Complex System Simulation: Interactions of NOM Molecules, Mineral Surfaces, and Microorganisms in Soils

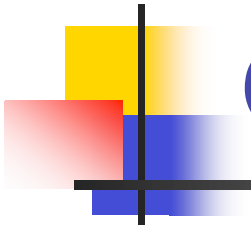
Greg Madey
Y-P Huang, X. Xiang, Eric Chanowich
University of Notre Dame

Steve Cabaniss
University of New Mexico

Simulation of NOM and Microbial-Environmental Interactions

- Funded in part by NSF-ITR (DEB)

- Co-PIs
  - Steve Cabaniss, Chemistry, University New Mexico
  - Greg Madey, Computer Science, Notre Dame
  - Robert Wershaw, USGS-Denver
  - Jerry Leenheer, USGS-Denver
  - Patricia Maurice, Geological Sciences, ND
  - Robert Wetzel, Biology, UNC-Chapel Hill
- Students
  - Yingping Huang, Computer Science, (MS Thesis)
  - Xiaorong Xiang, Computer Science, (MS Thesis)
  - Eric Chanowich, Computer Science, REU

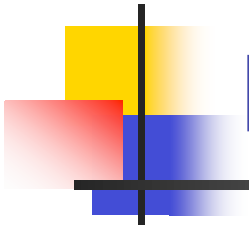


Overview

- Complex systems approach
- How to model complex systems?
- Why stochastic agent-based modeling?
- Our goals
- Our model
- Prototype demonstration

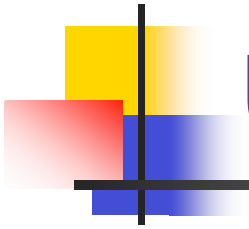
Complex Systems

- Complexity refers to the **dynamic web of interrelationships** within physical, biological, geochemical, hydrological, environmental, ecological, social, economic, engineered systems, etc.
- The study of complexity includes systems that range from molecular to global in scale, and exhibit properties that depend not only on the **individual actions** of their components, but also the **interactions among those components**.



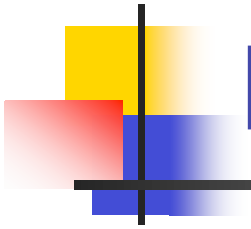
Properties of Complex Systems

- Many Entities (Typically Heterogeneous)
- Entities Have Individual Behaviors
- Interactions Between Entities Including Feedback (Often Nonlinear)
- Often Sensitive Dependence to Initial Conditions
- Self-Organization
- Emergence: Global Structures & Relationships



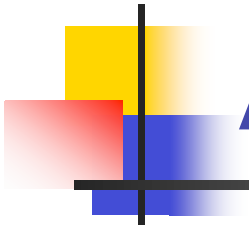
Understanding Complex Systems

- Parts versus the Whole
  - Limitations of the Reductionist Approach
- Sensitive Dependence on Initial Conditions
  - Limits to Predictability
  - Goal is to Understand the Invariant Global Properties and Mechanisms of the System
    - Stability, Periodicity, Chaotic
    - Bounded/Unbounded
    - Global Patterns, Webs of Relationships, Key Components
- Difficulties in Observing and Discovering Those Properties and Mechanisms in Nature!



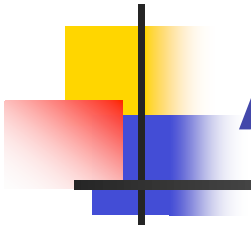
Modeling Complex Systems

- Mathematical Modeling (Mathematical “x”)
  - Limitations of analytic (pencil & paper) approaches
- Computer Simulation (Computational “x”)
  - Iteration/Recursion
  - Systems of Differential Equations
  - Numerical Methods
  - Limitations of traditional computational approaches
- Computer Simulation (Bottom-up Modeling)
  - Discrete-Event
    - **Agent-Based Modeling (Our approach!)**
      - **Heterogeneous interacting agents**
      - **Monte Carlo, stochastic, probabilistic behaviors**



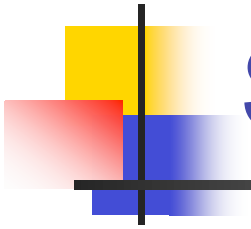
Agent-Based Modeling

- Object-Oriented Paradigm
  - Entities are Objects (Agents)
  - Objects have: Attributes (data) & Behaviors (methods)
  - Classes of Objects (heterogeneous)
  - Inheritance/Polymorphism
- Simulation Process
  - Model Entities with Classes: Attributes & Behaviors
  - Create (and destroy) Objects (Agents)
  - Model the Environment of the Objects (Agents)
  - Object Behaviors generate Interactions with Environment and other Objects (Agents)
  - Store State Information in Database/DataWarehouse (Oracle)
  - Post-Simulation Analysis (Data Mining/Knowledge Discovery)



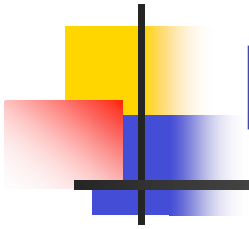
Agent-Based Modeling Tools

- Object Oriented Languages: C++, Java, Objective-C, SmallTalk
- Simulation Libraries (Class Packages)
  - Swarm
  - RePast
- Simulation Environments
  - Starlogo, StarLogoT, NetLogo
  - Agent Sheets
  - AScape
  - Integrated Modeling Toolkit (IMT)



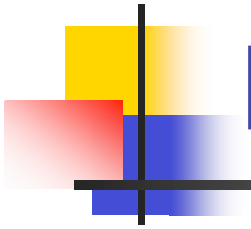
Swarm

- Agent-Based Modeling Library
- Open Source / Started at Santa Fe Institute - Chris Langton, A-Life
- ObjectiveC and Java
- Swarms
  - Collections of Agents
  - Swarms can be modeled hierarchically
  - Sub-Swarms



Background

- Prior modeling work often too simplistic to represent NOM heterogeneity and its complex behaviors in ecosystems (e.g., carbon cycling models), also …
- 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 …



Project Goals

- Develop stochastic model of NOM evolution — middle computational approach
  - Represent individual molecules and microbes as discrete objects
  - Model NOM evolution from biological precursor compounds
- Generate experimentally testable predictions about NOM systems (validation of simulation)
- Deploy Web-based simulation for testing, feedback and usage
- Open project site to environmental researchers
- Provide Web-based Collaboratory for NOM research & education

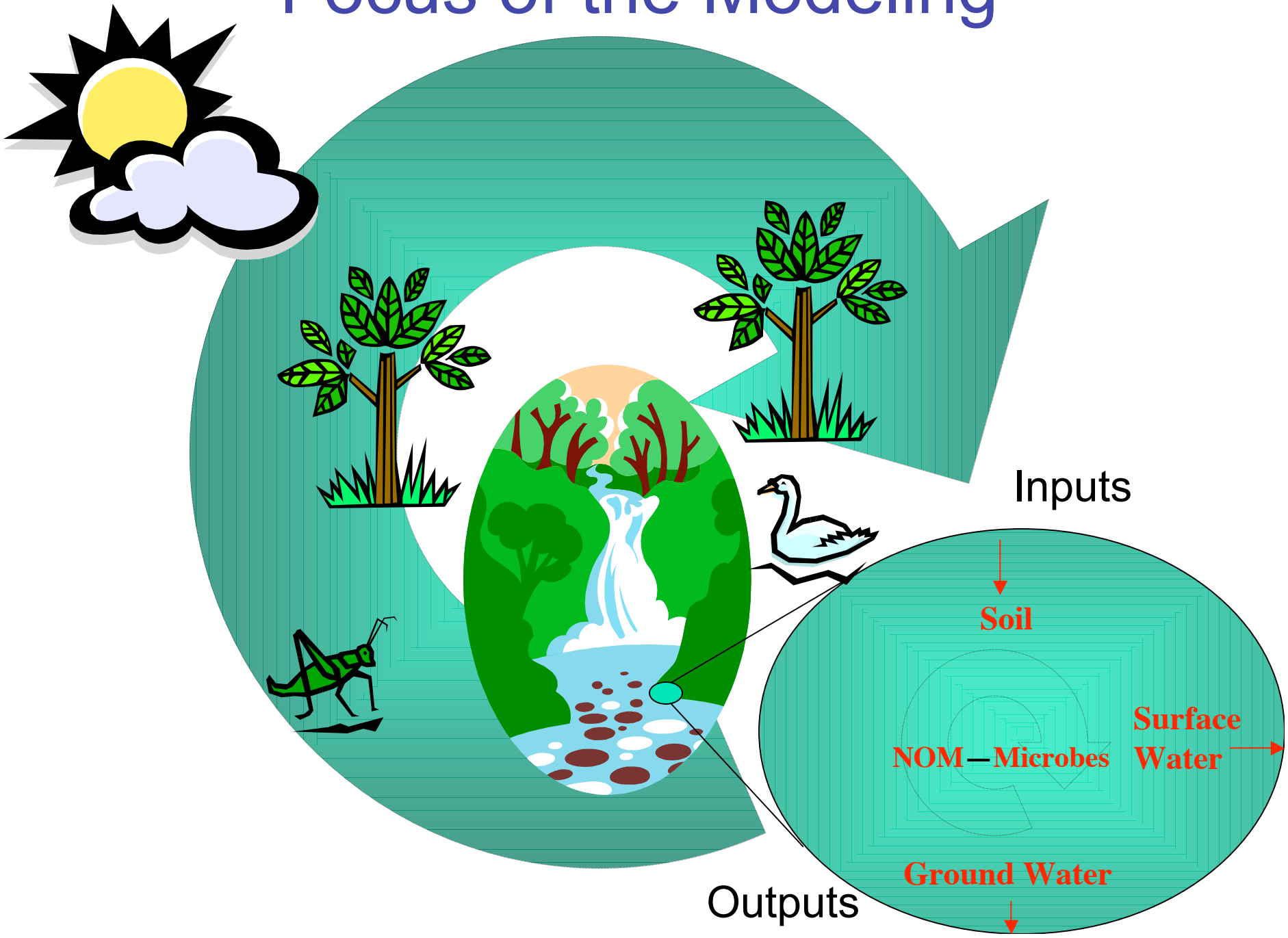
Collaboratory for NOM Research

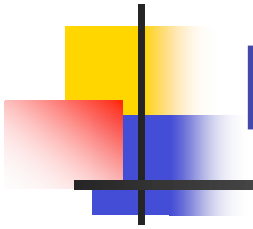
Goal: to produce digital capabilities for a web-based information management system in the form of interoperable databases and associated data management tools.

Tools include: software for NOM modeling & simulation, querying & data mining, data manipulation & analysis, scientific visualization, and electronic communication & collaboration between geographically distinct sites.

Databases & software tools: designed to be used by researchers & educators to better understand NOM evolution in terrestrial & aquatic environments.

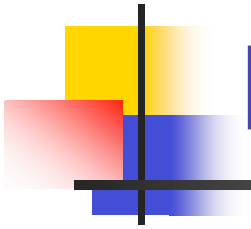
Focus of the Modeling





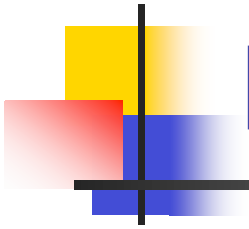
Modeling

- 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)

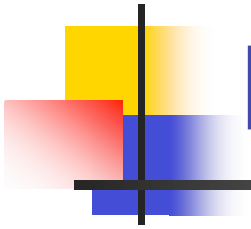
- Attributes
  - More specific than “percent carbon” but less detailed than a molecular connectivity map
  - Elemental composition
    - Number of **C, H, O, N, S** and **P** atoms in molecule
  - Functional group counts
    - Double-bonds
    - Ring structures
    - Phenyl groups
    - Alcohols
    - 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

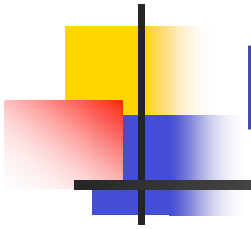
Modeling (cont)

- 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)

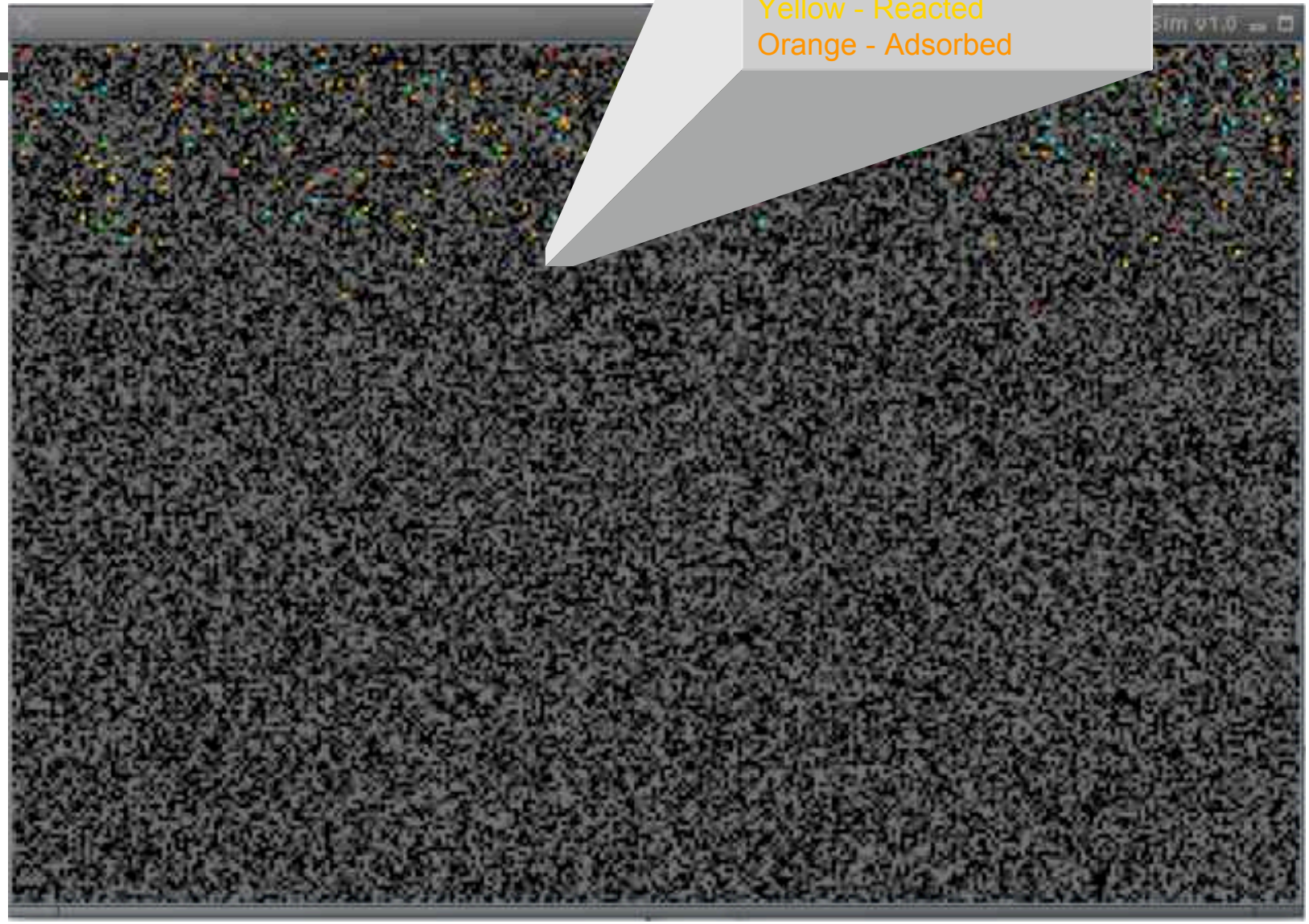
- Environmental parameters
  - Temperature
  - pH
  - Light intensity
  - Metal concentrations (e.g., Al and Fe)
  - Bacterial activity
  - Water flow rate/pressure gradient
- Environment: 2D Grid, mineral surfaces, soil pores
- Simulation parameters: run time, data collection



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

Visualization



Online NOM Simulation

Back Forward Stop Refresh Home AutoFill Print Mail Sherlock

Address: http://gemini.cse.nd.edu:8888/nom/homepage.jsp go

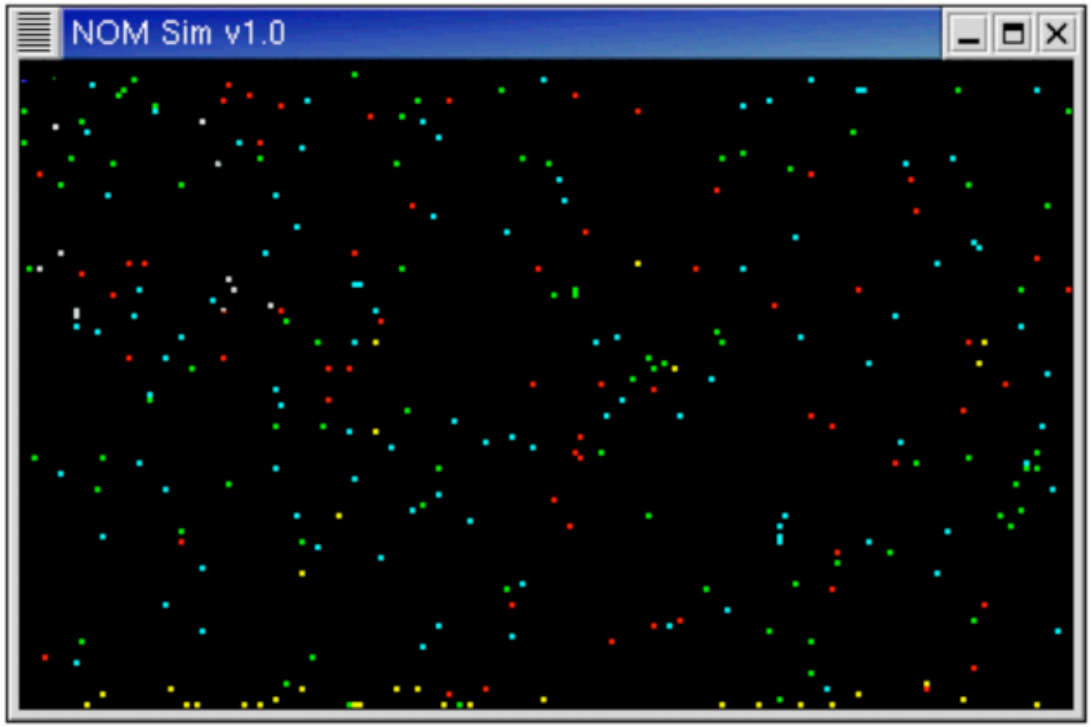
Live Home Page Apple Apple Support Apple Store iTools Mac OS X Microsoft MacTopia

Favorites History Search Scrapbook Page Holder

NOM Simulator

Welcome to NOM Research Group!

You must sign in to use the simulator!



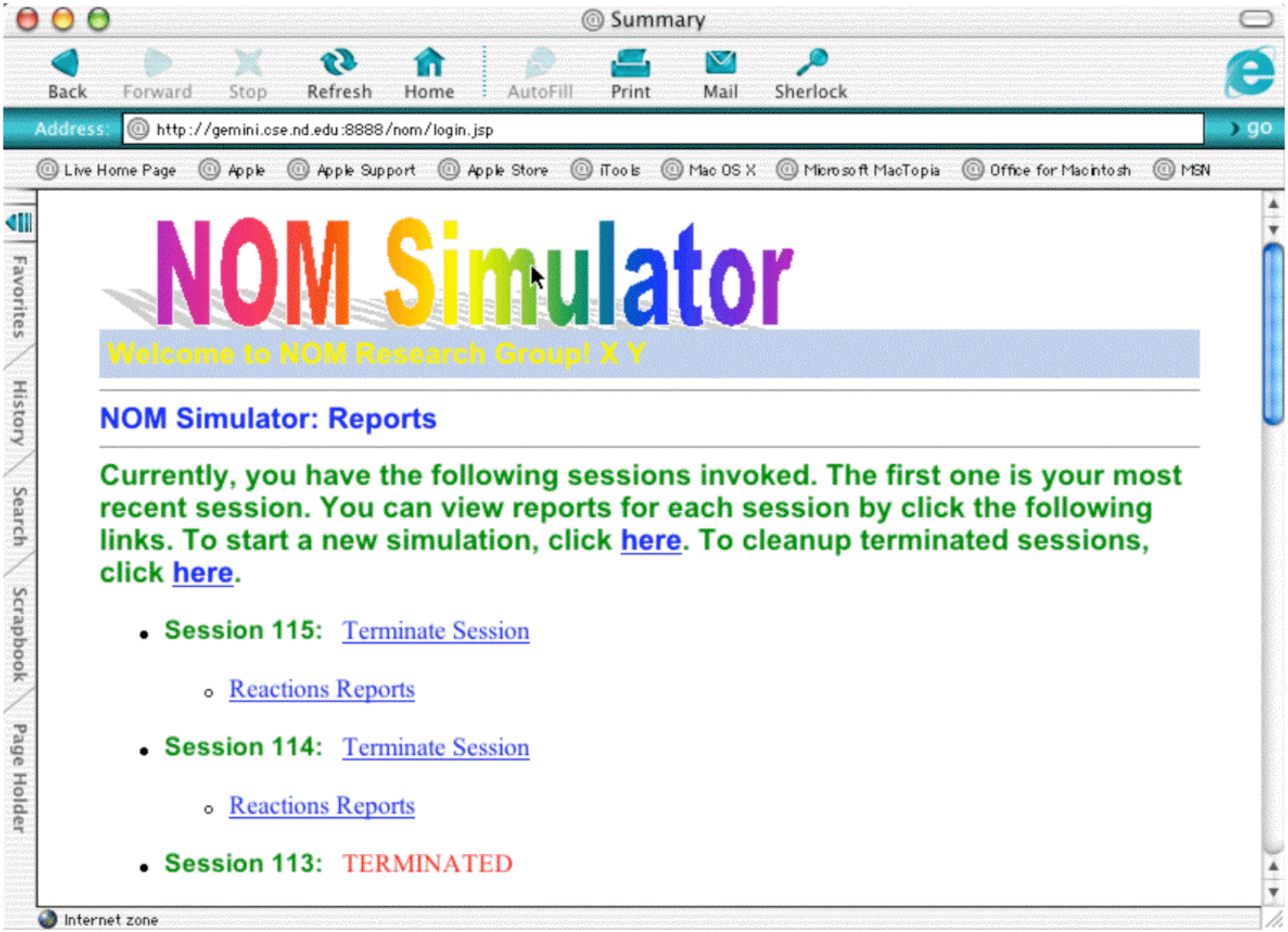
Existing Users
Enter your userid and password to sign in

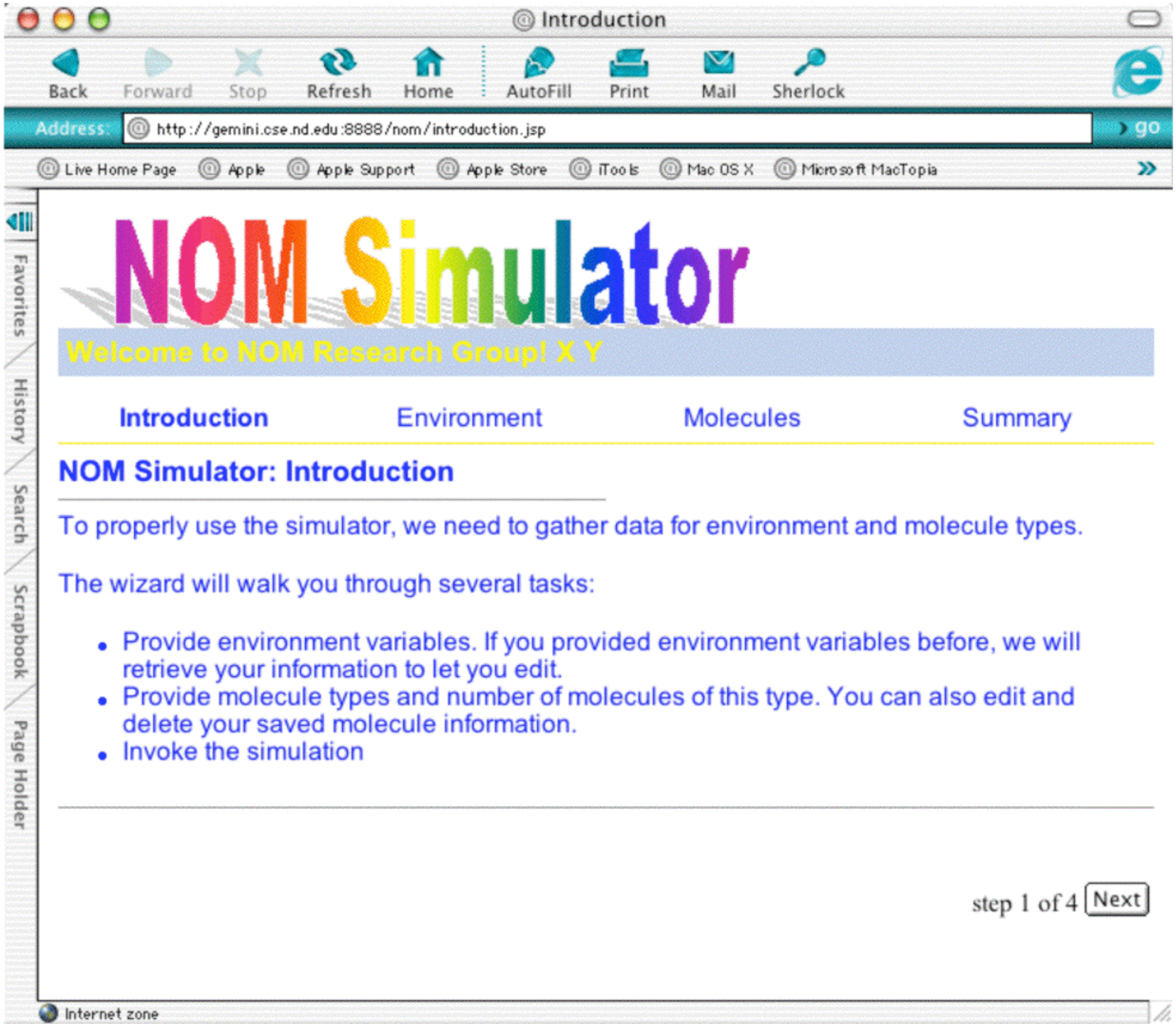
Userid:

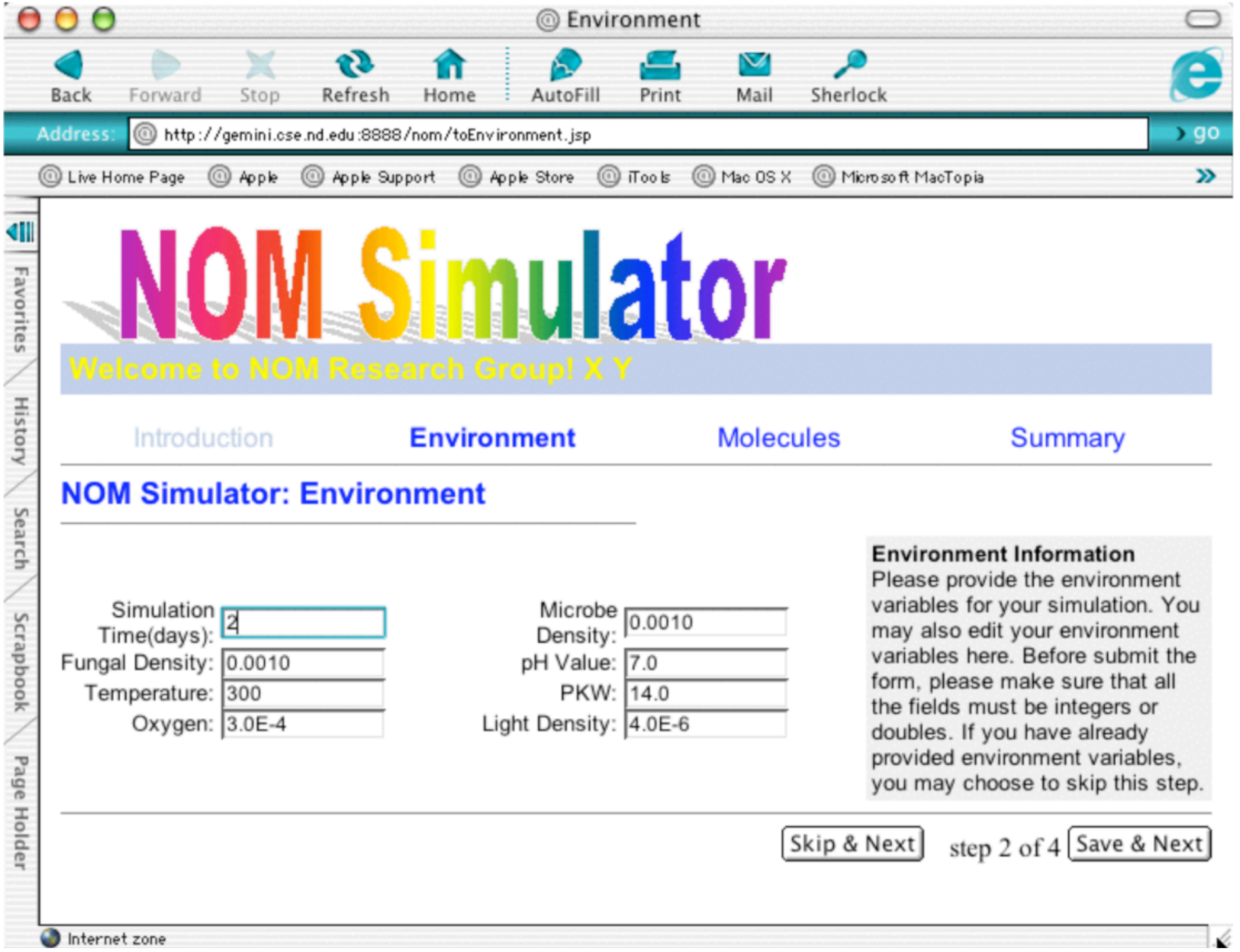
Password:

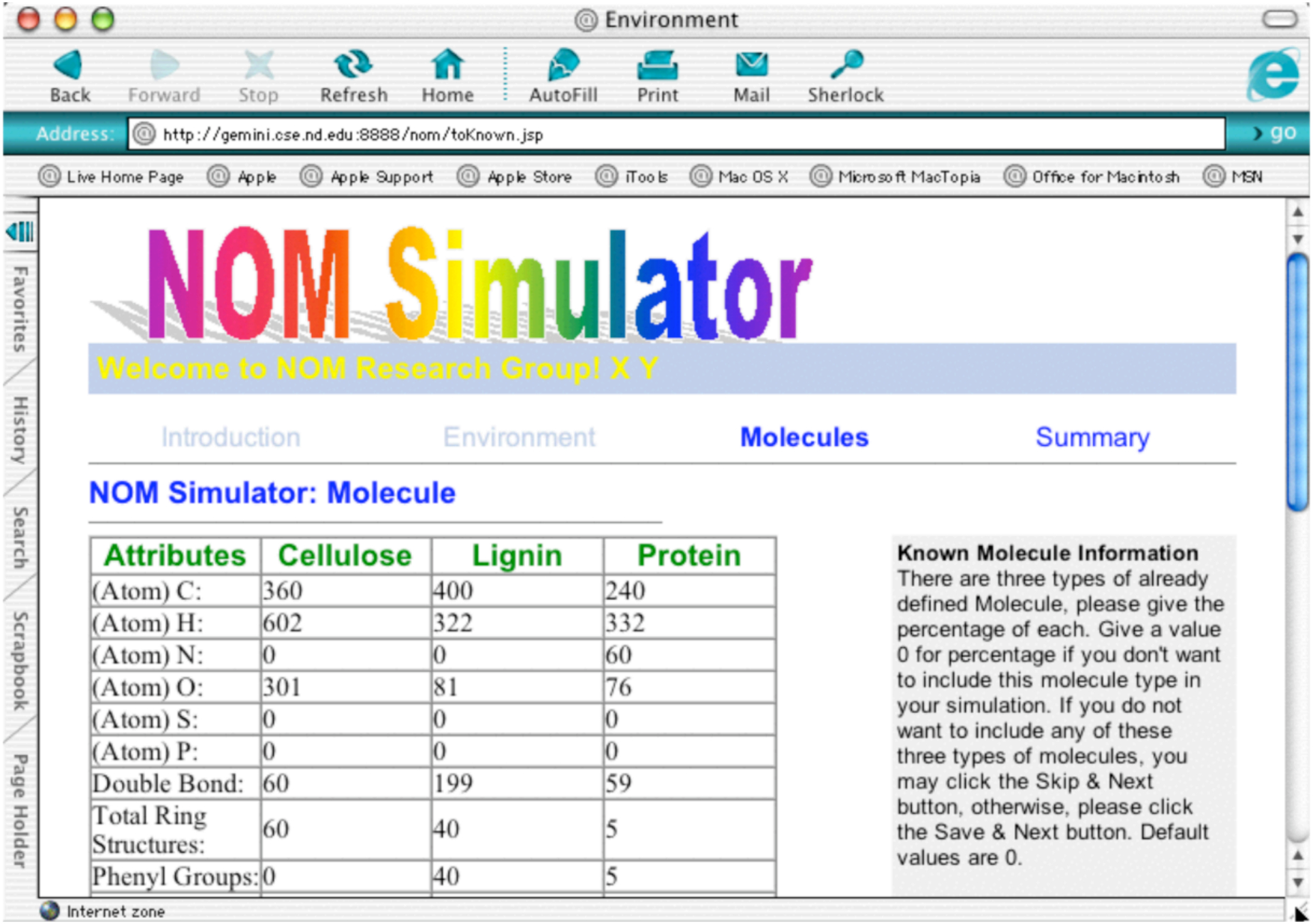
Sign In

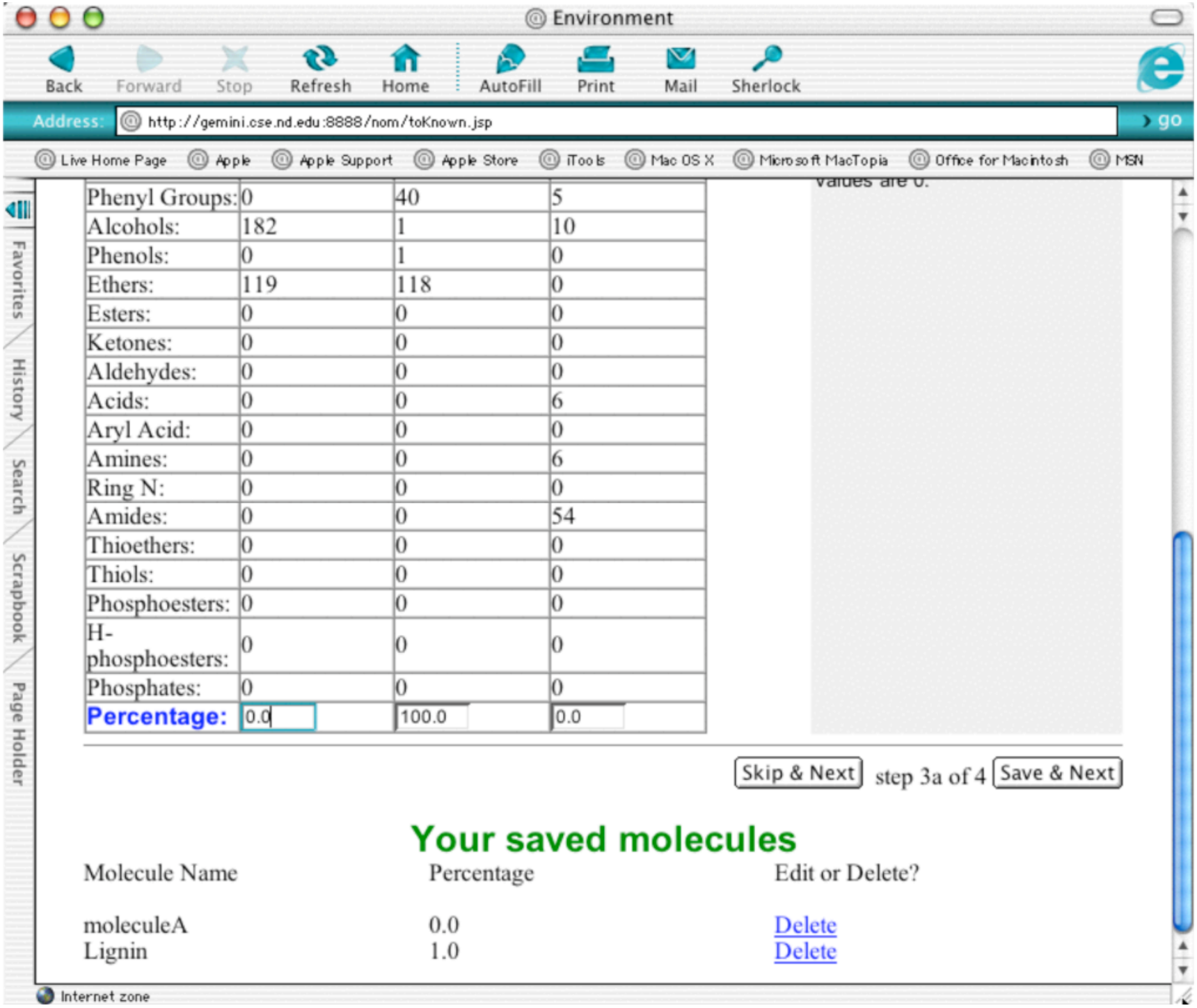
New users? Sign up now


Summary
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/login.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
NOM Simulator: Reports
Currently, you have the following sessions invoked. The first one is your most recent session. You can view reports for each session by click the following links. To start a new simulation, click here. To cleanup terminated sessions, click here.
Session 115: Terminate Session
Reactions Reports
Session 114: Terminate Session
Reactions Reports
Session 113: TERMINATED
Internet zone


Introduction
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/introduction.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
Environment
Molecules
Summary
NOM Simulator: Introduction
To properly use the simulator, we need to gather data for environment and molecule types.
The wizard will walk you through several tasks:
Provide environment variables. If you provided environment variables before, we will retrieve your information to let you edit.
Provide molecule types and number of molecules of this type. You can also edit and delete your saved molecule information.
Invoke the simulation
step 1 of 4
Next
Internet zone


Environment
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/toEnvironment.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
Environment
Molecules
Summary
NOM Simulator: Environment
Simulation Time(days): 2
Fungal Density: 0.0010
Temperature: 300
Oxygen: 3.0E-4
Microbe Density: 0.0010
pH Value: 7.0
PKW: 14.0
Light Density: 4.0E-6
Environment Information
Please provide the environment variables for your simulation. You may also edit your environment variables here. Before submit the form, please make sure that all the fields must be integers or doubles. If you have already provided environment variables, you may choose to skip this step.
Skip & Next
step 2 of 4
Save & Next
Internet zone


Environment
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/toKnown.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
Environment
Molecules
Summary
NOM Simulator: Molecule
Attributes
Cellulose
Lignin
Protein
(Atom) C:
360
400
240
(Atom) H:
602
322
332
(Atom) N:
0
0
60
(Atom) O:
301
81
76
(Atom) S:
0
0
0
(Atom) P:
0
0
0
Double Bond:
60
199
59
Total Ring Structures:
60
40
5
Phenyl Groups:
0
40
5
Known Molecule Information
There are three types of already defined Molecule, please give the percentage of each. Give a value 0 for percentage if you don't want to include this molecule type in your simulation. If you do not want to include any of these three types of molecules, you may click the Skip & Next button, otherwise, please click the Save & Next button. Default values are 0.
Internet zone


Environment
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/toKnown.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
Page Holder
values are 0.
Phenyl Groups: 0 40 5
Alcohols: 182 1 10
Phenols: 0 1 0
Ethers: 119 118 0
Esters: 0 0 0
Ketones: 0 0 0
Aldehydes: 0 0 0
Acids: 0 0 6
Aryl Acid: 0 0 0
Amines: 0 0 6
Ring N: 0 0 0
Amides: 0 0 54
Thioethers: 0 0 0
Thiols: 0 0 0
Phosphoesters: 0 0 0
H-phosphoesters: 0 0 0
Phosphates: 0 0 0
Percentage: 0.0 100.0 0.0
Skip & Next
step 3a of 4
Save & Next
Your saved molecules
Molecule Name
Percentage
Edit or Delete?
moleculeA 0.0 Delete
Lignin 1.0 Delete
Internet zone

NOM Simulator

Welcome to NOM Research Group! X Y

Introduction | Environment | **Molecules** | Summary

NOM Simulator: Molecule

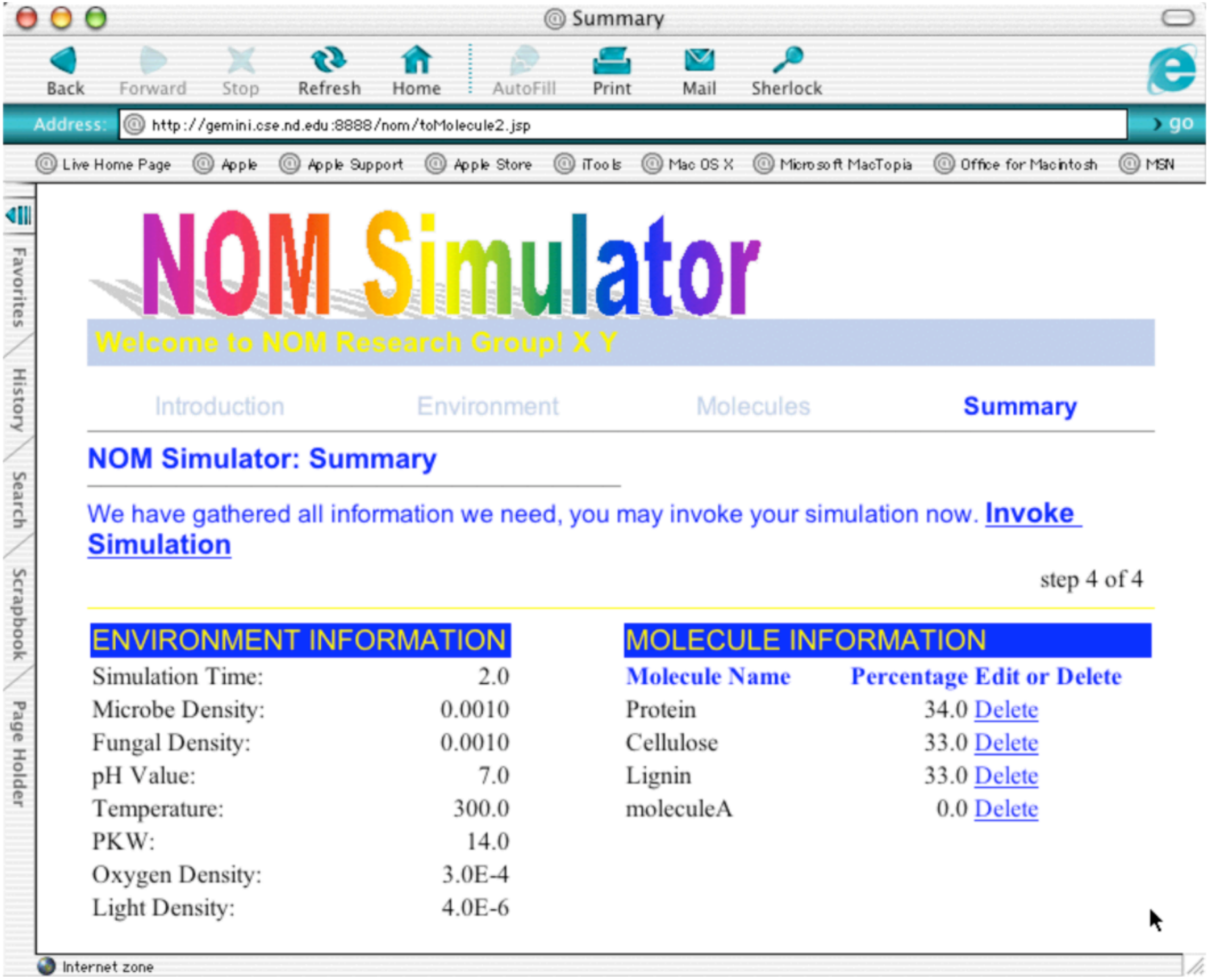
Molecule Name:	name	Percentage:	29.0
(Atom) C:	0	(Atom) H:	0
(Atom) N:	0	(Atom) O:	0
(Atom) S:	0	(Atom) P:	0

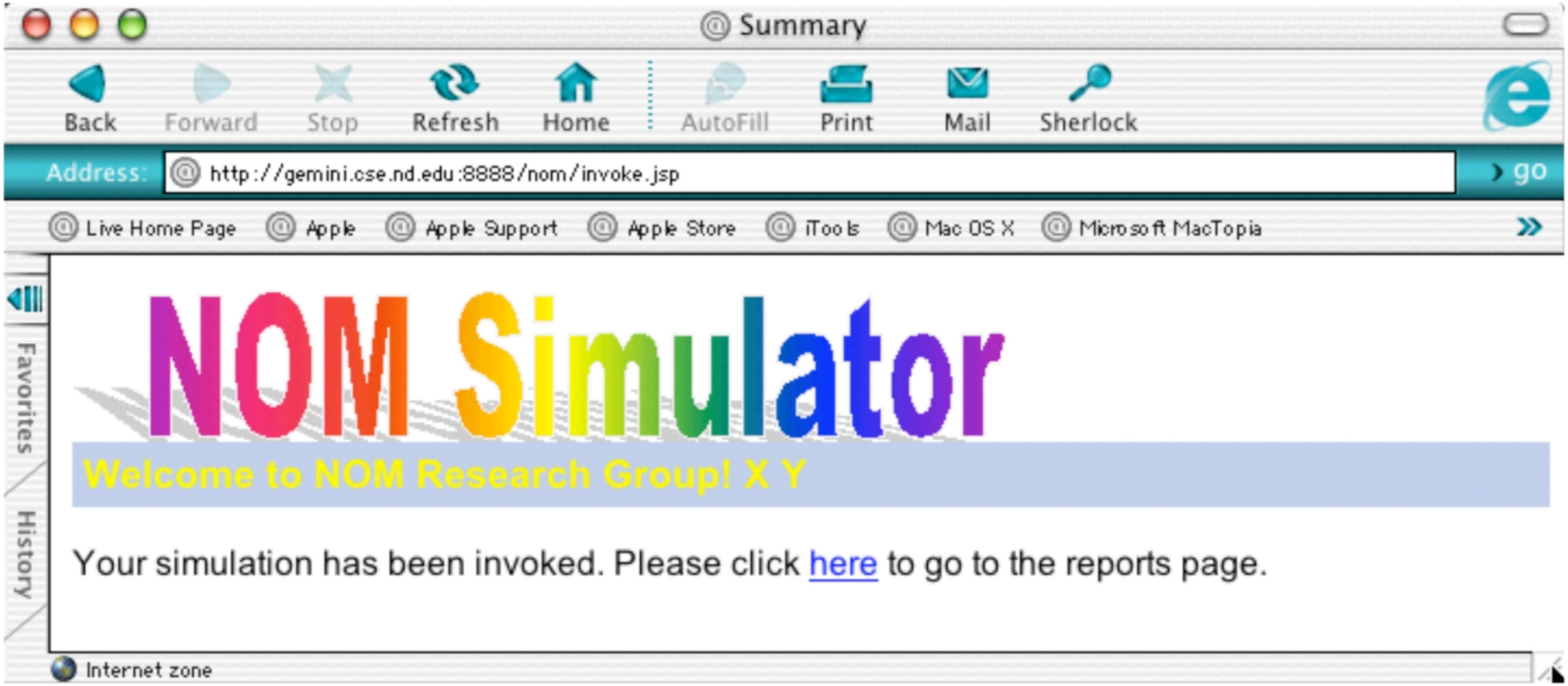
Molecule Information
Please provide molecule's name, percentage, number of atoms of molecules for your simulation. Please remember, except "Molecule Name", all fields should be integers or doubles. "Percentage" should be between 0 and 100.

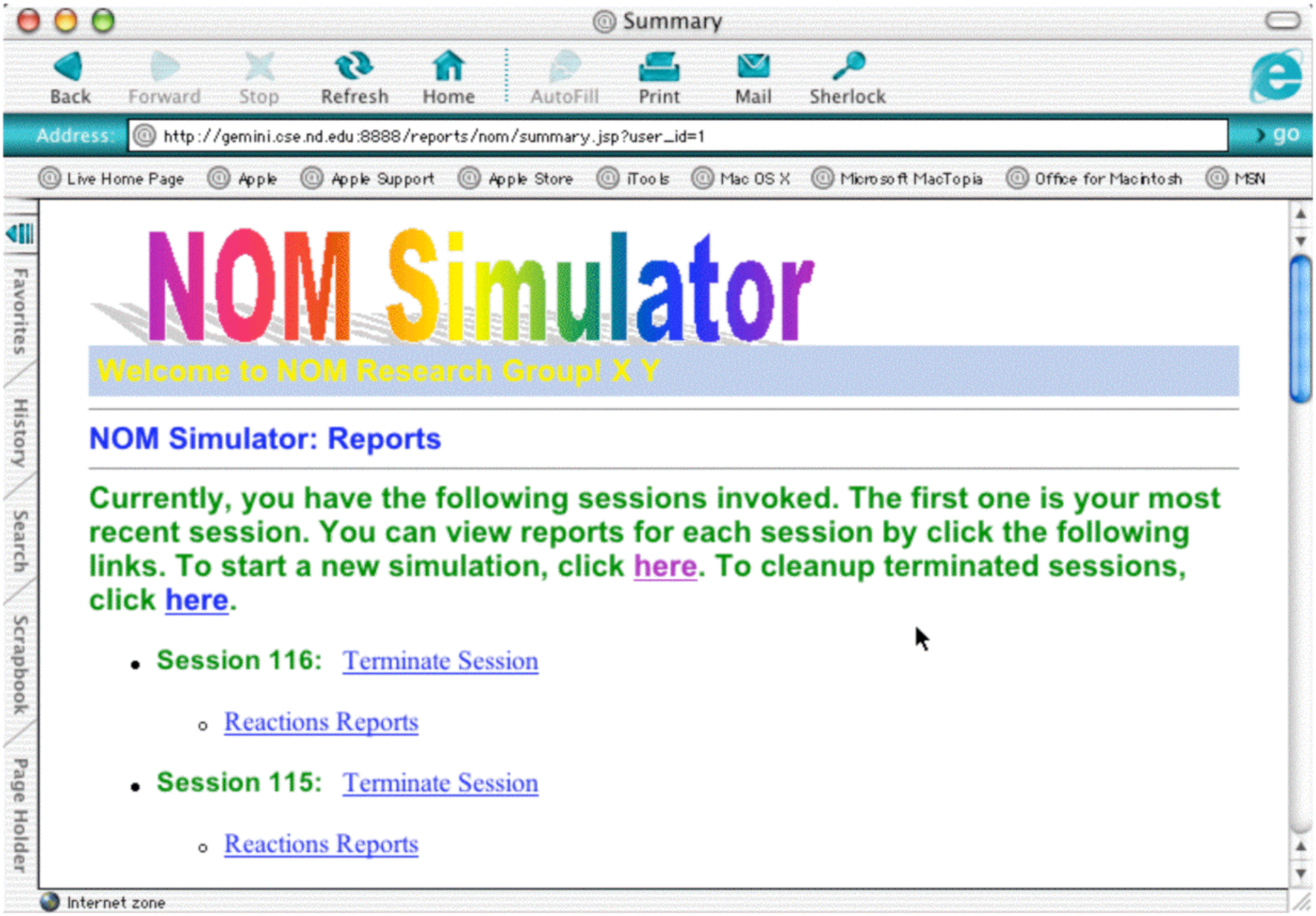
Doublebond:	0	Arylacids:	0
Rings:	0	Amines:	0
Phenyl:	0	RingN:	0
Alcohols:	0	Amides:	0
Phenols:	0	Thioethers:	0
Ethers:	0	Thiols:	0
Esters:	0	Phosphoesters:	0
Ketones:	0	HPhosphoesters:	0
Aldehydes:	0	Phosphates:	0
Acids:	0		

Functional Groups
Please provide a number for each functional group. Default value is 0.

step 3b of 4 Save & Next


Summary
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/toMolecule2.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
Environment
Molecules
Summary
NOM Simulator: Summary
We have gathered all information we need, you may invoke your simulation now. Invoke Simulation
step 4 of 4
ENVIRONMENT INFORMATION
Simulation Time: 2.0
Microbe Density: 0.0010
Fungal Density: 0.0010
pH Value: 7.0
Temperature: 300.0
PKW: 14.0
Oxygen Density: 3.0E-4
Light Density: 4.0E-6
MOLECULE INFORMATION
Molecule Name
Percentage
Edit or Delete
Protein 34.0 Delete
Cellulose 33.0 Delete
Lignin 33.0 Delete
moleculeA 0.0 Delete
Internet zone


Summary
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/invoke.jsp
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Favorites
History
NOM Simulator
Welcome to NOM Research Group! X Y
Your simulation has been invoked. Please click here to go to the reports page.
Internet zone

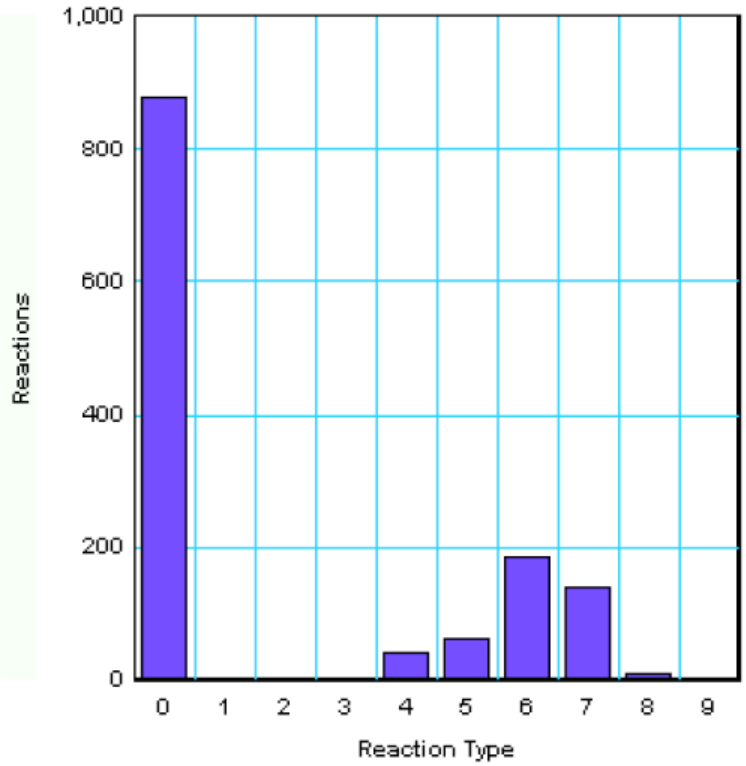

Summary
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/reports/nom/summary.jsp?user_id=1
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
Page Holder
NOM Simulator
Welcome to NOM Research Group! X Y
NOM Simulator: Reports
Currently, you have the following sessions invoked. The first one is your most recent session. You can view reports for each session by click the following links. To start a new simulation, click here. To cleanup terminated sessions, click here.
Session 116: Terminate Session
Reactions Reports
Session 115: Terminate Session
Reactions Reports
Internet zone

NOM Simulator

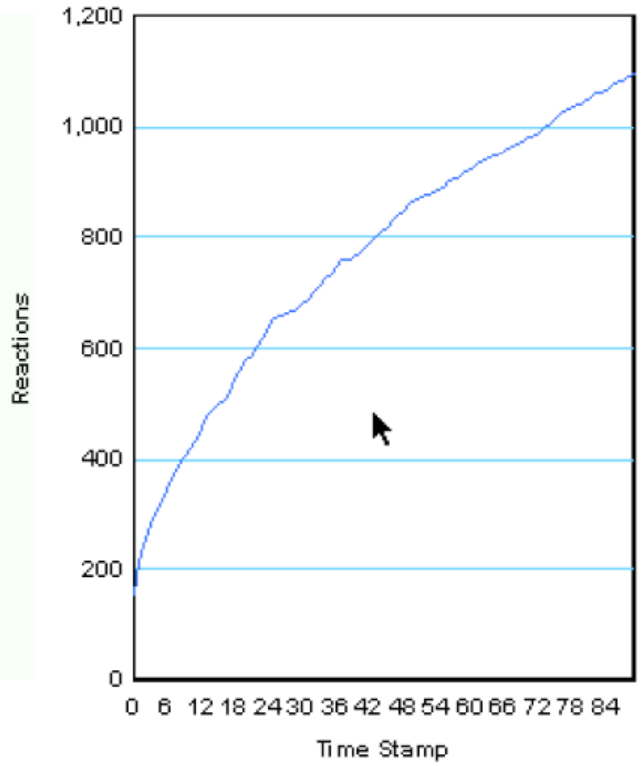
Welcome to NOM Research Group! X Y

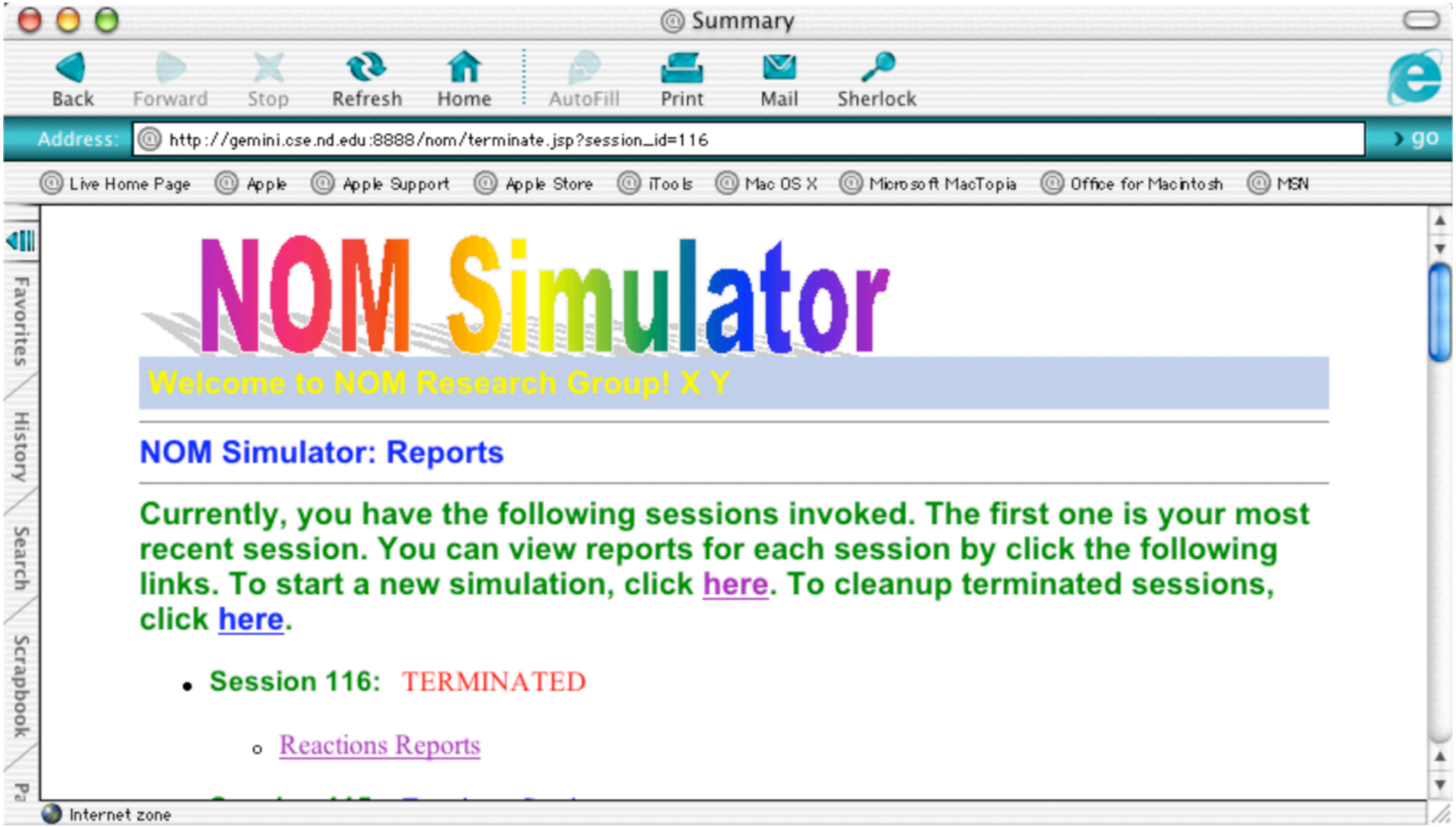
NOM Simulator: Reports

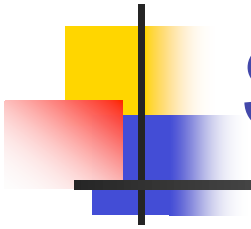
Reactions By Type



Reactions vs Time




Summary
Back
Forward
Stop
Refresh
Home
AutoFill
Print
Mail
Sherlock
Address:
http://gemini.cse.nd.edu:8888/nom/terminate.jsp?session_id=116
go
Live Home Page
Apple
Apple Support
Apple Store
iTools
Mac OS X
Microsoft MacTopia
Office for Macintosh
MSN
Favorites
History
Search
Scrapbook
NOM Simulator
Welcome to NOM Research Group! X Y
NOM Simulator: Reports
Currently, you have the following sessions invoked. The first one is your most recent session. You can view reports for each session by click the following links. To start a new simulation, click here. To cleanup terminated sessions, click here.
Session 116: TERMINATED
Reactions Reports
Internet zone



Summary

- Work in progress
- Complexity Perspective
- Middle computational approach
- Agent-Based Modeling approach
- Stochastic (Monte Carlo based simulation)
- NOM Molecules & Microbes as Agents
- Web-based Databases, Data warehouse, Visualization, Database Queries, Data Mining
- Web-based Collaboratory for NOM Research