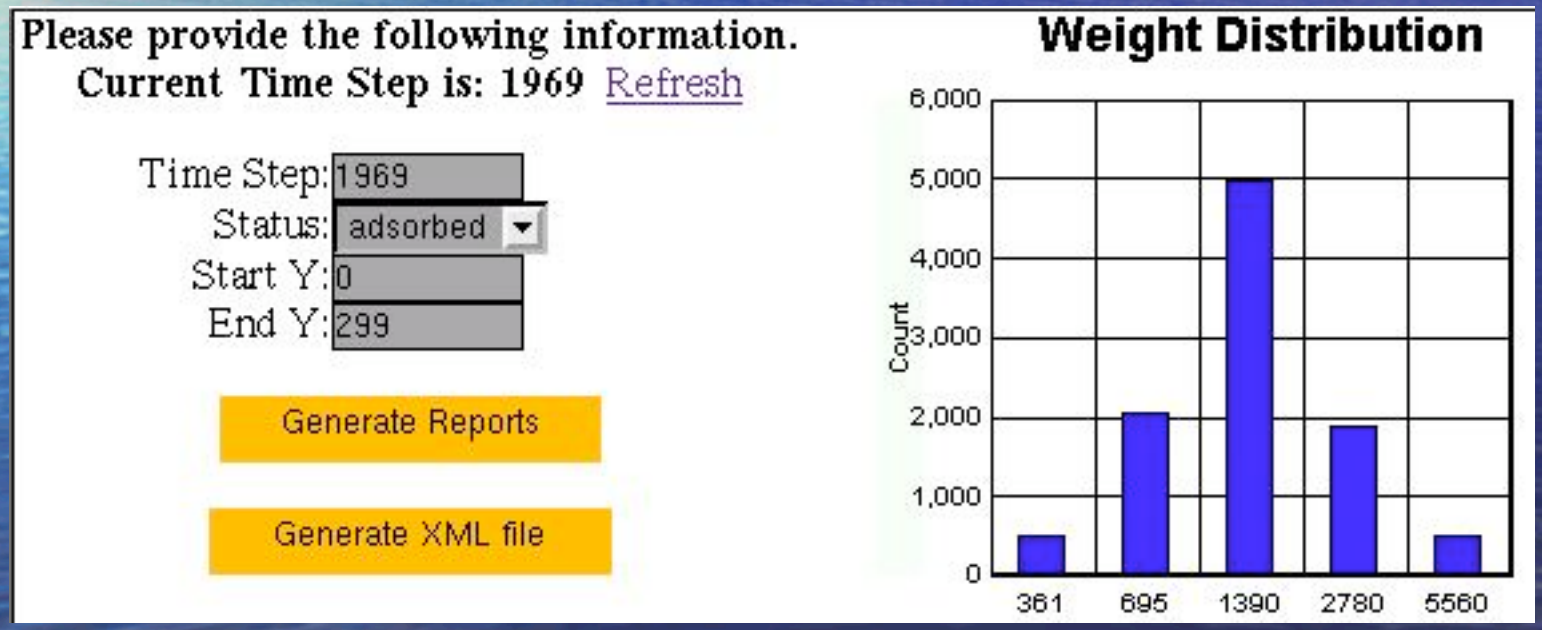
Create New Molecule Type

Visualization

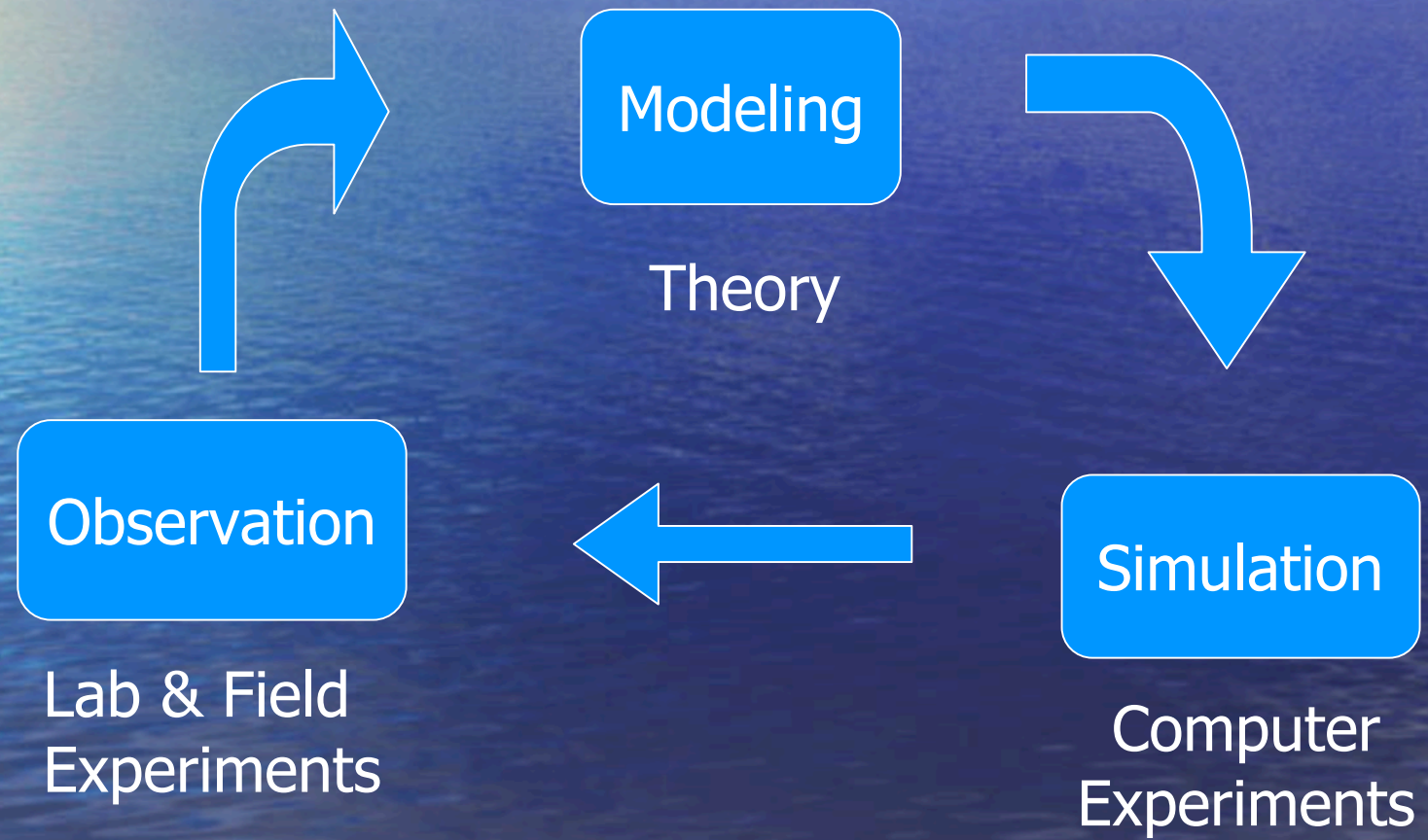
Color coded molecules
- Solution
- Adsorbed
- Mw



Web-based Reports



Modeling and Simulation in support of Biocomplexity Research



Summary

- Challenges for biocomplexity research
- New computer science tools
- Middle computational approach
- Agent-Based Modeling approach
- Stochastic (Monte Carlo based simulation)
- NOM Molecules & Microbes as Agents
- Web-based Simulation, databases, data warehouse, visualization, database queries, data mining
- Invitation to collaborate …

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