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

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Overview

- Modeling of Complexity
- Stochastic Simulation of Natural Organic Matter (NOM) and Environmental/Microbial Interactions
- Another study (NSF - CISE/IIS)
  - Agent-Based Model of the Open Source Software (OSS) Development Phenomenon

Simulation of NOM and Microbial-Environmental Interactions

- Funded in part by NSF-ITR (DEB)
  - Co-PIs
    - Robert Wershaw, USGS-Denver
    - Jerry Leenheer, USGS-Denver
    - Patricia Maurice, Geological Sciences, ND
      - USGS - 5 years, New Jersey
    - Steve Cabaniss, Chemistry, UNM
    - Robert Wetzel, Biology, UNC-Chapel Hill
  - Students
    - Yingping Huang, CSE, (MS Thesis)
    - Xiaorong Xiang, CSE, (MS Thesis)
    - Eric Chanwich, CSE, REU

My Definition …. and Inspiration

- 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

- Entities (Often Many & Heterogeneous)
- Entity Behaviors
- Interactions Between Entities Including Feedback (Possibly Nonlinear)
- Often Sensitive Dependence to Initial Conditions
- Self-Organization (Self-Assembly?)
- Emergence

Understanding Complex Systems

- Parts versus the Whole
  - Limitations of the Reductionist Approach
- Sensitive Dependence on Initial Conditions
  - Limits to Predictability
- Understand the Properties of the System
  - Stability
  - Periodicity
  - Chaotic
  - Bounded/Unbounded
  - System Behaviors, Processes, Mechanisms, and Interactions

Modeling Complex Systems

- Mathematical Analysis
  - Stochastic Analysis
- Computer Simulation (Computational “x”)
  - Iteration/Recursion
  - Numerical Methods
- Computer Simulation (Bottom-up Modeling)
  - Discrete-Event
  - Agent-Based Modeling (includes CA)
- Very Large Computer Databases
  - Sensor Arrays, NanoSensors, Data Warehouses
  - Data Mining and Knowledge Discovery

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
  - Instantiate (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
  - 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)

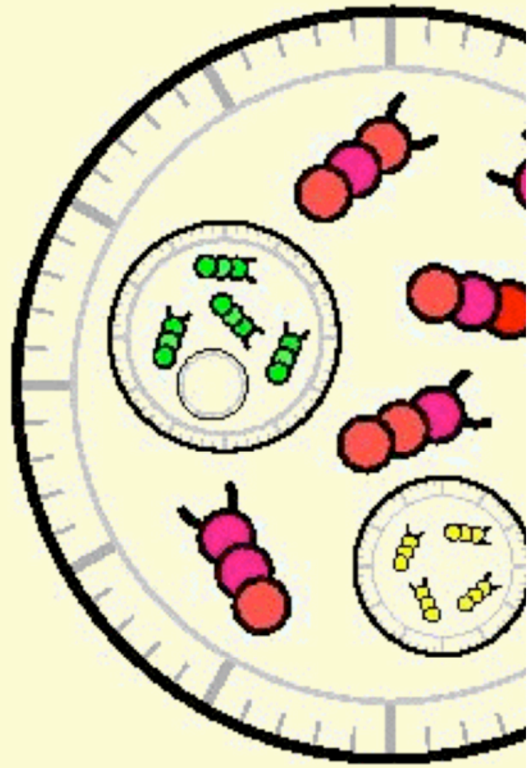
SWARM

- 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

SDG
www.swarm.org

SWARM 2003

Meeting Announcement



Seventh Annual Swarm Users/
Researchers Meeting

Notre Dame, Indiana USA

April 13 - 15, 2003

- The Registration Page will be available shortly.
- Mark your calendars!
- Call for papers, tutorials, and posters!

The Department of Computer Science & Engineering at the University of Notre Dame, and the Development Group (SDG) are pleased to announce the **Seventh Annual SWARM Users/R** **Meeting** to be held on the campus of the University of Notre Dame, on April 13-15, 2003.

At **Swarm 2003**, scientists, modellers, and programmers working in a wide variety of domains opportunity to share their research, knowledge and experience with multi-agent modelling inclu restricted to) the Swarm simulation system. The Swarm Development Group also uses the meet determine future development priorities, so come and tell us what's on your mind! The meeting section of the community, historically including content suitable for both inexperienced and exp and researchers.

Simulation of NOM and Microbial-Environmental Interactions

- NSF - ITR - Division of Environmental Biology
- Interdisciplinary project
  - Chemist
  - Geomicrobiologist
  - Biologist
  - Ecologist
  - Computer Scientist
- Stochastic Simulation of Environmental Transformations of Natural Organic Matter
  - In soil
  - In solution

Natural Organic Matter

- Ubiquitous in terrestrial, aquatic and marine ecosystems
- Important role in compositional evolution and fertility of soil
- Impacts mobility and transport of pollutants, e.g., trace metals, radionuclides and hydrophobic organic compounds
- Impacts availability of nutrients for microorganisms and plant communities
- Impacts growth and dissolution of minerals

Natural Organic Matter (cont)

Hardwood
Swamp

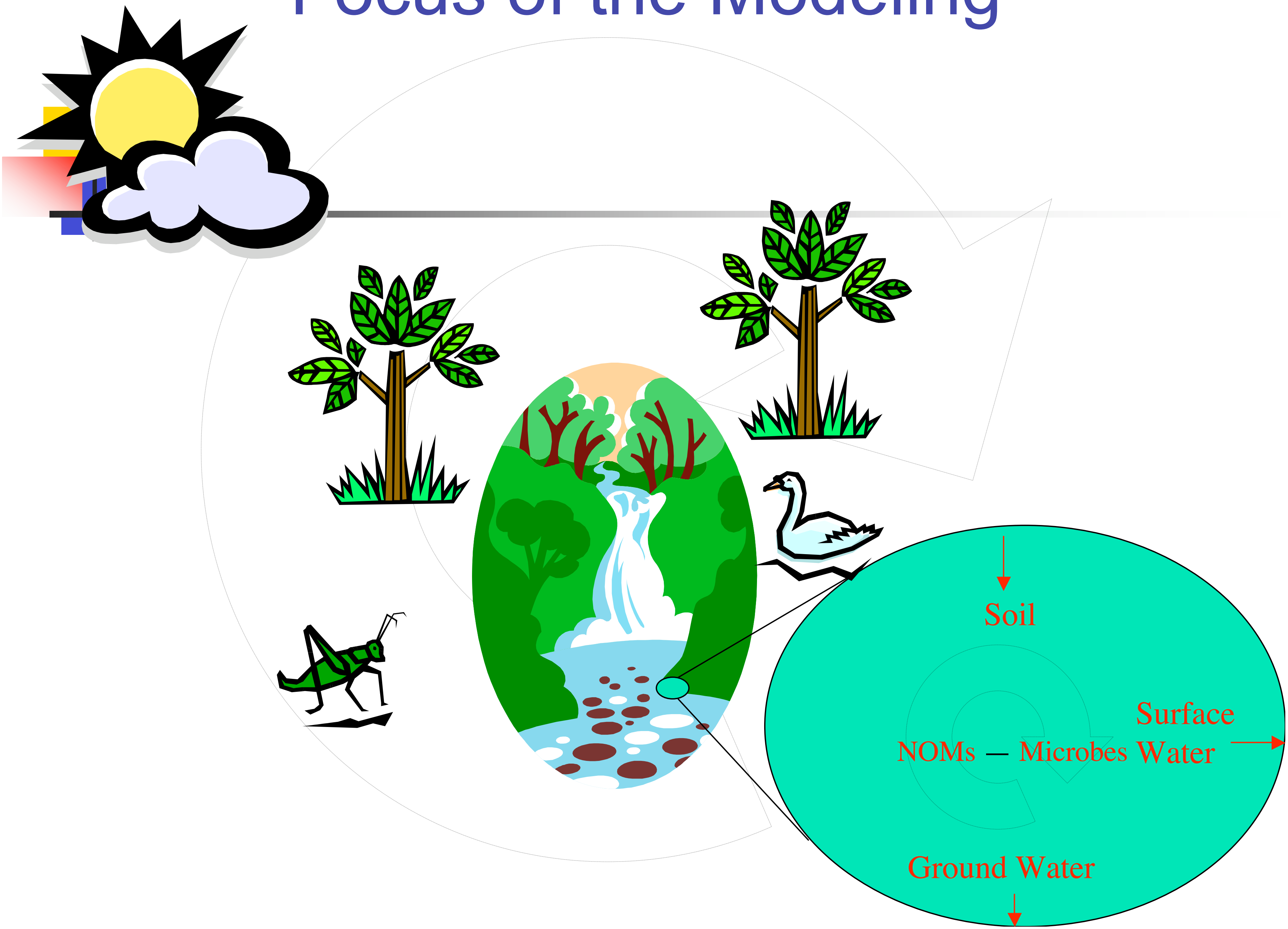
Natural Organic Matter (cont)

Open
Channel

Natural Organic Matter (cont)

Cedar Swamp

Focus of the Modeling



Background

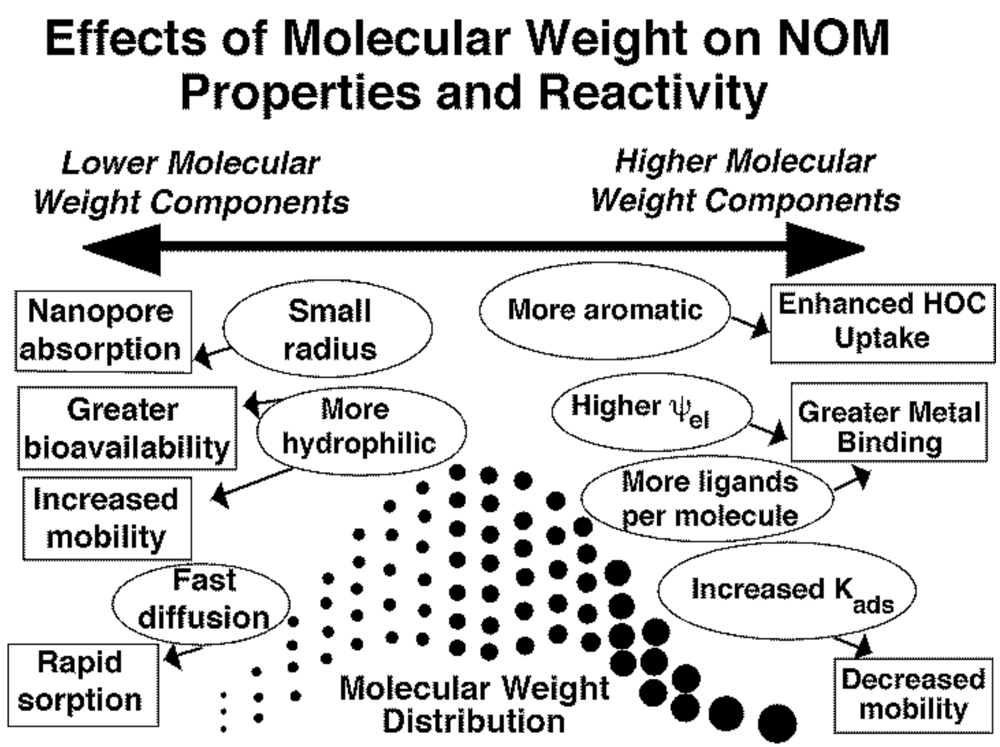
- Compositional evolution of NOM is an interesting problem
- Important aspect of predictive environmental modeling
- Prior modeling work is often too simplistic to represent the heterogeneous structure of NOM and its complex behaviors in ecosystems (e.g., carbon cycling models), also …
- Prior modeling work is 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

- Stochastic model of NOM evolution — middle computational approach
  - Algorithms
  - Parameters
- Represent individual molecules as discrete objects with
  - Specified elemental and functional group composition
  - Size/weight
  - Reactivity
- Model the evolution of NOM from biological precursor compounds
  - Lignins
  - Polysaccharides
  - Proteins
- Deploy web-based simulation for testing, feedback and usage
- Generate experimentally testable predictions about NOM evolution and properties - validation of simulation

Generate Experimentally Testable Predictions about NOM Evolution and Properties

Molecular weight is a key property controlling the reactivity of NOM.



(From Cabaniss et al., 2000)

Modeling

- Molecules and microbes are objects
- Molecules and microbes have attributes
  - Heterogeneous, distributions
  - Currently 1,000 objects, preferably 10,000 or 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
    - Polynucleotinde, tannin, lignin, polyterpene, cutin
  - Smaller molecules
    - Phospholipids
    - Sugars
    - Amino acids
    - Flavinoids
    - Quinoines
  - Microbes

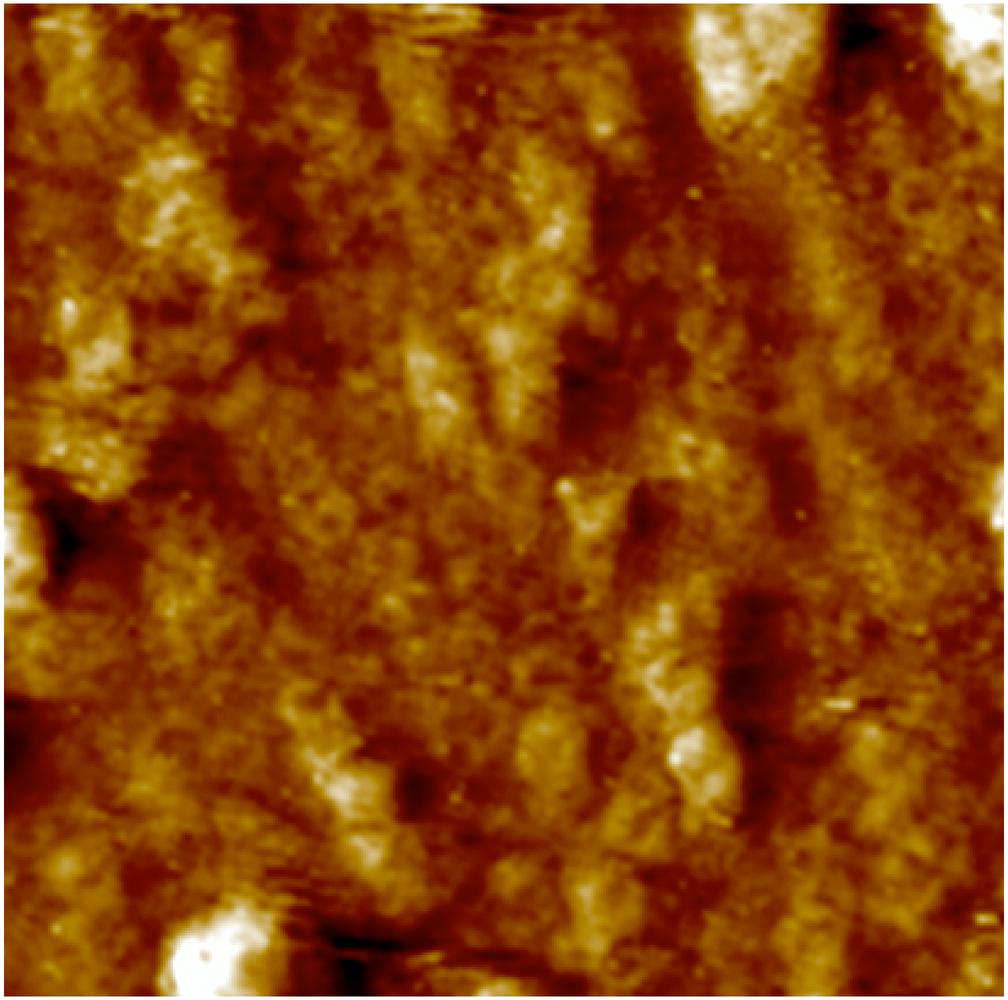
Modeling (cont)

- 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

AFM Image of NOM Adsorbtion



NOM
Rings

Maurice, 1999

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

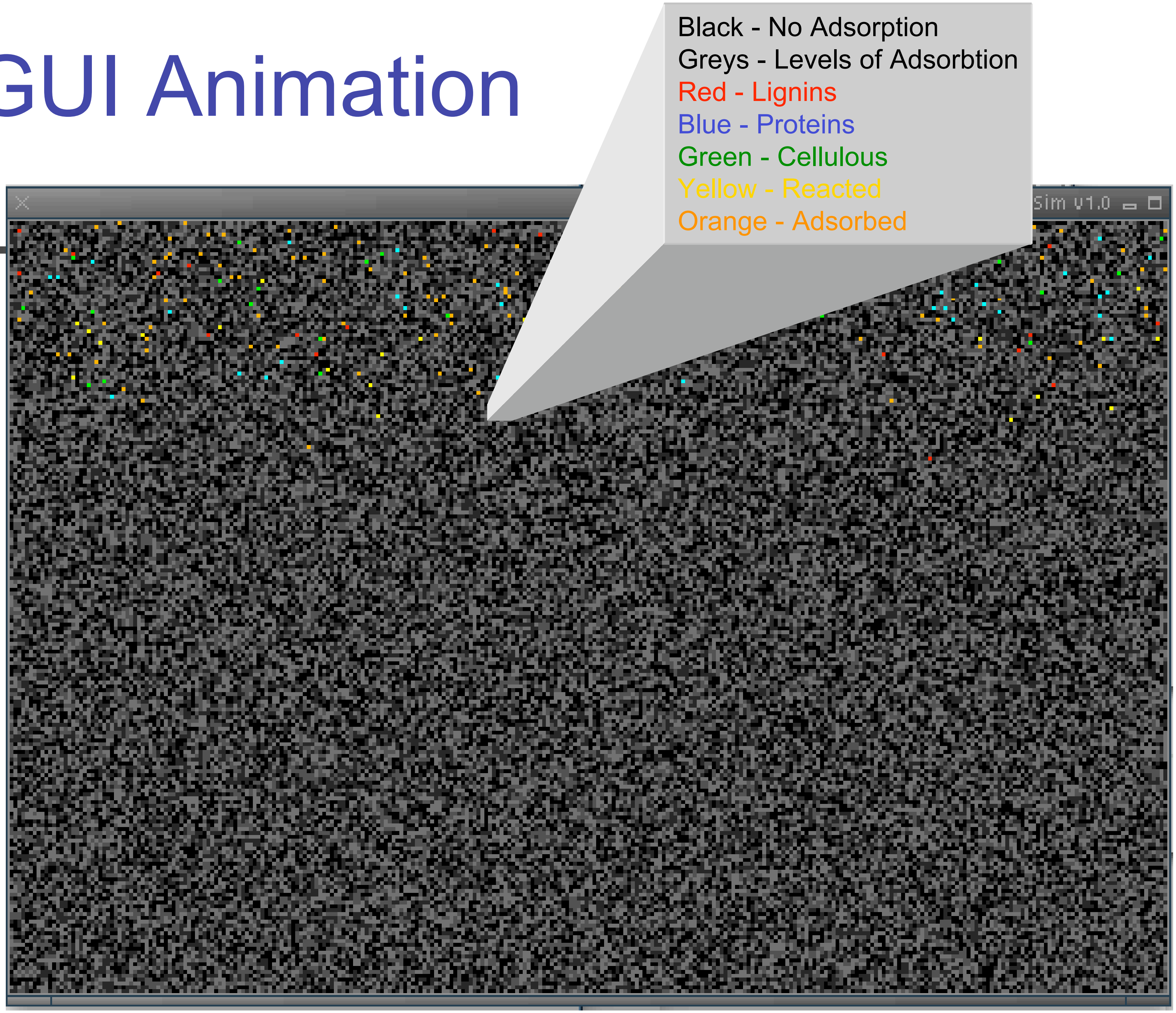
Modeling (cont)

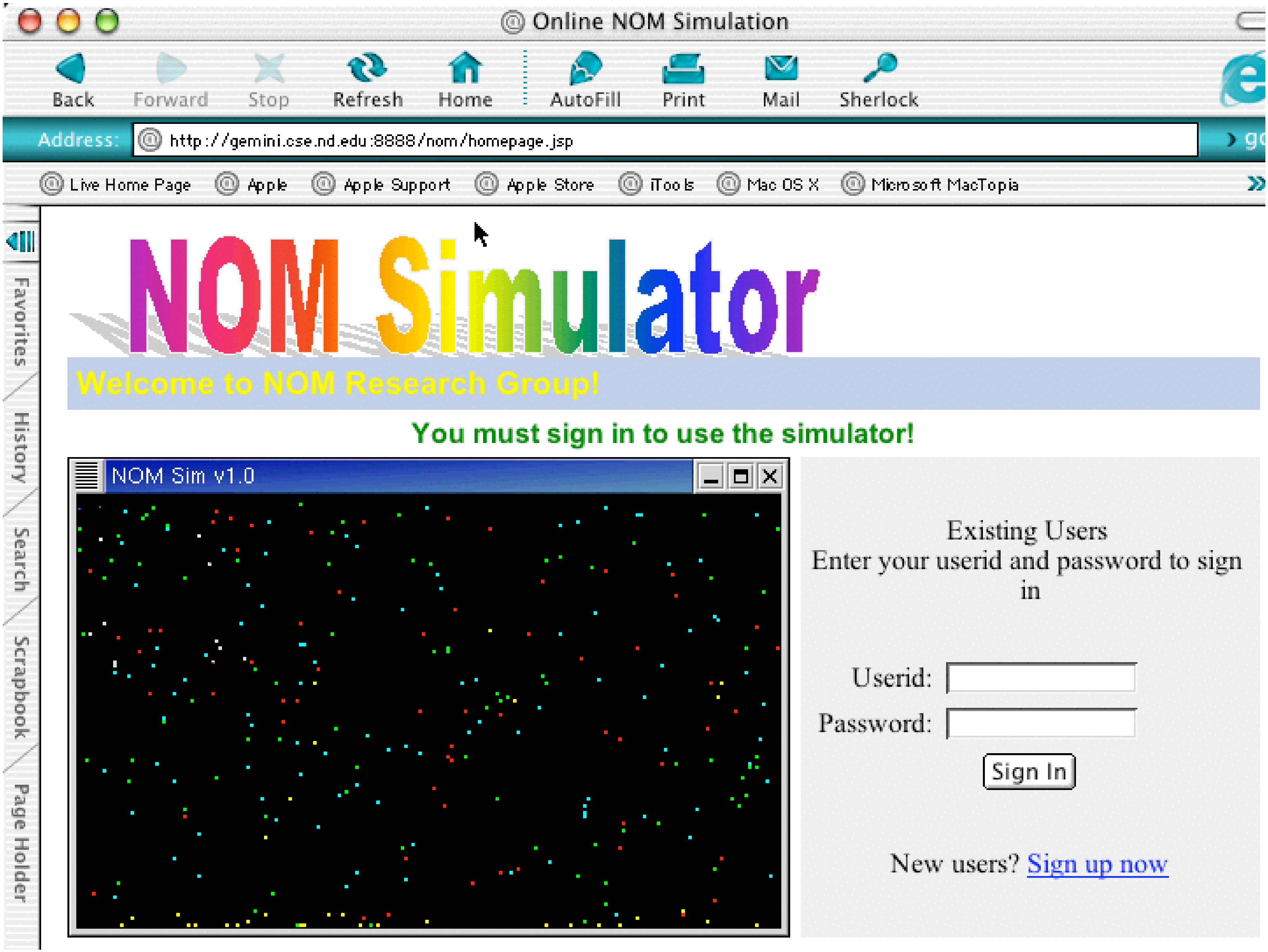
- Environmental parameters
  - Temperature
  - pH
  - Light intensity
  - Metal concentrations (e.g., Al(III) and Fe)
  - Bacterial activity
  - Water flow rate/pressure gradient
  - Surface area

NOM 1.0

- GUI Version - Stand Alone
  - Simulation and Animation of Molecules
- Web-Based Collaboratory
  - Standard Browser Interface
    - HTML Forms / JSP
    - Java Servlets
    - JDBC - Oracle Database
    - Oracle Forms and Reports
  - Model Development
  - Shared Data and Simulations
  - Collaboration Support

GUI Animation

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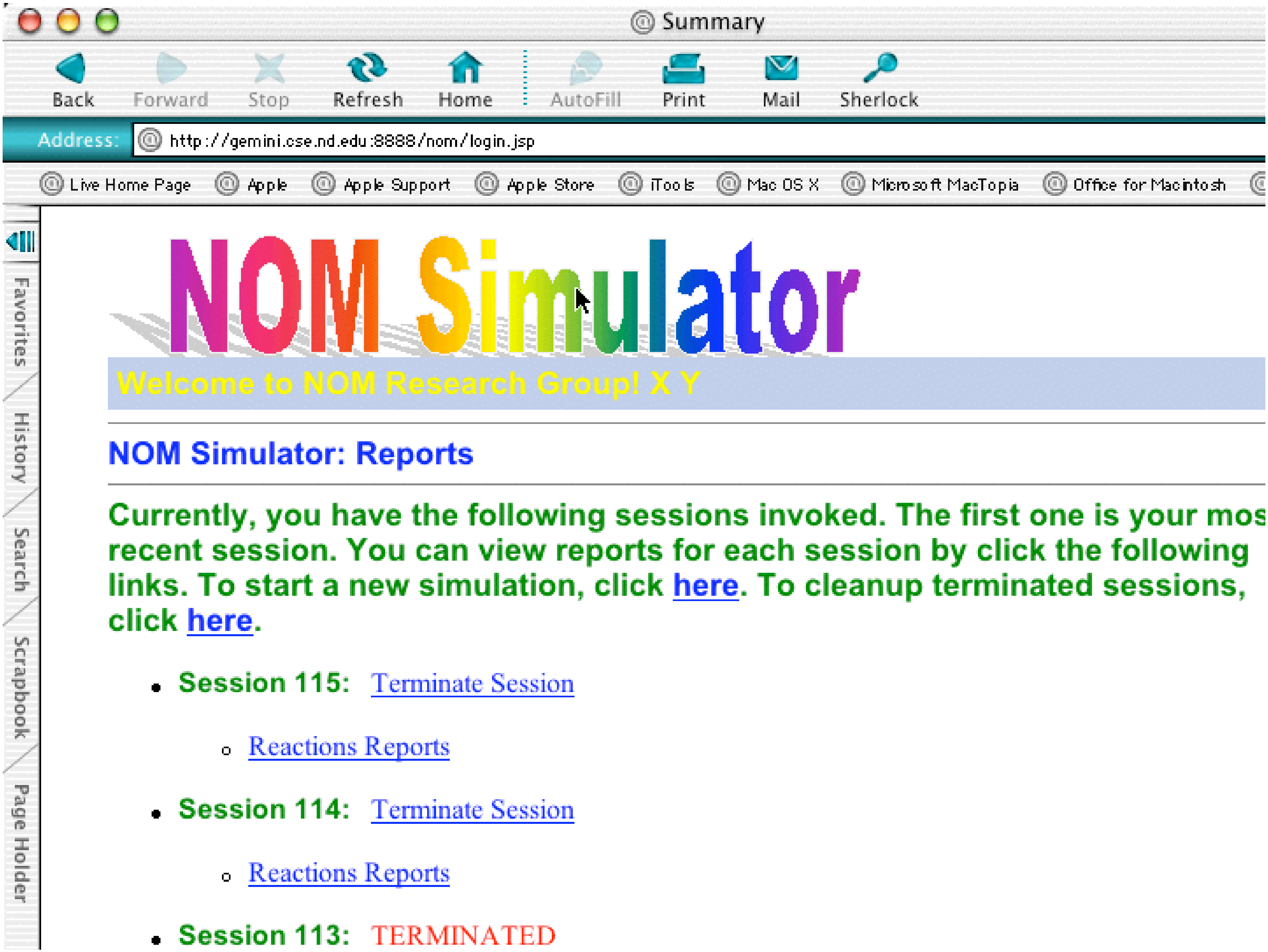
Welcome to NOM Research Group!
You must sign in to use the simulator!
NOM Sim v1.0
Existing Users
Enter your userid and password to sign in
Userid:
Password:
Sign In
New users? Sign up now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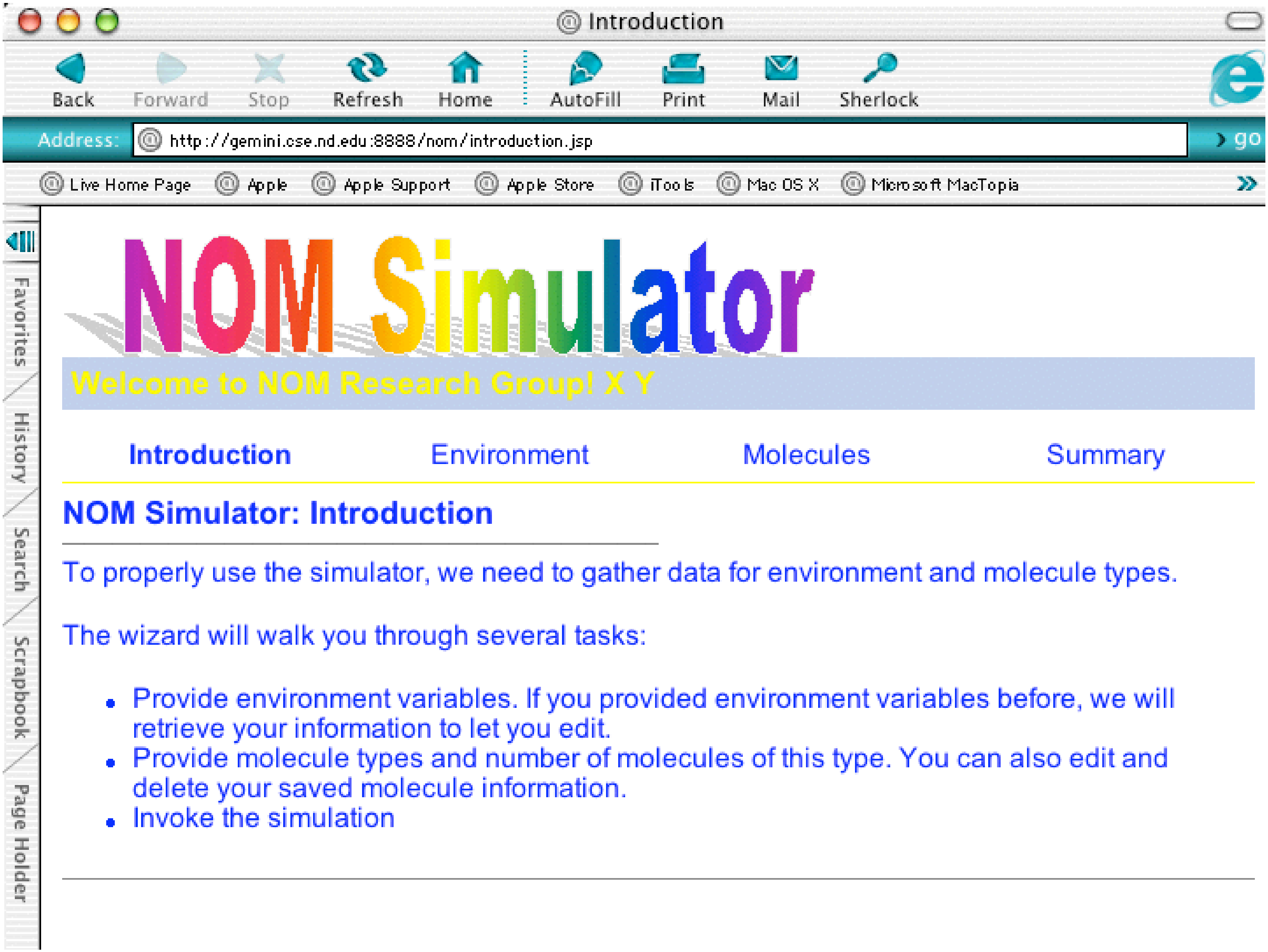
Session 115: Terminate Session
Reactions Reports
Session 114: Terminate Session
Reactions Reports
Session 113: TERMINATED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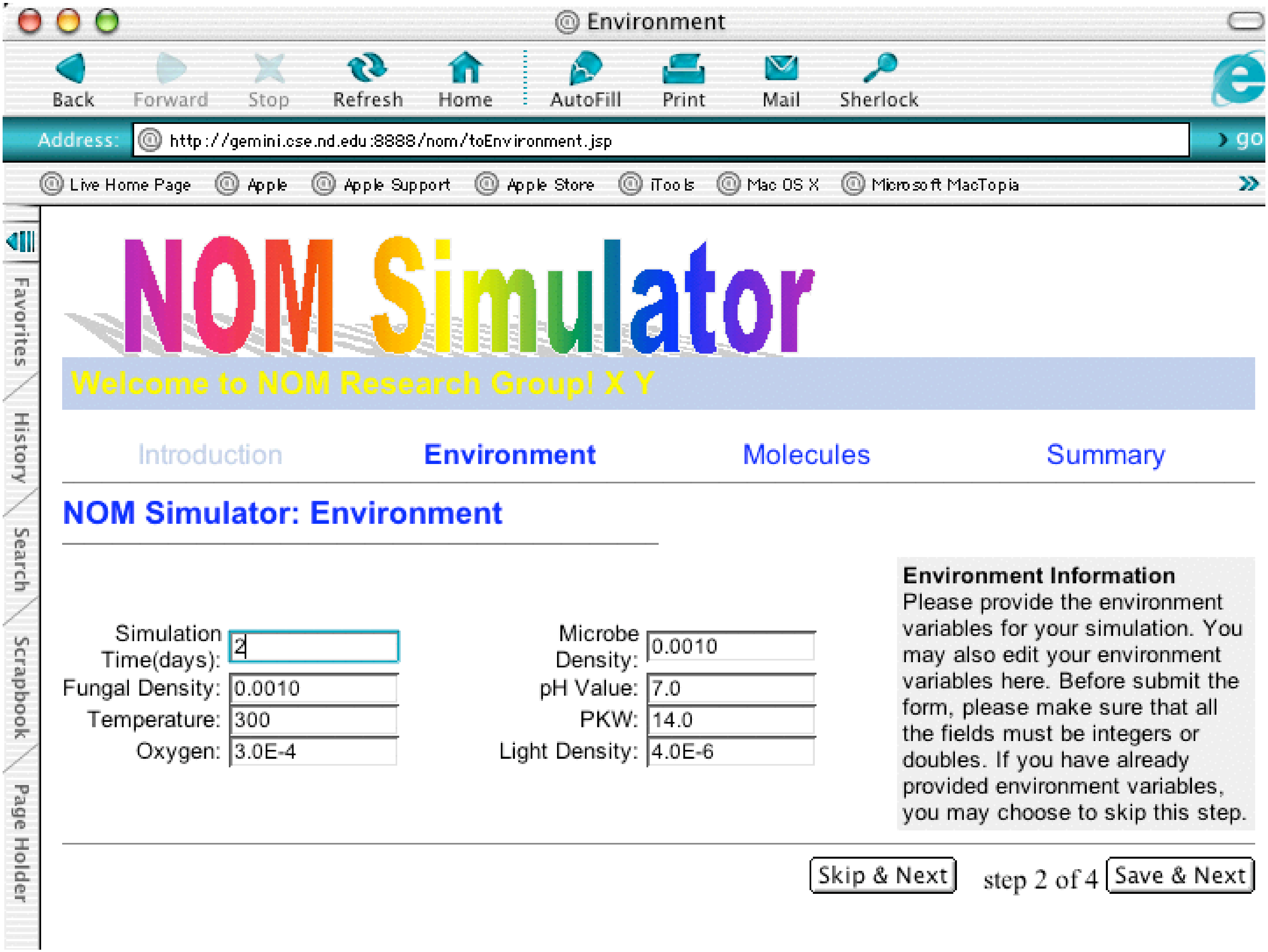
NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
Environment
Molecules
Summary
NOM Simulator: Introduction
To properly use the simulator, we need to gather data for environment and molecule types.
The wizard will walk you through several tasks:
Provide environment variables. If you provided 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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NOM Simulator
Welcome to NOM Research Group! X Y
Introduction
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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

Environment

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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.

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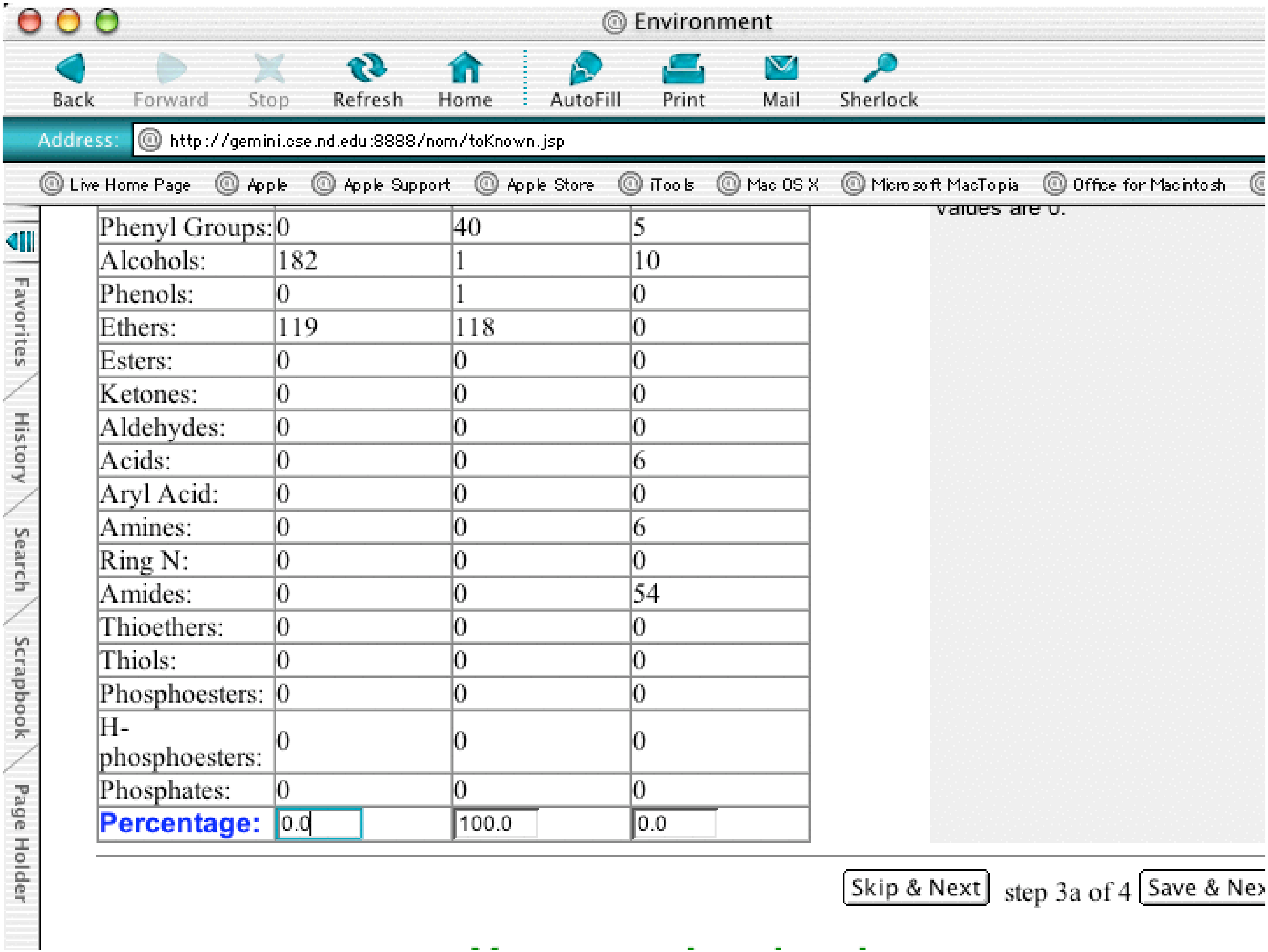

Phenyl Groups:	0	40	5
Alcohols:	182	1	10
Phenols:	0	1	0
Ethers:	119	118	0
Esters:	0	0	0
Ketones:	0	0	0
Aldehydes:	0	0	0
Acids:	0	0	6
Aryl Acid:	0	0	0
Amines:	0	0	6
Ring N:	0	0	0
Amides:	0	0	54
Thioethers:	0	0	0
Thiols:	0	0	0
Phosphoesters:	0	0	0
H-phosphoesters:	0	0	0
Phosphates:	0	0	0
Percentage:	0.0	100.0	0.0

NOM Simulator

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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 na
percentage, number of atoms
molecules for your simulatior
Please remember, except
"Molecule Name", all fields
should be integers or doubles
"Percentage" should be betw
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
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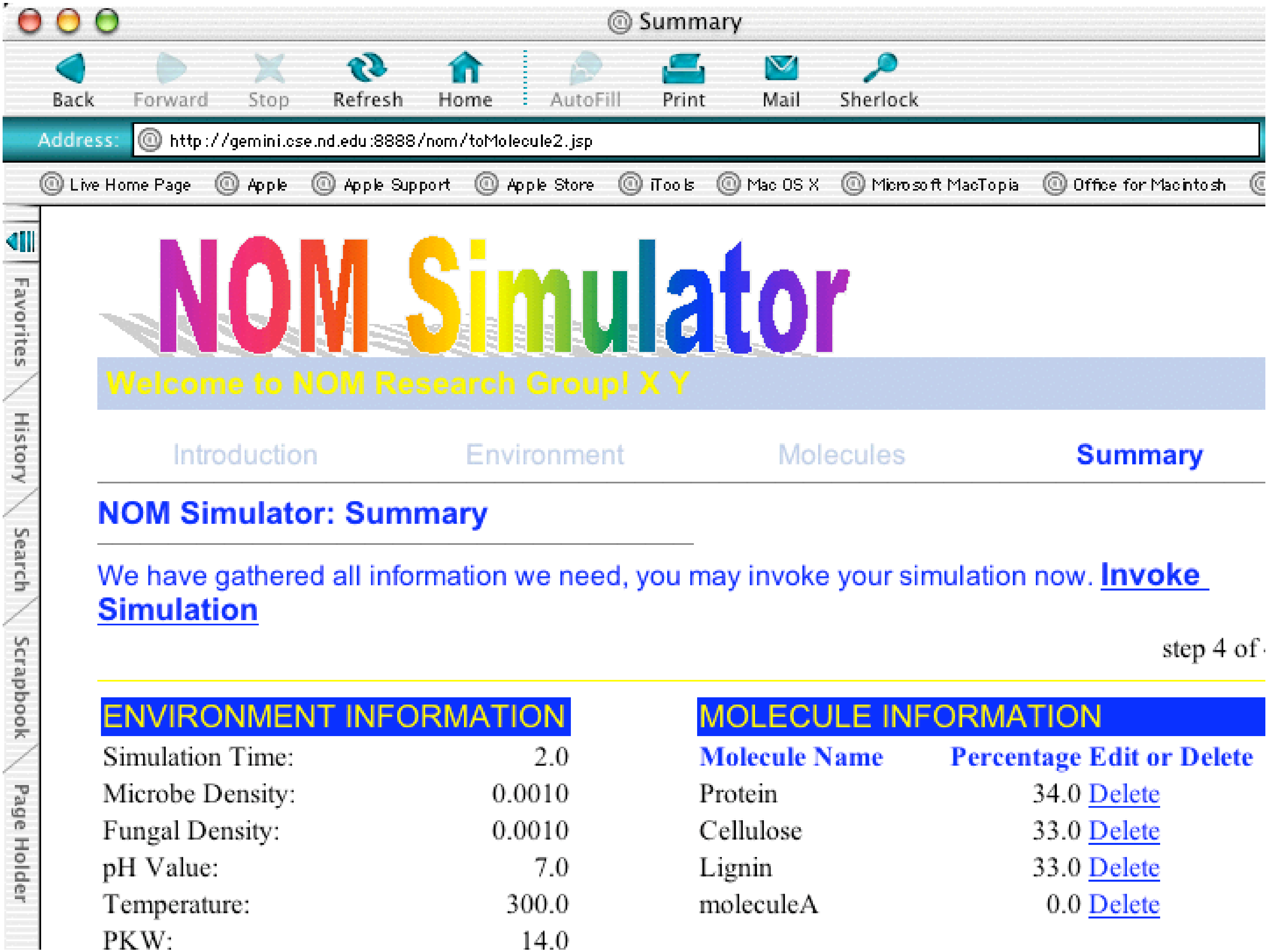
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We have gathered all information we need, you may invoke your simulation now. Invoke Simulation
step 4 of
ENVIRONMENT INFORMATION
Simulation Time: 2.0
Microbe Density: 0.0010
Fungal Density: 0.0010
pH Value: 7.0
Temperature: 300.0
PKW: 14.0
MOLECULE INFORMATION
Molecule Name
Percentage
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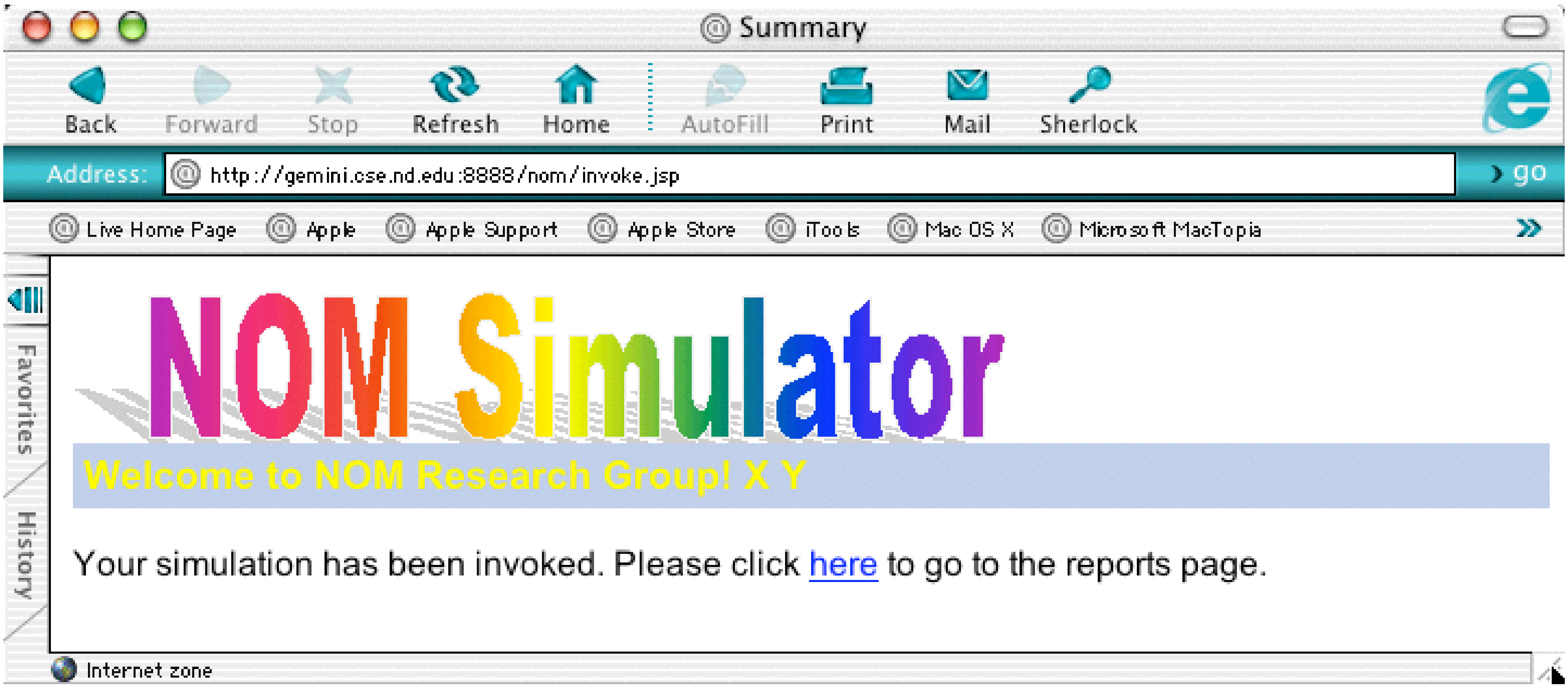
Protein 34.0 Delete
Cellulose 33.0 Delete
Lignin 33.0 Delete
moleculeA 0.0 Delete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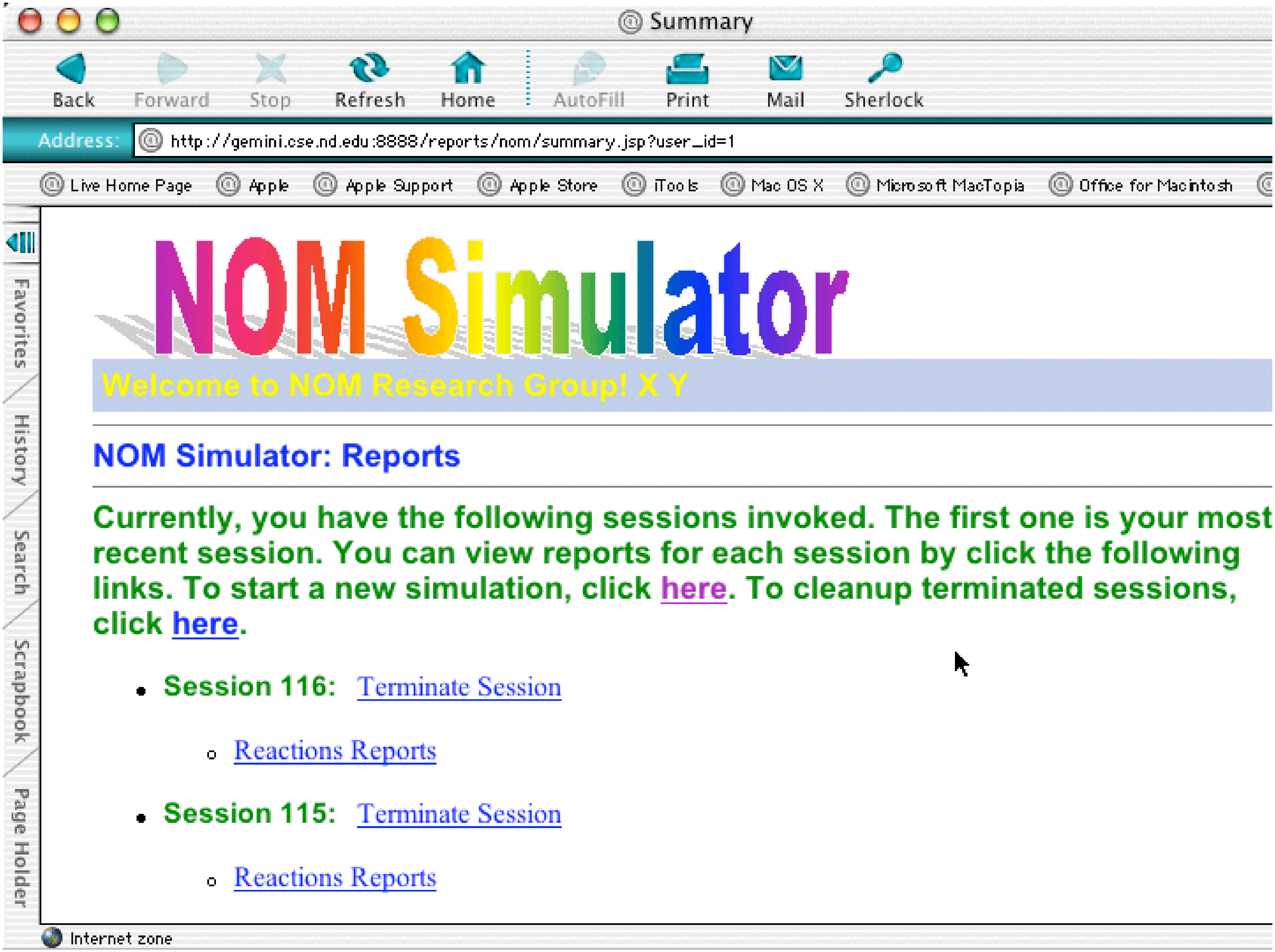
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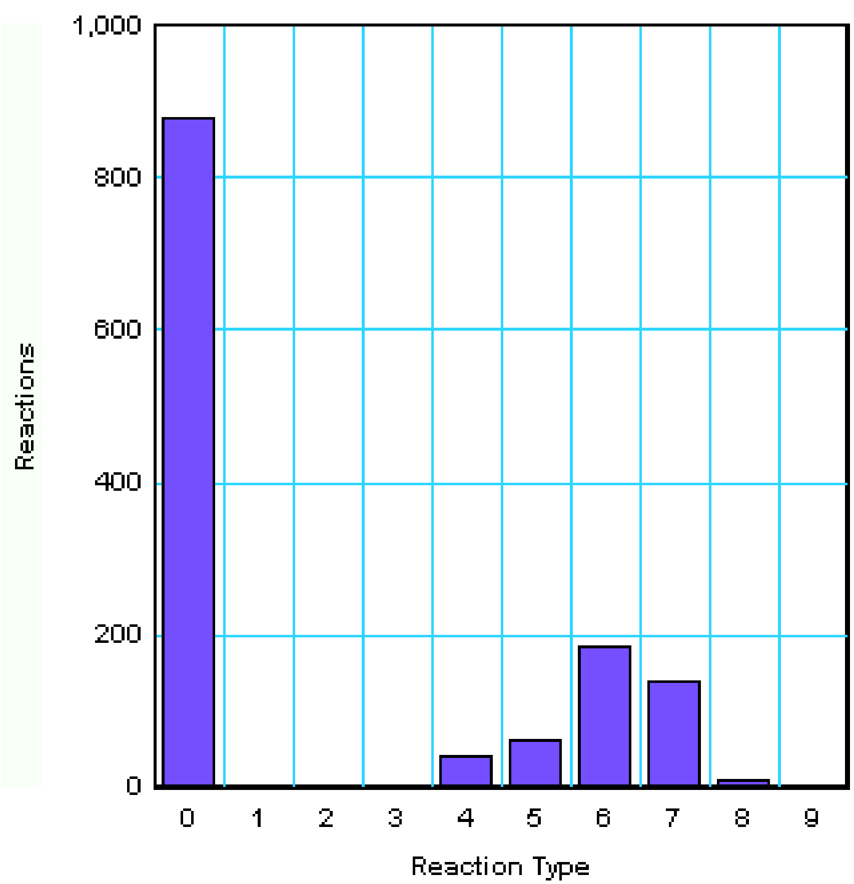
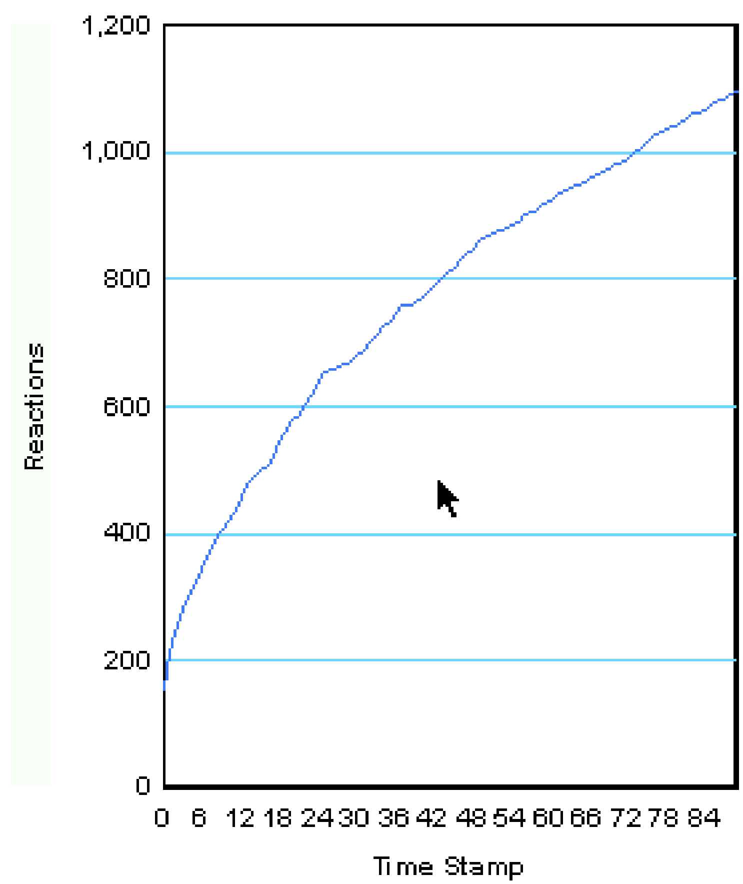
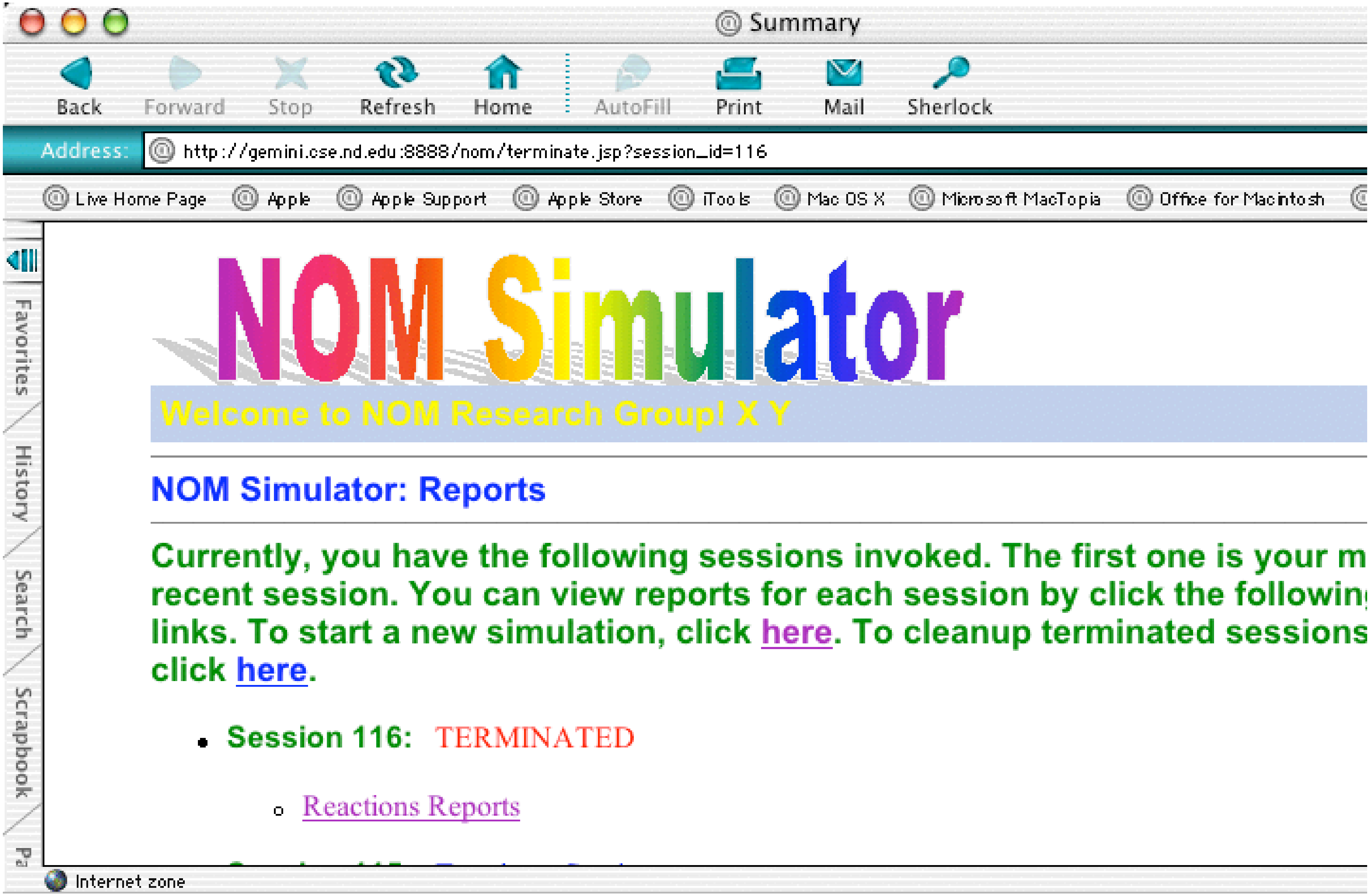
NOM Simulator: Reports

Reactions By Type



Reactions vs Time

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Summary

- Agent-Based Modeling approach
- Swarm and other tools
- Natural Organic Matter
- Molecules as Agents (objects)
- Web-based collaboratory

NOM 1.0 - Status/Plans

- Distributed System
  - Two Simulation Servers
  - Three Database Servers
  - Reports/Forms Server
  - Load Balancing / Fail Over
- Continue to Work on Core Simulation
- Get Researchers to Test and Provide Feedback
- Ad Hoc Queries to the Database
- Add Data Mining Interface/Capabilities
  - Clustering, Classification, Association Rules, Model Selection

Agent-Based Modeling of OSS

- NSF - CISE - Division of Information & Intelligent Systems
- Develop an Understanding of the Open Source Software (OSS) Development Phenomenon
  - Self-organized
  - Decentralized
  - Emergent Properties
  - Complex Adaptive Process
- Research Activity
  - Data collection
  - Social Network Models
  - SWARM-Based Simulation

Open Source Software (OSS)

- Free …
  - to view source
  - to modify
  - to share
  - of cost
- Examples
  - Apache
  - Perl
  - GNU
  - Linux
  - Sendmail
- Development
  - Mostly volunteer
  - Global teams
  - Virtual teams
  - Self-organized
  - Self-managed
  - Often large numbers of developers, testers, support help
  - Rapid, frequent releases
  - Mostly unpaid

Open Source Software (OSS): Significance

- Contradicts traditional wisdom:
  - Software engineering
  - Coordination, large numbers
  - Motivation of developers
  - Quality
  - Security
  - Business strategy
- Significant component of e-Business infrastructure
- Little Research Done to Date
- Great Research Opportunity
  - Almost all activity in online
  - Much of activity is archived
  - SourceForge Repository

- Research issues:
  - Understanding motives
  - Understanding processes
  - Intellectual property
  - Digital divide
  - Self-organization
  - Government policy
  - Impact on innovation
  - Ethics
  - Economic models
  - Cultural issues

Open Source Software (OSS)

- Major Component of e-Technology Infrastructure with major presence in
  - e-Business
  - e-Science
  - e-Government
  - e-Learning
- Apache has over 60% market share of Internet Web servers
- Linux on over 7 million computers
- Most Internet e-mail runs on Sendmail
- Tens of thousands of quality products
- Part of product offerings of companies like IBM
  - Apache in Websphere, Linux on mainframe
  - Corporate employees participating on OSS projects

Open Source Software (OSS)

- Seems to challenge traditional economic assumptions
- Model for software engineering
- New business strategies
  - Cooperation with competitors
  - Beyond trade associations, shared industry research, and standards processes — shared product development!
- Virtual, self-organizing and self-managing teams
- Intellectual property issues
- Government policy issues

Related Research

- Feller and Fitzgerald (ICIS, 2000)
  - Research framework and analysis of the OSS phenomenon
- Hars and Ou (HICSS 2001)
  - Survey of OSS developers
  - Reported on motivations of developers
- Scacchi (IEE Proceedings - Software, 2002)
  - Study of socio-technical processes associated with OSS development practices
- Wolf, Lakhani, and Bates (BCG/MIT Sloan, 2002)
  - Survey of Source Forge Developers
- Hann, Roberts, Slaughter, and Fielding (ICSE, 2002)
  - Survey of Apache developers - economic incentives
- Madey, Freeh, and Tynan (ICSE 2002, AMCIS 2002)

Self-Organizing Systems

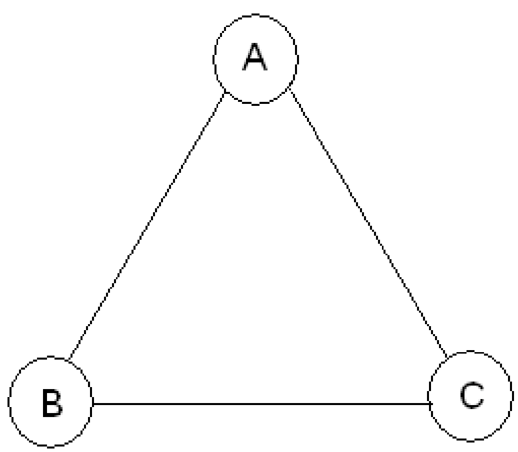
- Large numbers of locally interacting agents
- Simple rules for agent behavior
- Heterogeneous agents: attributes and behaviors
- Often unexpected and difficult to predict global properties emerge
- Emergence
- Complexity: hence, need for agent-based simulation

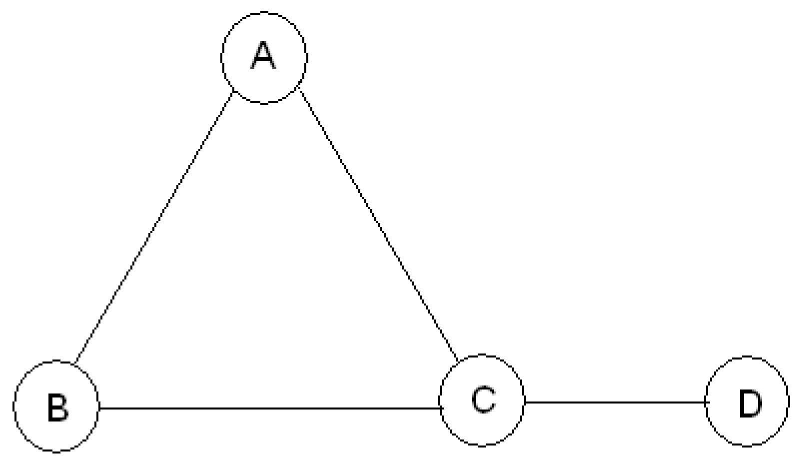
Modeling Social Systems

- Agent-Based Approach
  - Schelling (1978)
    - Micro and Macro Motives, racial housing patterns
  - Axelrod (1984)
    - Iterated prisoners dilemma, strategies
  - Epstein and Axtell (1996)
    - Political behavior
- Goal is not to predict, but to understand the processes that lead to emergent behavior
- Swarm Simulation: Agent Based Modeling
- Social Network Theory

OSS as a Social Network

- Social Network Theory
  - Agents are nodes on a graph (developers)
  - Edges are relationships (project participation)
  - Growth of network: random or preferential attachment, formation of clusters
  - Network attributes: diameter, average degree





Collaborative Social Networks

- Six degrees of separation
  - Small World Phenomenon
  - MS => 1 degree of Separation
- Research on joint authorship
- Movie Co-Stars
  - Kevin Bacon Game
  - IMDB.com
- Open Source Software Development
- Linked: The New Science of Networks, by Albert-László Barabási

Data Collection — Monthly

- Web crawler (scripts)
  - Python
  - Perl
  - AWK
  - Sed
- Monthly
- Since Jan 2001
- Project ID
- User ID
- Anonymized

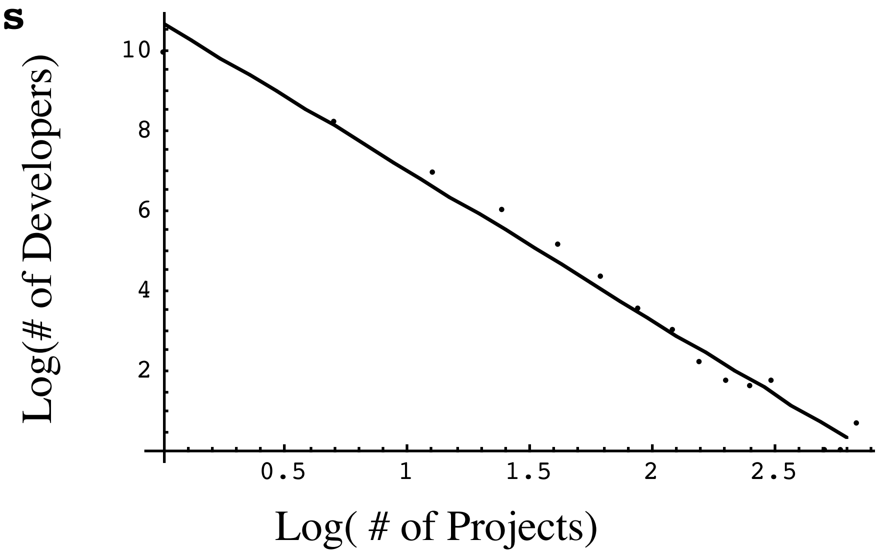
8001|dev378
8001|dev8975
8001|dev9972
8002|dev27650
8005|dev31351
8006|dev12509
8007|dev19395
8007|dev4622
8007|dev35611
8008|dev7698

Sample Summary Data

- SourceForge.net (May 2002)
  - Statistical data
    - 56,144 developers
    - 39,025 projects
  - Structural data
    - 43,871 developers on only one project
    - 16,821 isolated developers (no collaborative links)
  - Pareto distributions
    - Project sizes
    - Developer participation (number of projects a member of)
  - Trend data

Regression: Number of projects that developers are on

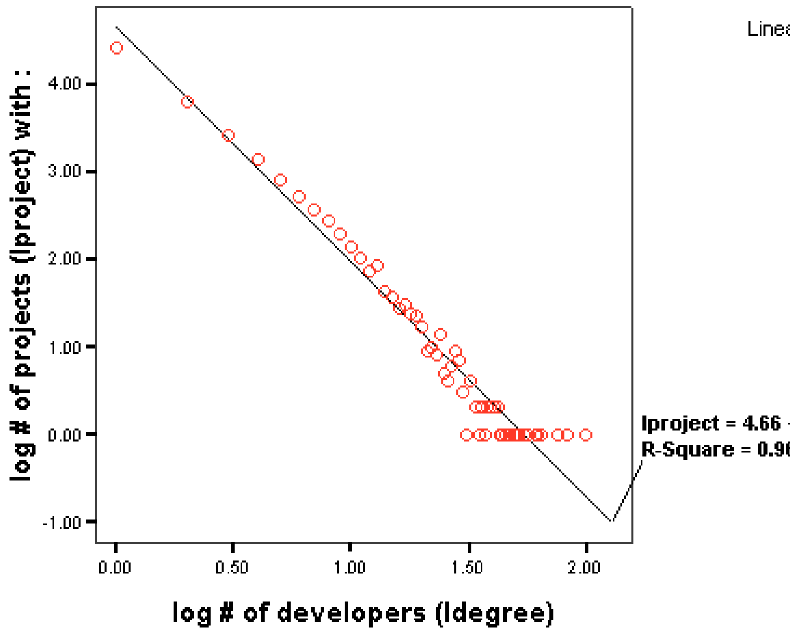
# projects	# of developers on that many projects
1	21488
2	3688
3	1086
4	413
5	177
6	76
7	35
8	21
9	9
10	6
11	5
12	6
15	1
16	1
17	1

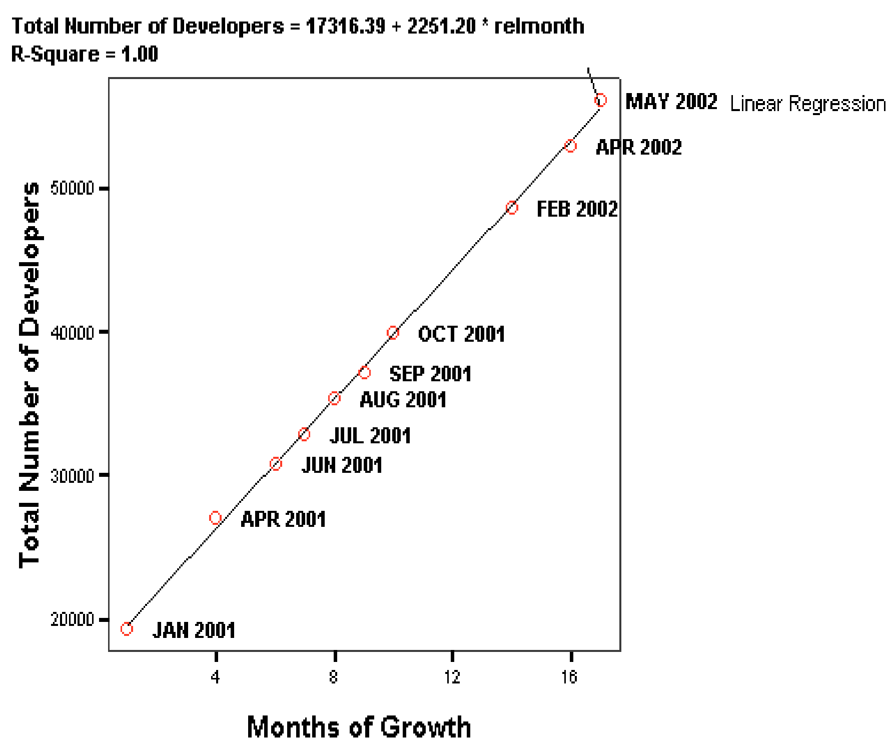


$$y = 10.6905 - 3.70892\,x$$

$$R^2 = 0.979906$$

More Empirical Data





Prototype Simulation

- Java Swarm / JDBC
- Developer class
- Each simulated developer is an instance of "Developer" with random attributes and behaviors
  - Local decision logic
  - Simulates self-organization
  - Create new projects
  - Join existing projects
  - Abandon a project

Prototype Simulation

- Simulating individual agent behavior stochastically
- Tuning simulation to fit empirical data

Parameter Name	**Description of Value**
probCreateInitially	Probability that a developer creates a project during his first time slice
probCreateEachPeriod	Probability that developer creates a project during any time slice after his first
probJoinEachPeriod	Probability that developer joins a project during any time slice after his first
probAbandonEachPeriod	Probability that developer abandons a project during any time slice after his first
developersPerPeriod	The number of developers introduced to the network each period
endTime	The duration of the simulation in time slices (days)

Prototype Simulation

- Oracle Tables
  - DEVELOPERS
  - PROJECTS
  - LINKS
    - Format identical to SourceForge empirical DB
    - Reuse of scripts for analysis of simulation data

Results/Limitations/Future Work

- Prototype currently models high level empirical statistics of SourceForge
- Currently simulating random attachment
- Plan to implement preferential attachment
- Plan to fit simulation with lower level statistics and structural data from SourceForge, e.g., Pareto Distribution
- Interpretation
- Survey instruments to collect additional data on developer behavior

Discussion