Online Collaboratory for NOM Research: Agent-based Simulations, Data-Mining, and Knowledge-Discovery

Madey, G.R., Cabaniss, S.E., Maurice, P.A., Xiang, X., Arthurs, L., Kennedy, R., Huang, Y

University of Notre Dame

University of New Mexico

ASLO 2005

February 24, 2005

Overview

- Project Background
- E-Science Background
- The NOM e-Science Collaboratory
- Invitation to Test, Contribute, Participate
- Summary

Background

- Small NSF-ITR involving Computer Scientists and Environmental Scientists
- Focus: “Stochastic Synthesis: Simulating the environmental transformations of NOM”
- IT Focus: e-Science, Web-Based Science, Agent-Based Simulation, Data Mining

E-Science Background

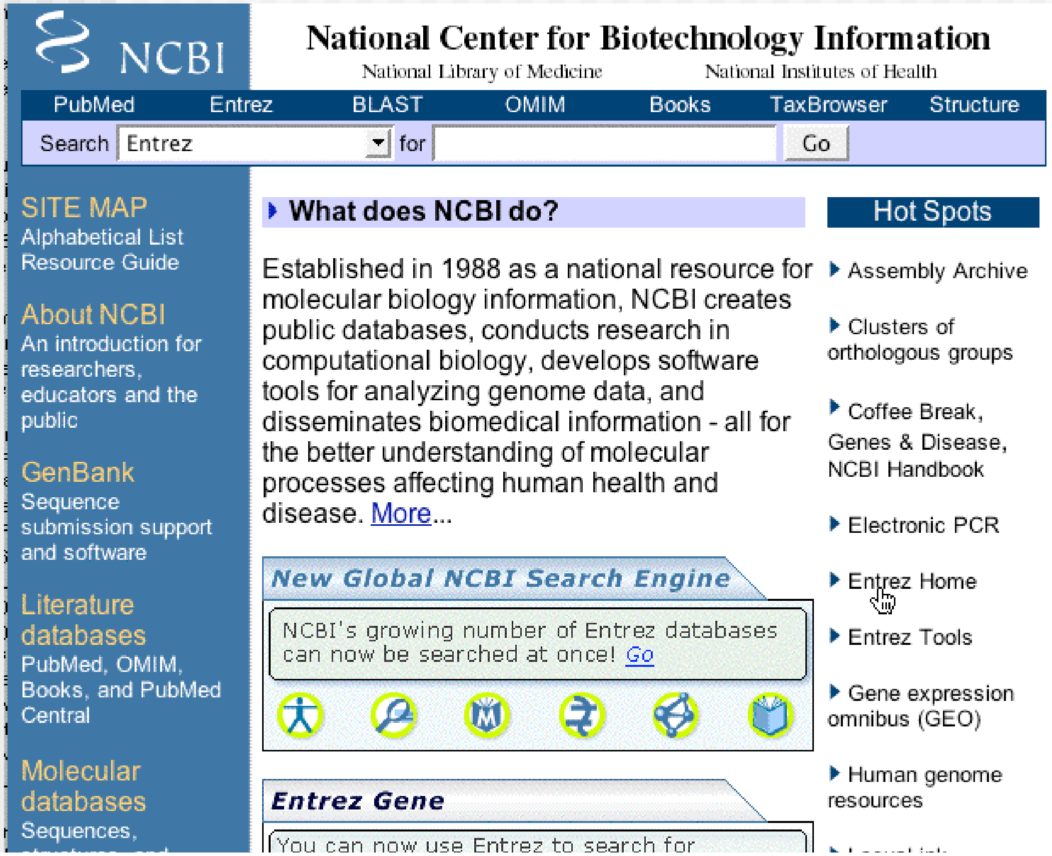
- NSF Cyberinfrastructure Program
  - Sensor networks
  - Large amounts of data => discovery through datamining
  - Online linked data repositories
  - Online analysis programs: search, extraction, matching, simulation, visualizations, etc.

E-Science Background (cont)

- WWW Telescope
- Virtual Observatories
  - NASA Skyview
  - US National Virtual Observatory
  - International Virtual Observatory Alliance
- More and more research done without every using a telescope => use of distributed data already collected

E-Science Background (cont)

- NCBI (National Center for Biotechnology Information)



NCBI

National Center for Biotechnology Information

National Library of Medicine National Institutes of Health

SITE MAP
Alphabetical List
Resource Guide

About NCBI
An introduction for researchers, educators and the public

GenBank
Sequence submission support and software

Literature databases
PubMed, OMIM, Books, and PubMed Central

Molecular databases
Sequences,

What does NCBI do?

Established in 1988 as a national resource for molecular biology information, NCBI creates public databases, conducts research in computational biology, develops software tools for analyzing genome data, and disseminates biomedical information - all for the better understanding of molecular processes affecting human health and disease. More...

New Global NCBI Search Engine

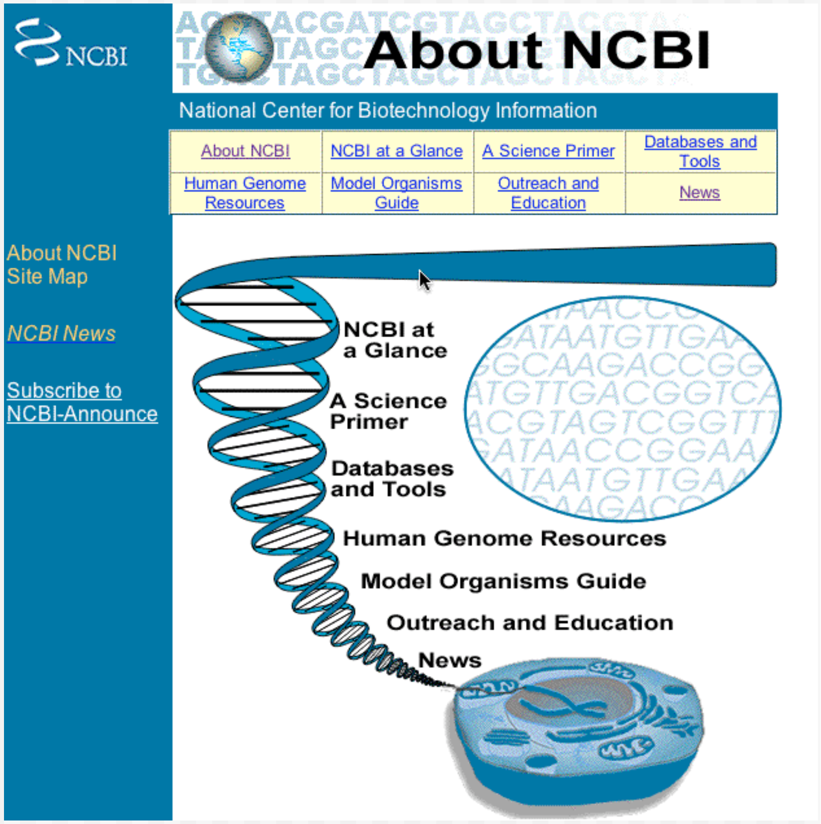
NCBI's growing number of Entrez databases can now be searched at once! Go

Entrez Gene

You can now use Entrez to search for

Hot Spots

- Assembly Archive
- Clusters of orthologous groups
- Coffee Break, Genes & Disease, NCBI Handbook
- Electronic PCR
- Entrez Home
- Entrez Tools
- Gene expression omnibus (GEO)
- Human genome resources



NCBI

About NCBI

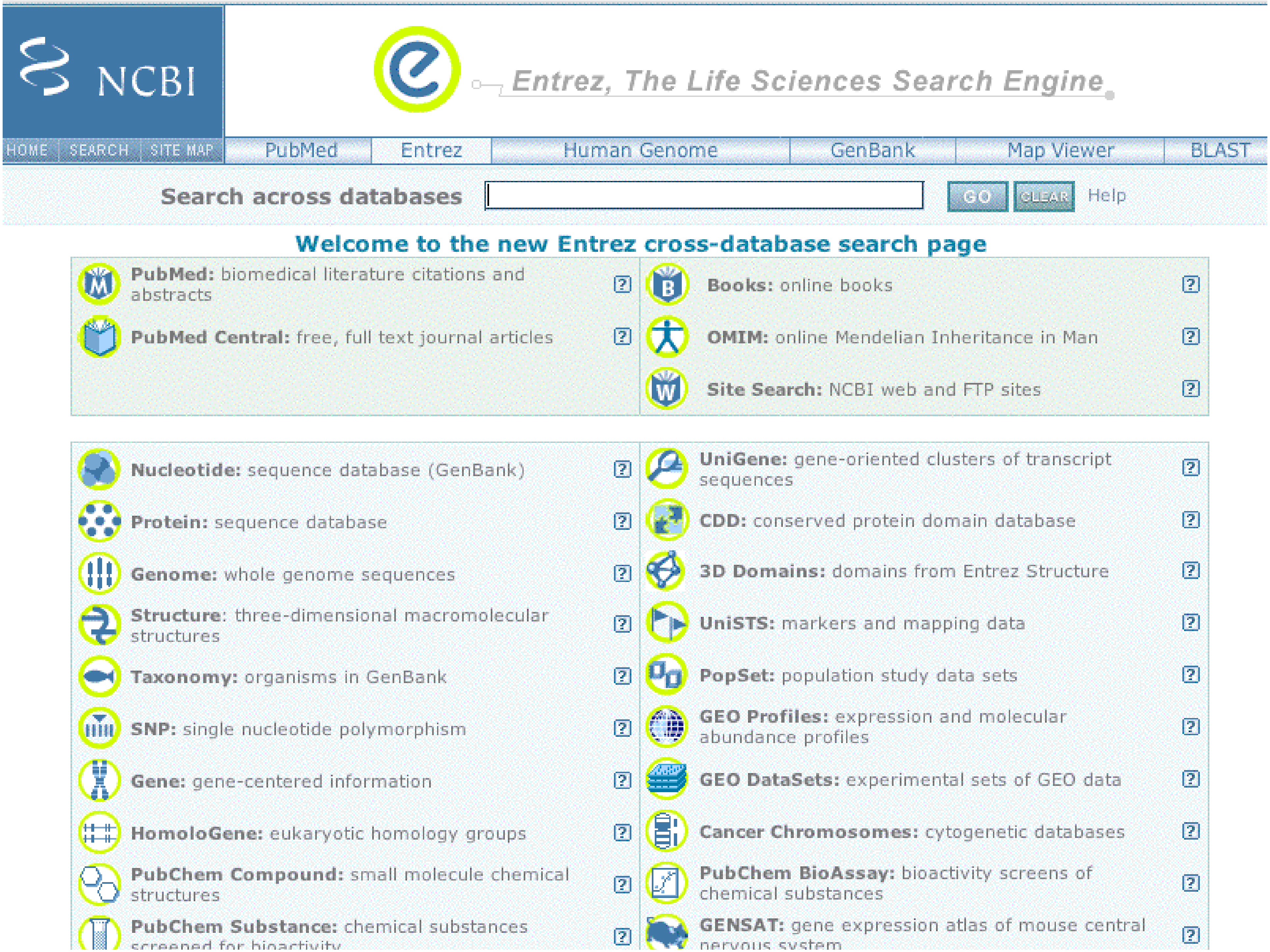
National Center for Biotechnology Information

About NCBI	NCBI at a Glance	A Science Primer	Databases and Tools
Human Genome Resources	Model Organisms Guide	Outreach and Education	News

About NCBI
Site Map

NCBI News

Subscribe to NCBI-Announce



Search across databases

Welcome to the new Entrez cross-database search page

PubMed: biomedical literature citations and abstracts

PubMed Central: free, full text journal articles

Books: online books

OMIM: online Mendelian Inheritance in Man

Site Search: NCBI web and FTP sites

Nucleotide: sequence database (GenBank)

Protein: sequence database

Genome: whole genome sequences

Structure: three-dimensional macromolecular structures

Taxonomy: organisms in GenBank

SNP: single nucleotide polymorphism

Gene: gene-centered information

HomoloGene: eukaryotic homology groups

PubChem Compound: small molecule chemical structures

PubChem Substance: chemical substances screened for bioactivity

UniGene: gene-oriented clusters of transcript sequences

CDD: conserved protein domain database

3D Domains: domains from Entrez Structure

UniSTS: markers and mapping data

PopSet: population study data sets

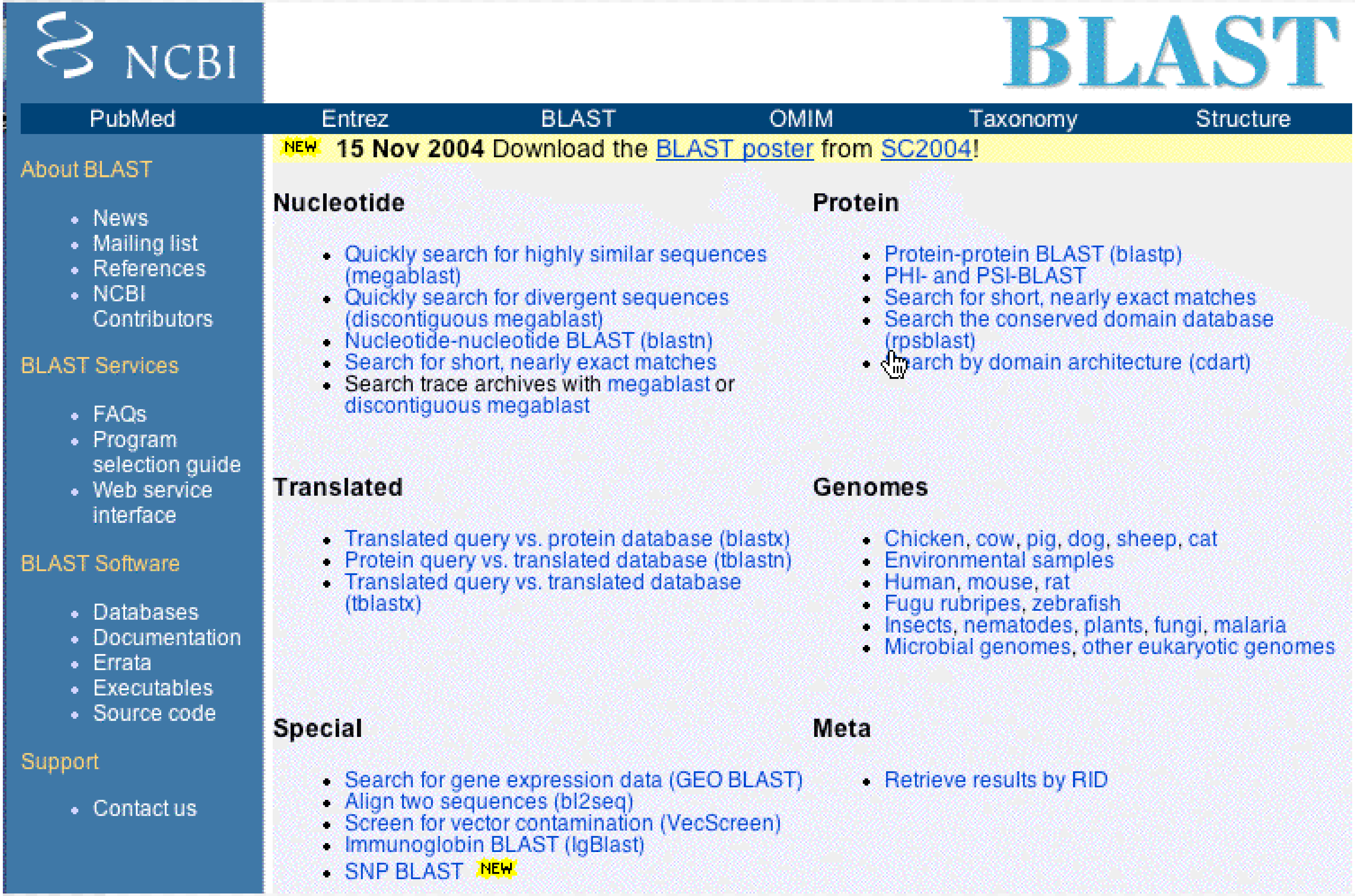
GEO Profiles: expression and molecular abundance profiles

GEO DataSets: experimental sets of GEO data

Cancer Chromosomes: cytogenetic databases

PubChem BioAssay: bioactivity screens of chemical substances

GENSAT: gene expression atlas of mouse central nervous system



NCBI

BLAST

PubMed Entrez BLAST OMIM Taxonomy Structure

NEW **15 Nov 2004** Download the BLAST poster from SC2004!

About BLAST

- News
- Mailing list
- References
- NCBI Contributors

BLAST Services

- FAQs
- Program selection guide
- Web service interface

BLAST Software

- Databases
- Documentation
- Errata
- Executables
- Source code

Support

- Contact us

Nucleotide

- Quickly search for highly similar sequences (megablast)
- Quickly search for divergent sequences (discontiguous megablast)
- Nucleotide-nucleotide BLAST (blastn)
- Search for short, nearly exact matches
- Search trace archives with megablast or discontiguous megablast

Protein

- Protein-protein BLAST (blastp)
- PHI- and PSI-BLAST
- Search for short, nearly exact matches
- Search the conserved domain database (rpsblast)
- Search by domain architecture (cdart)

Translated

- Translated query vs. protein database (blastx)
- Protein query vs. translated database (tblastn)
- Translated query vs. translated database (tblastx)

Genomes

- Chicken, cow, pig, dog, sheep, cat
- Environmental samples
- Human, mouse, rat
- Fugu rubripes, zebrafish
- Insects, nematodes, plants, fungi, malaria
- Microbial genomes, other eukaryotic genomes

Special

- Search for gene expression data (GEO BLAST)
- Align two sequences (bl2seq)
- Screen for vector contamination (VecScreen)
- Immunoglobin BLAST (IgBlast)
- SNP BLAST NEW

Meta

- Retrieve results by RID

Model Organism e-Science Sites

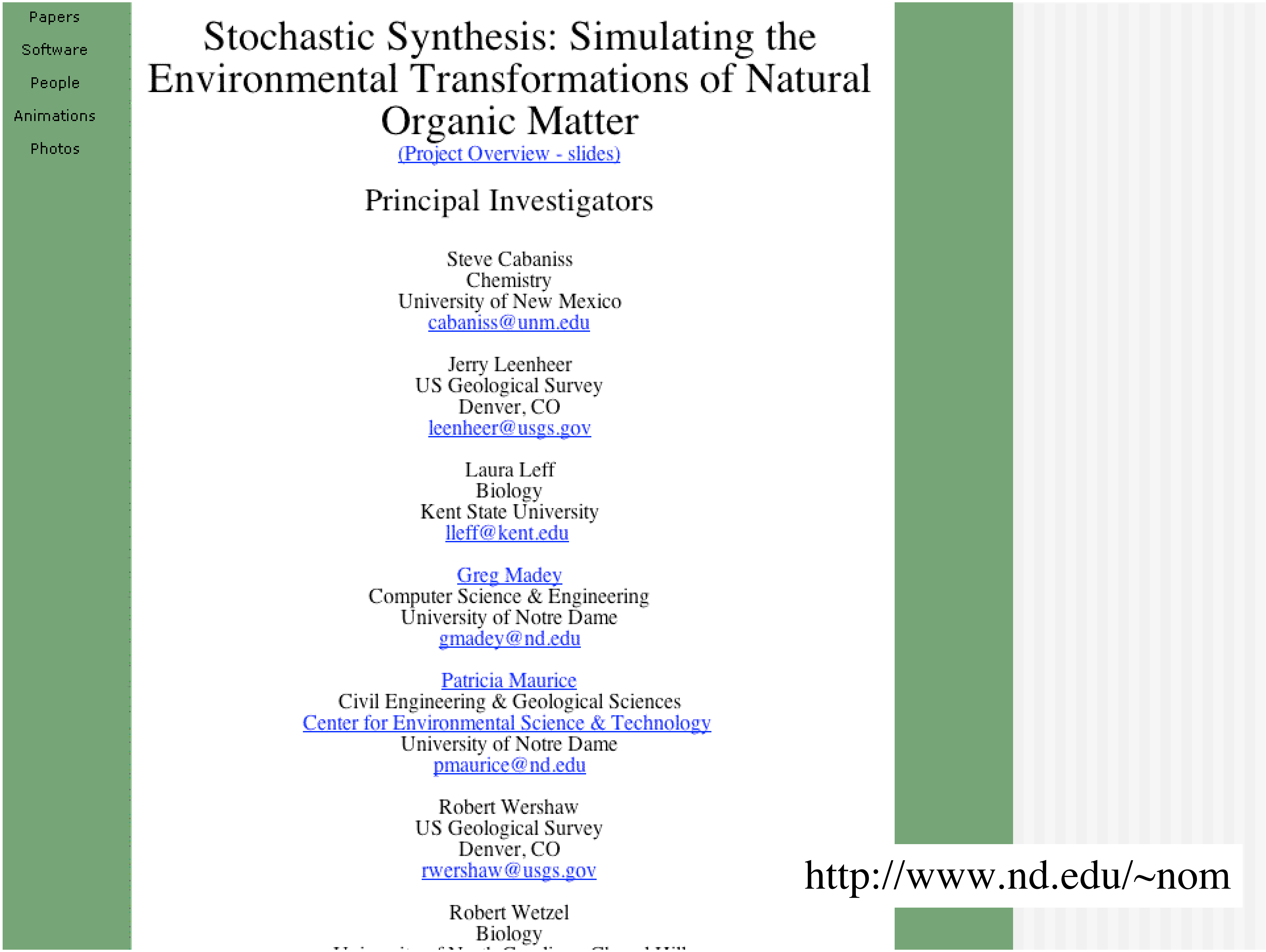
- FlyBase: Drosophila
- WormBase: C. elegans
- VectorBase: Mosquitos
- Mouse Genome
- DictyBase
- Etc.
- So many => GMOD

Questions?

- Has this research community begun to participate in the e-Science initiatives?
- Would this community benefit from e-Science initiatives?
- Is this community interested in an e-Science initiatives?
- Is this community willing to experiment?

The NOM e-Science Collaboratory

- Web-based
- Back-end database
- A cluster of simulation servers
- Shared simulation results
- Shared simulation configurations
- Other collaboratory features



Stochastic Synthesis: Simulating the Environmental Transformations of Natural Organic Matter

(Project Overview - slides)

Principal Investigators

Steve Cabaniss
Chemistry
University of New Mexico
cabaniss@unm.edu

Jerry Leenheer
US Geological Survey
Denver, CO
leenheer@usgs.gov

Laura Leff
Biology
Kent State University
lleff@kent.edu

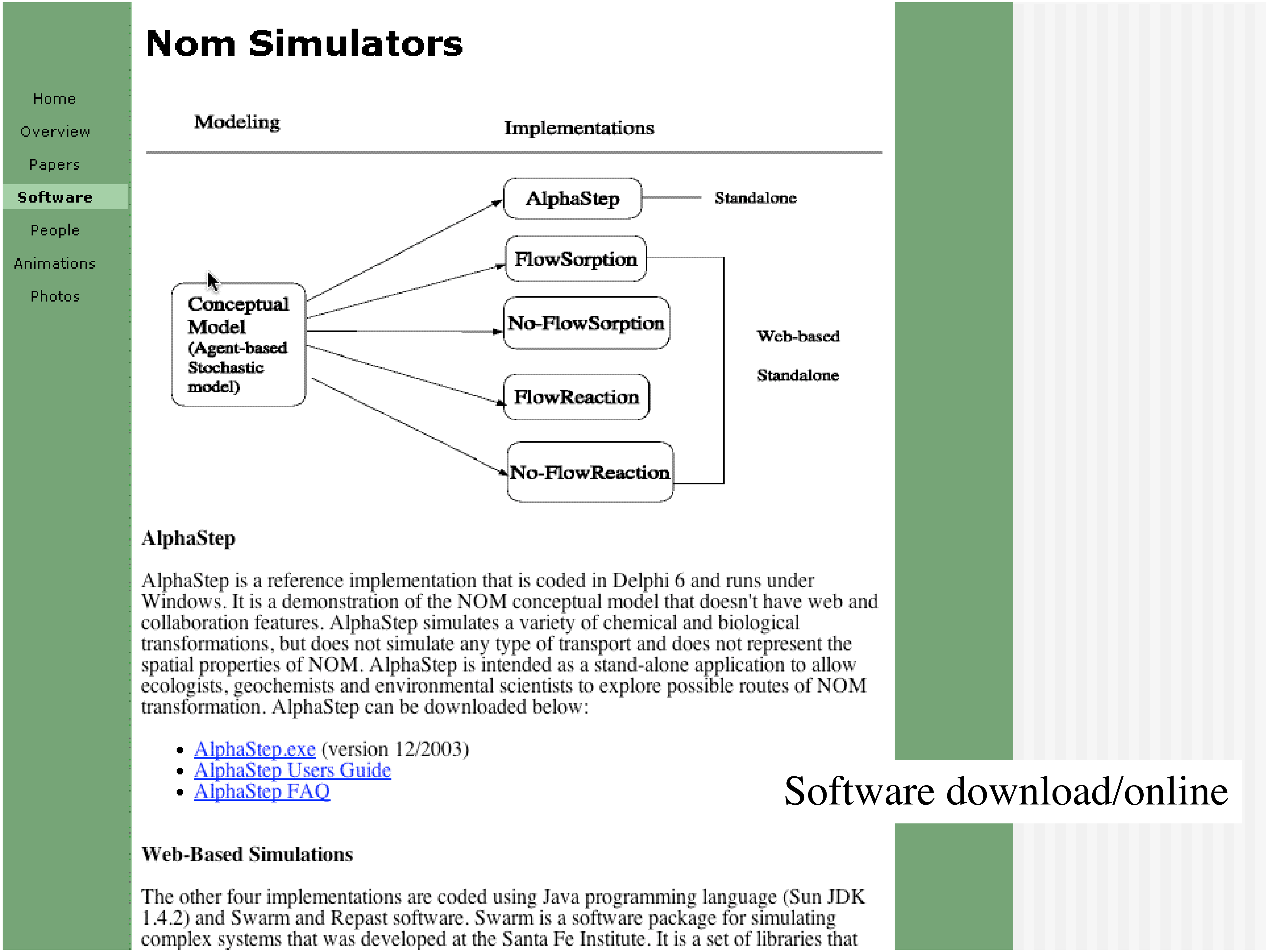
Greg Madey
Computer Science & Engineering
University of Notre Dame
gmadey@nd.edu

Patricia Maurice
Civil Engineering & Geological Sciences
Center for Environmental Science & Technology
University of Notre Dame
pmaurice@nd.edu

Robert Wershaw
US Geological Survey
Denver, CO
rwershaw@usgs.gov

Robert Wetzel
Biology
University of North Carolina, Chapel Hill

http://www.nd.edu/~nom



Nom Simulators

AlphaStep

AlphaStep is a reference implementation that is coded in Delphi 6 and runs under Windows. It is a demonstration of the NOM conceptual model that doesn't have web and collaboration features. AlphaStep simulates a variety of chemical and biological transformations, but does not simulate any type of transport and does not represent the spatial properties of NOM. AlphaStep is intended as a stand-alone application to allow ecologists, geochemists and environmental scientists to explore possible routes of NOM transformation. AlphaStep can be downloaded below:

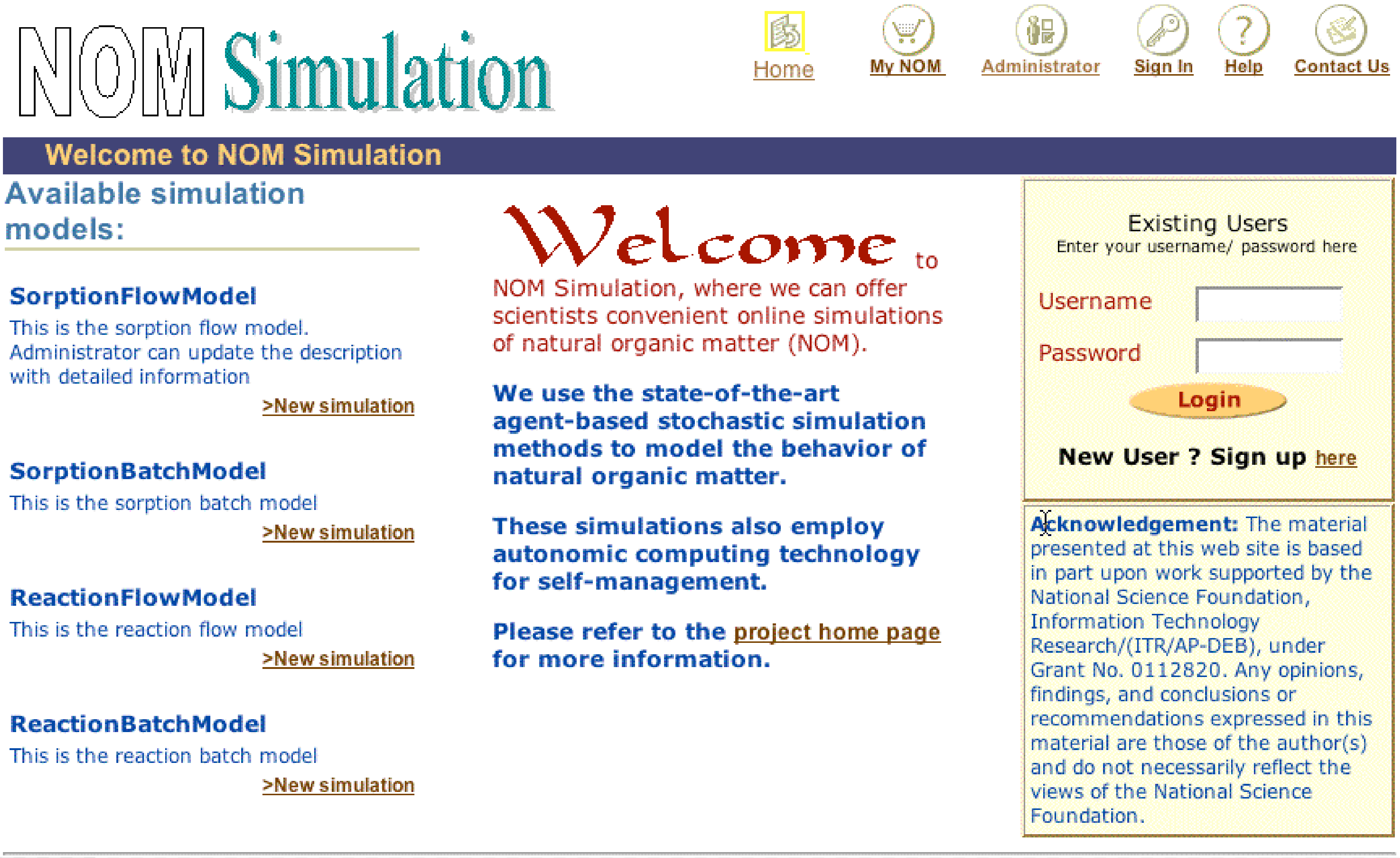
- AlphaStep.exe (version 12/2003)
- AlphaStep Users Guide
- AlphaStep FAQ

Web-Based Simulations

The other four implementations are coded using Java programming language (Sun JDK 1.4.2) and Swarm and Repast software. Swarm is a software package for simulating complex systems that was developed at the Santa Fe Institute. It is a set of libraries that

Software download/online

Simulation HomePage: http://tobit.cse.nd.edu/



Welcome to NOM Simulation

Available simulation models:

SorptionFlowModel

This is the sorption flow model. Administrator can update the description with detailed information

>New simulation

SorptionBatchModel

This is the sorption batch model

>New simulation

ReactionFlowModel

This is the reaction flow model

>New simulation

ReactionBatchModel

This is the reaction batch model

>New simulation

Welcome to NOM Simulation, where we can offer scientists convenient online simulations of natural organic matter (NOM).

We use the state-of-the-art agent-based stochastic simulation methods to model the behavior of natural organic matter.

These simulations also employ autonomic computing technology for self-management.

Please refer to the project home page for more information.

Existing Users

Enter your username/ password here

Username

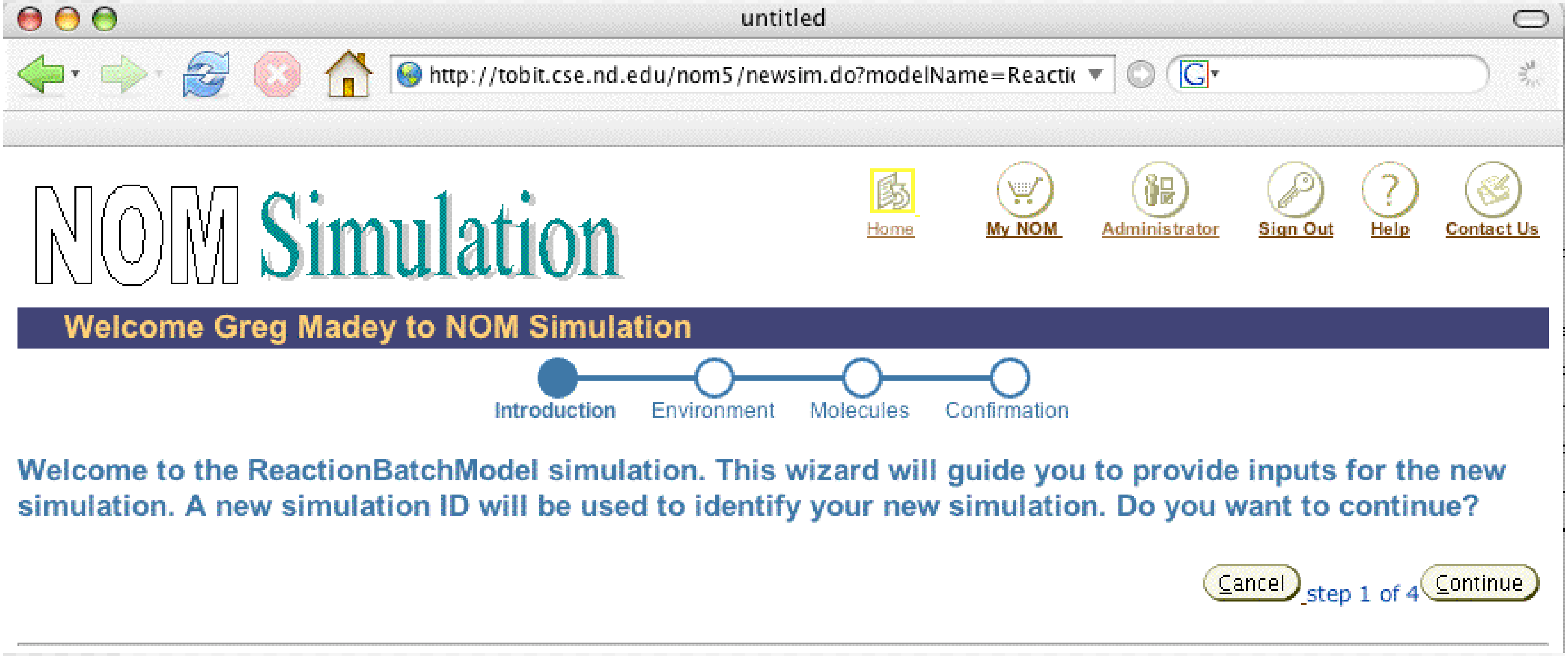
Password

Login

New User ? Sign up here

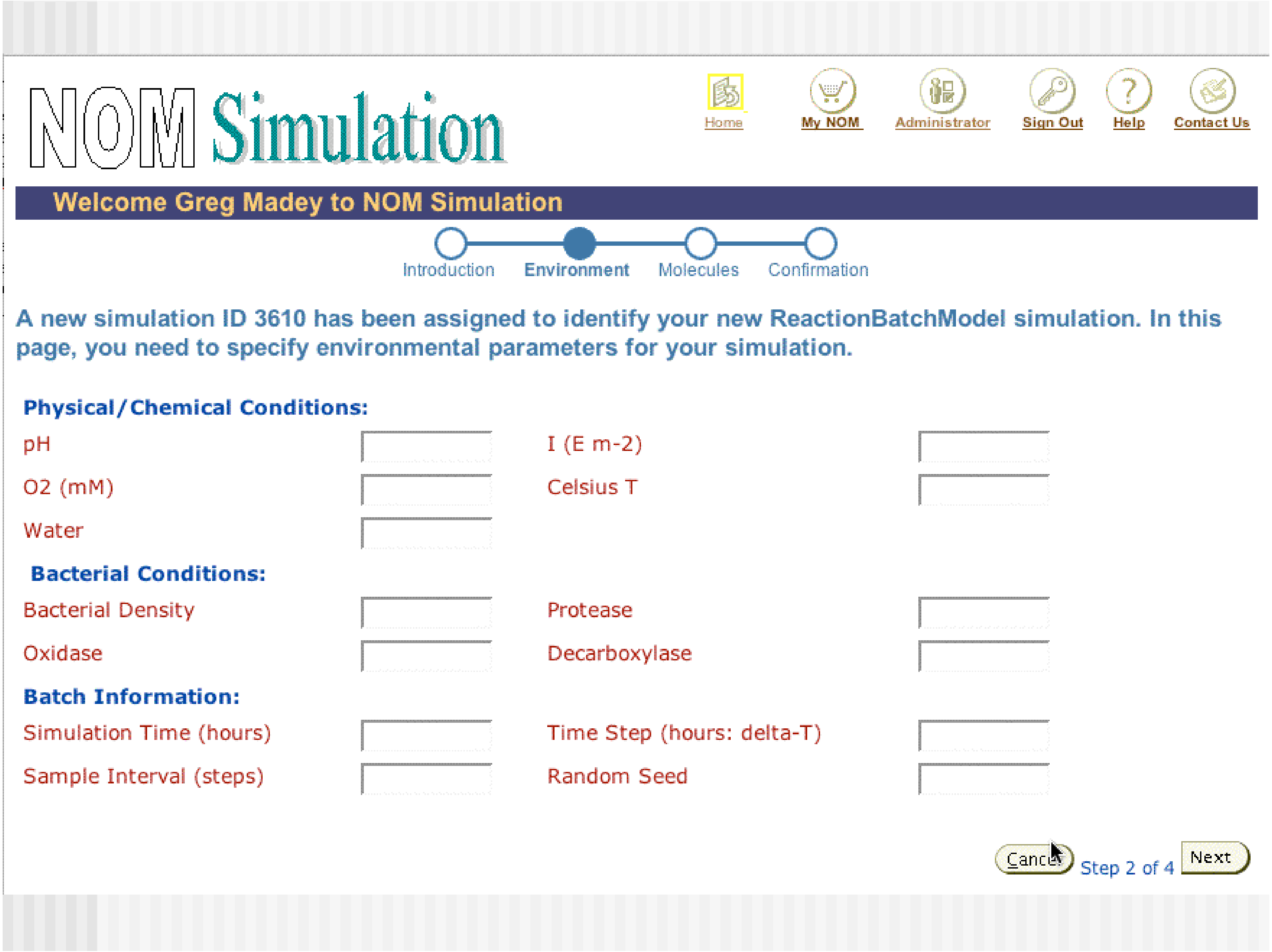
Acknowledgement: The material presented at this web site is based in part upon work supported by the National Science Foundation, Information Technology Research/(ITR/AP-DEB), under Grant No. 0112820. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

Reaction Batch Model



Welcome Greg Madey to NOM Simulation

Welcome to the ReactionBatchModel simulation. This wizard will guide you to provide inputs for the new simulation. A new simulation ID will be used to identify your new simulation. Do you want to continue?



Welcome Greg Madey to NOM Simulation

A new simulation ID 3610 has been assigned to identify your new ReactionBatchModel simulation. In this page, you need to specify environmental parameters for your simulation.

Physical/Chemical Conditions:

pH		I (E m-2)	
O2 (mM)		Celsius T	
Water			

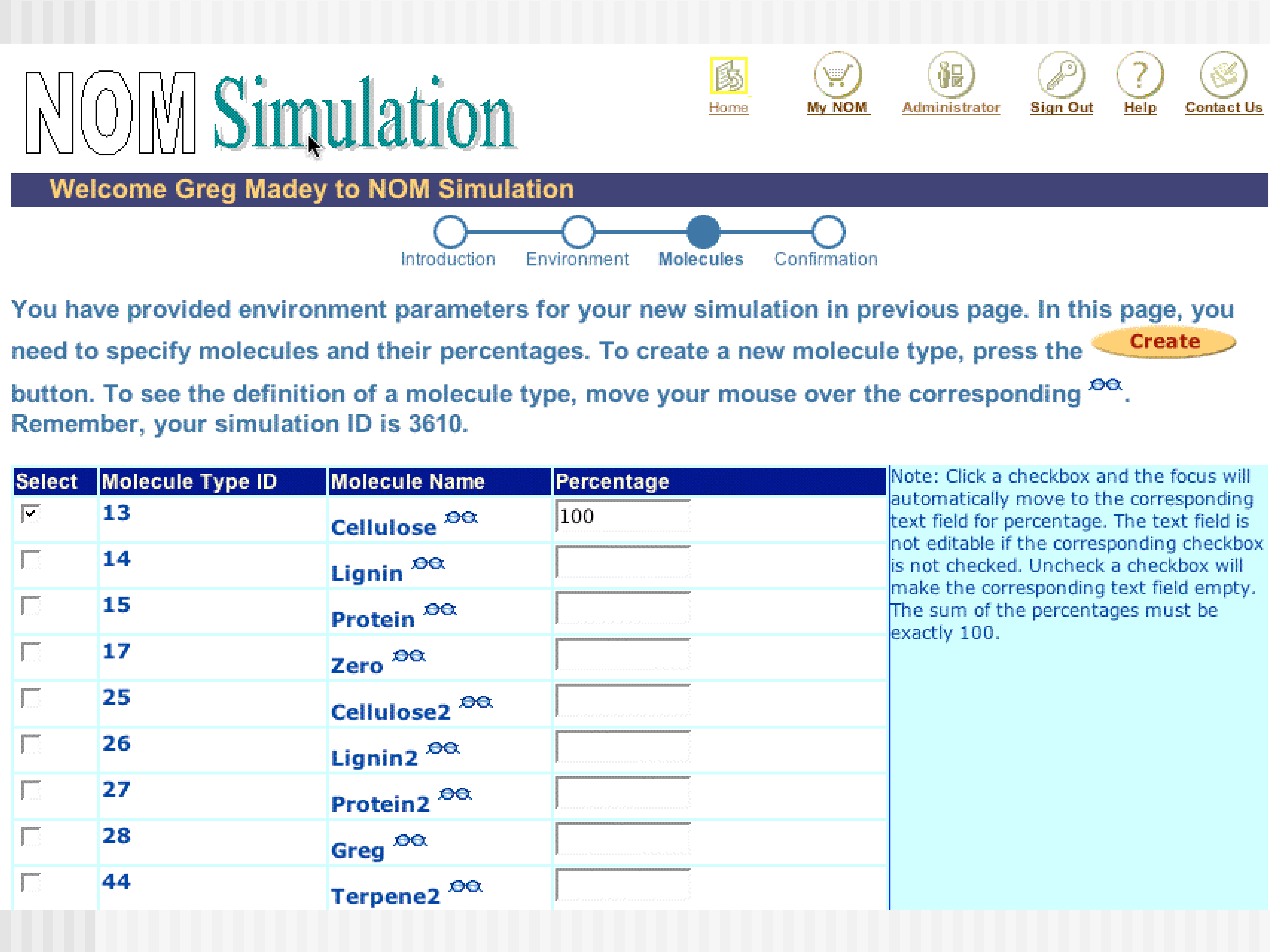
Bacterial Conditions:

Bacterial Density		Protease	
Oxidase		Decarboxylase	

Batch Information:

Simulation Time (hours)		Time Step (hours: delta-T)	
Sample Interval (steps)		Random Seed	

Step 2 of 4



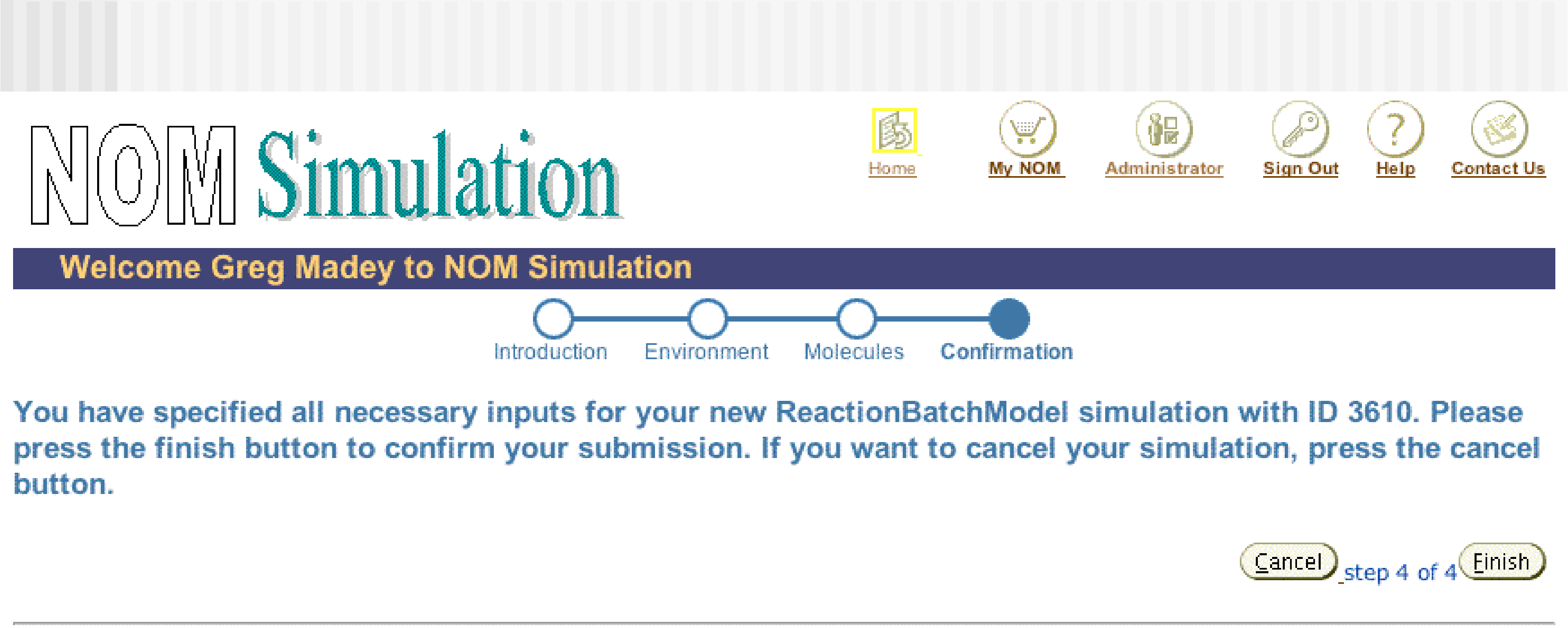
NOM Simulation

Welcome Greg Madey to NOM Simulation

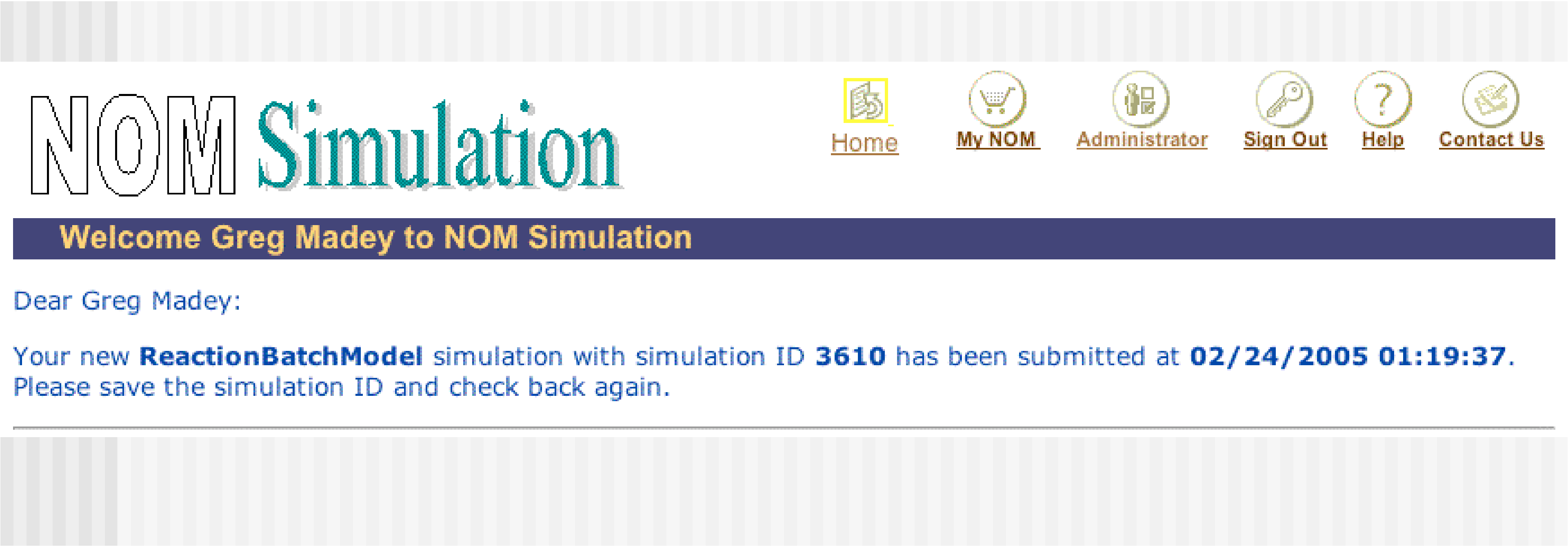
You have provided environment parameters for your new simulation in previous page. In this page, you need to specify molecules and their percentages. To create a new molecule type, press the **Create** button. To see the definition of a molecule type, move your mouse over the corresponding 👓. Remember, your simulation ID is 3610.

Select	Molecule Type ID	Molecule Name	Percentage
☑	13	Cellulose 👓	100
□	14	Lignin 👓	
□	15	Protein 👓	
□	17	Zero 👓	
□	25	Cellulose2 👓	
□	26	Lignin2 👓	
□	27	Protein2 👓	
□	28	Greg 👓	
□	44	Terpene2 👓	

Note: Click a checkbox and the focus will automatically move to the corresponding text field for percentage. The text field is not editable if the corresponding checkbox is not checked. Uncheck a checkbox will make the corresponding text field empty. The sum of the percentages must be exactly 100.

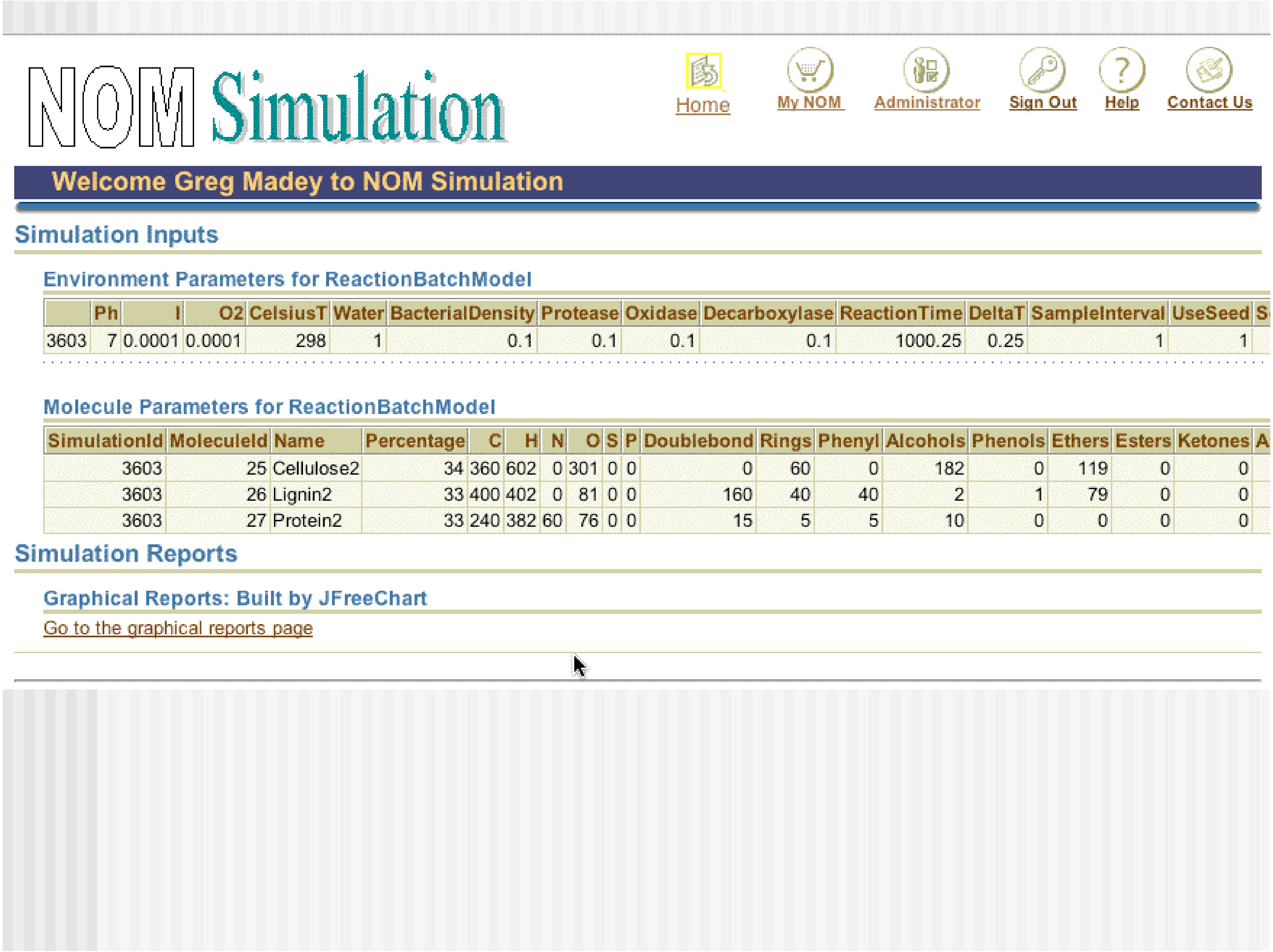


You have specified all necessary inputs for your new ReactionBatchModel simulation with ID 3610. Please press the finish button to confirm your submission. If you want to cancel your simulation, press the cancel button.



Dear Greg Madey:

Your new **ReactionBatchModel** simulation with simulation ID **3610** has been submitted at **02/24/2005 01:19:37**. Please save the simulation ID and check back again.



Welcome Greg Madey to NOM Simulation

Simulation Inputs

Environment Parameters for ReactionBatchModel

	Ph	I	O2	CelsiusT	Water	BacterialDensity	Protease	Oxidase	Decarboxylase	ReactionTime	DeltaT	SampleInterval	UseSeed	S
3603	7	0.0001	0.0001	298	1	0.1	0.1	0.1	0.1	1000.25	0.25	1	1	

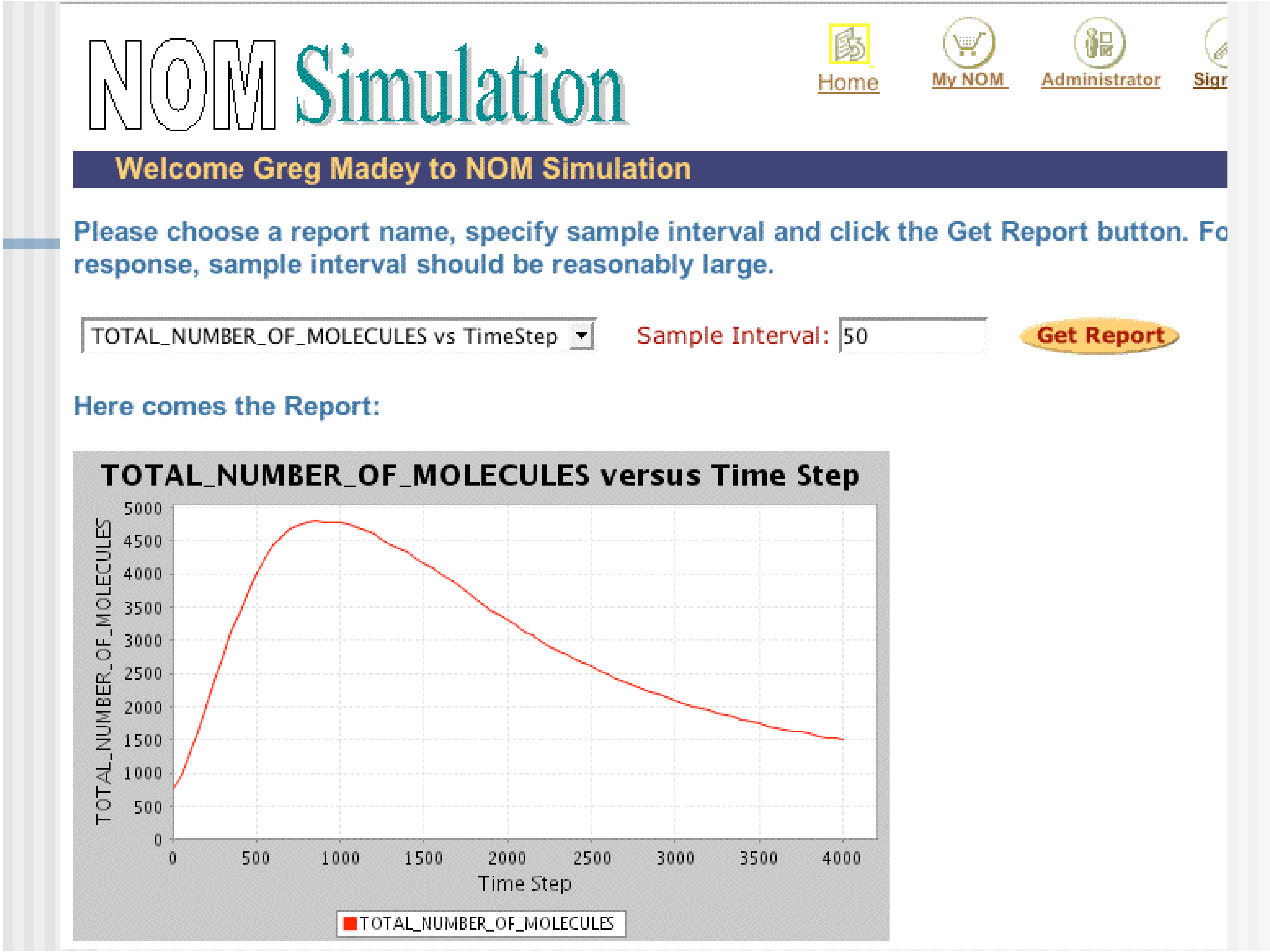
Molecule Parameters for ReactionBatchModel

SimulationId	MoleculeId	Name	Percentage	C	H	N	O	S	P	Doublebond	Rings	Phenyl	Alcohols	Phenols	Ethers	Esters	Ketones	A
3603	25	Cellulose2	34	360	602	0	301	0	0	0	60	0	182	0	119	0	0	
3603	26	Lignin2	33	400	402	0	81	0	0	160	40	40	2	1	79	0	0	
3603	27	Protein2	33	240	382	60	76	0	0	15	5	5	10	0	0	0	0	

Simulation Reports

Graphical Reports: Built by JFreeChart

Go to the graphical reports page



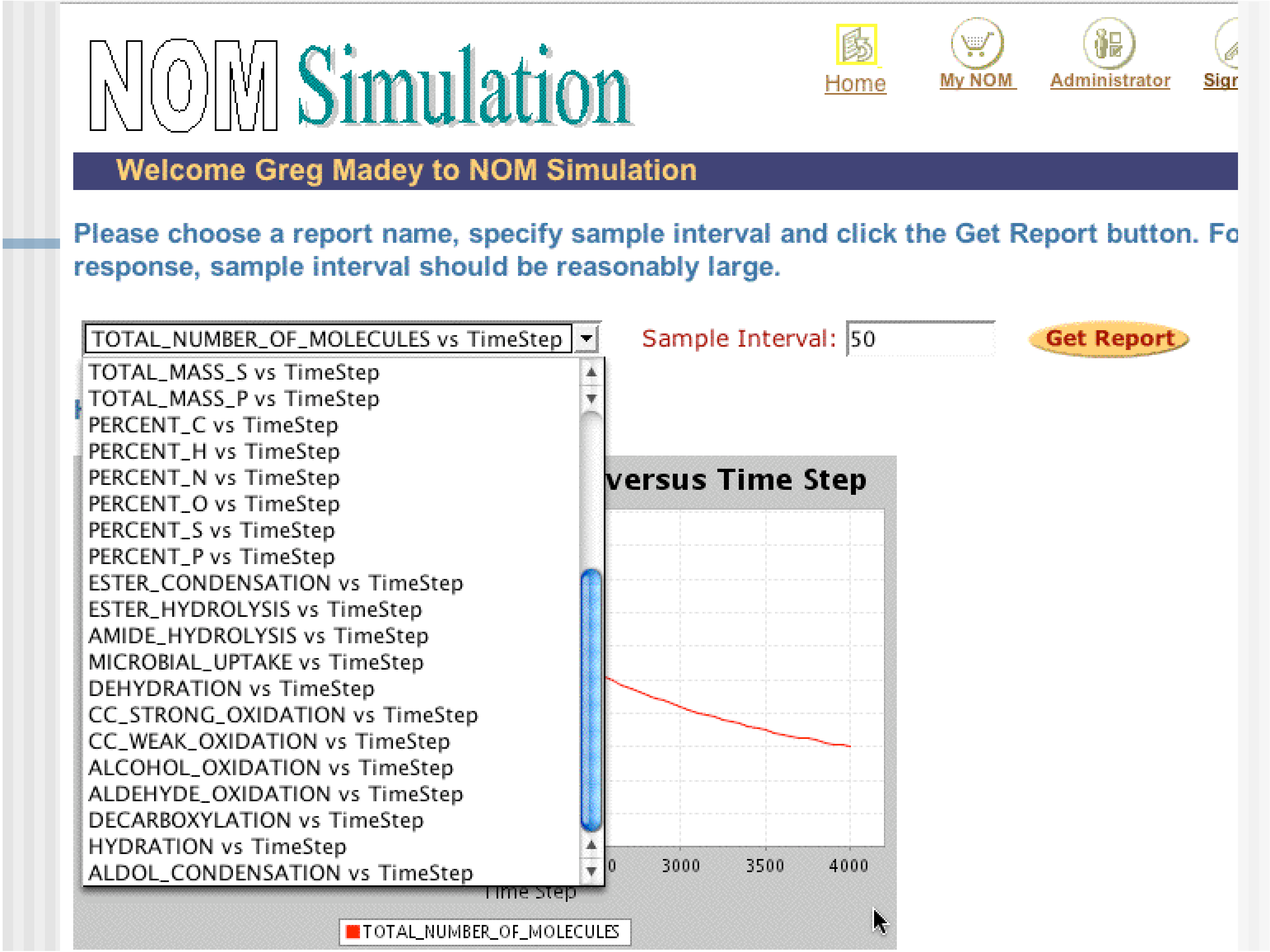
Welcome Greg Madey to NOM Simulation

Please choose a report name, specify sample interval and click the Get Report button. Fo response, sample interval should be reasonably large.

TOTAL_NUMBER_OF_MOLECULES vs TimeStep

Sample Interval: 50

Here comes the Report:



NOM Simulation
Home
My NOM
Administrator
Sigr

Welcome Greg Madey to NOM Simulation

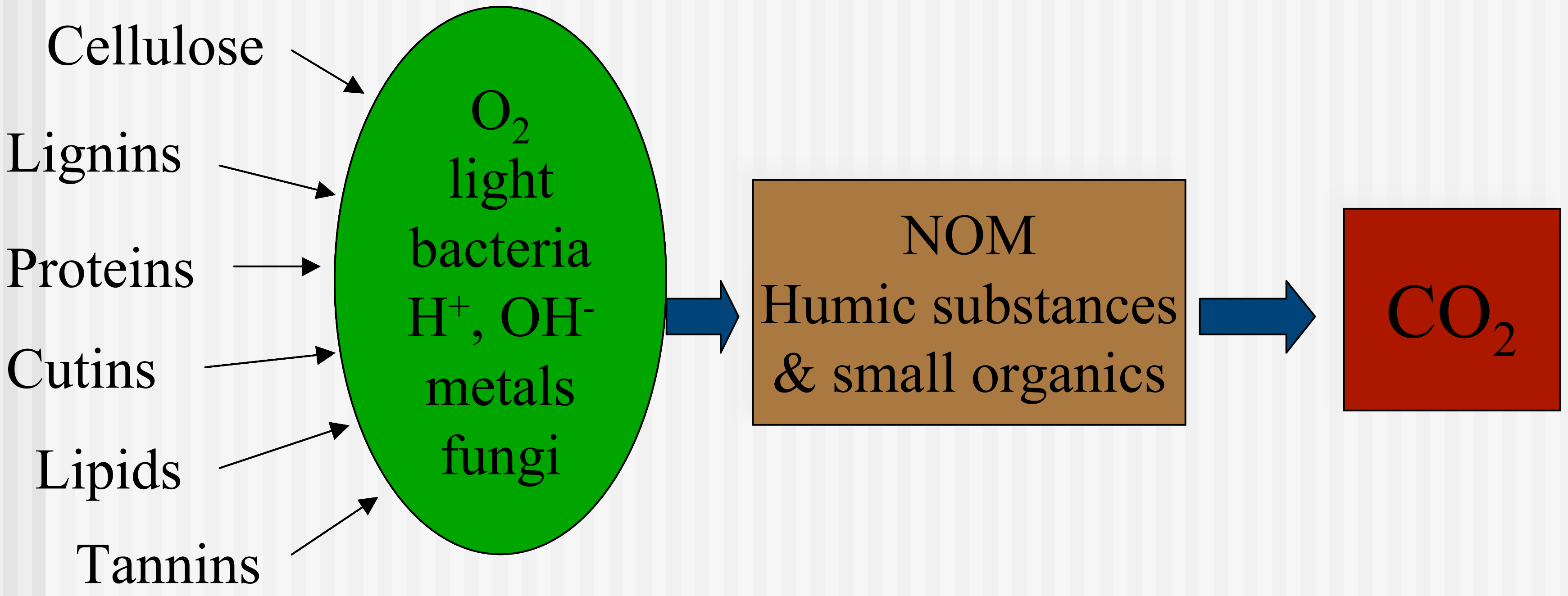
Please choose a report name, specify sample interval and click the Get Report button. Fo
response, sample interval should be reasonably large.

TOTAL_NUMBER_OF_MOLECULES vs TimeStep

Sample Interval: 50

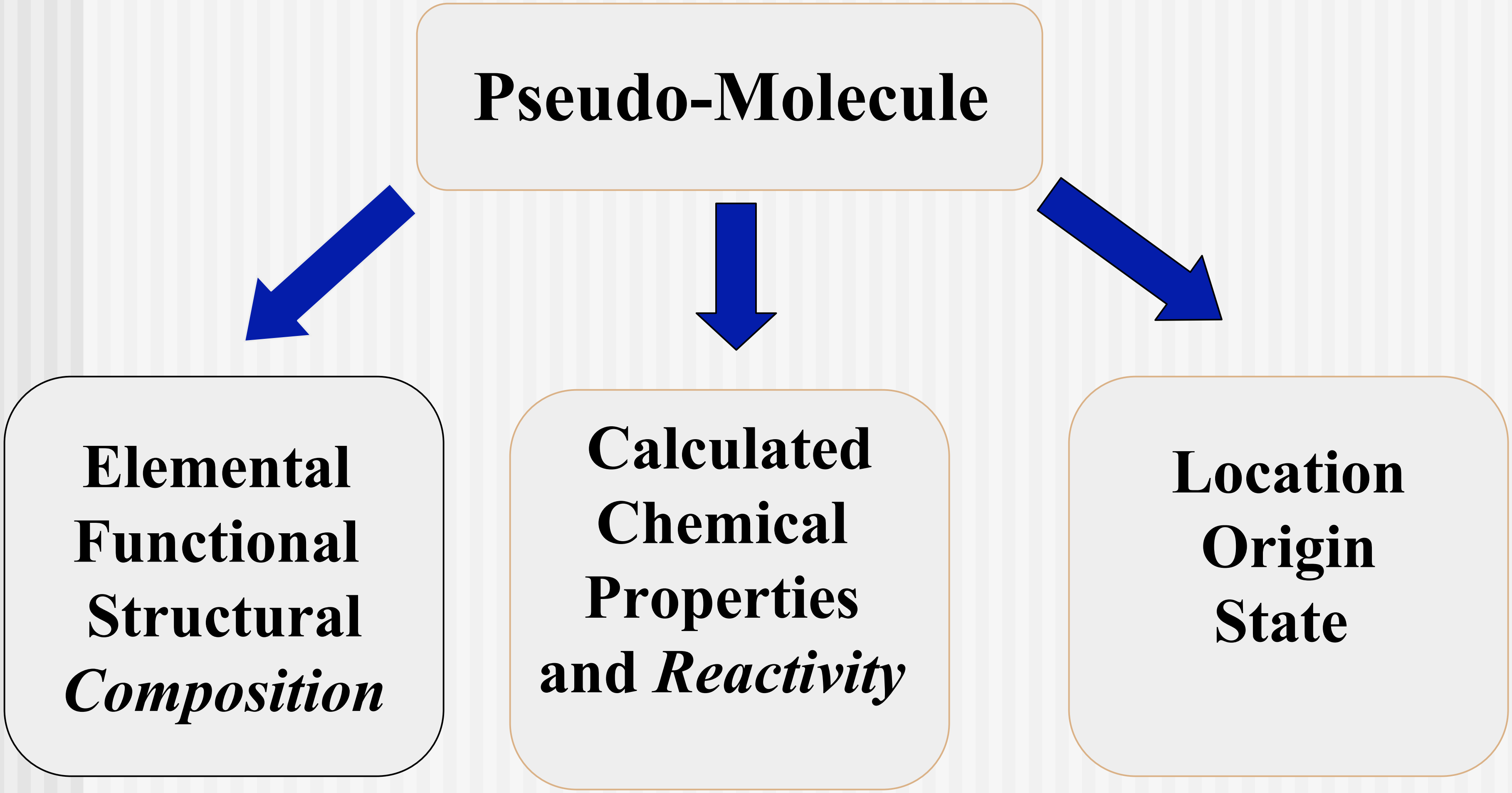
Get Report
TOTAL_MASS_S vs TimeStep
TOTAL_MASS_P vs TimeStep
PERCENT_C vs TimeStep
PERCENT_H vs TimeStep
PERCENT_N vs TimeStep
PERCENT_O vs TimeStep
PERCENT_S vs TimeStep
PERCENT_P vs TimeStep
ESTER_CONDENSATION vs TimeStep
ESTER_HYDROLYSIS vs TimeStep
AMIDE_HYDROLYSIS vs TimeStep
MICROBIAL_UPTAKE vs TimeStep
DEHYDRATION vs TimeStep
CC_STRONG_OXIDATION vs TimeStep
CC_WEAK_OXIDATION vs TimeStep
ALCOHOL_OXIDATION vs TimeStep
ALDEHYDE_OXIDATION vs TimeStep
DECARBOXYLATION vs TimeStep
HYDRATION vs TimeStep
ALDOL_CONDENSATION vs TimeStep
versus Time Step
0
3000
3500
4000
Time Step
TOTAL_NUMBER_OF_MOLECULES

Agent-Based Modeling of NOM



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

Data model



Pseudo-Molecule

Elemental
Functional
Structural
Composition

Calculated
Chemical
Properties
and *Reactivity*

Location
Origin
State

Environmental Parameters

Physical:
Temperature
Light Intensity

Chemical:
Water
pH
[O_2]

Biological:
Bacterial Density
Oxidase Activity
Protease Activity
Decarboxylase Activity

Invitation to Test, Contribute, Participate

- HTTP://www.nd.edu/~nom/
- HTTP://tobit.cse.nd.edu/

Summary

- Growing phenomenon of e-Science based research
- One small “environmental science” e-Science site: http://tobit.cse.nd.edu
- Invitation to test, download, evaluate, contribute, build your own, etc.
- Description of Agent-based NOM Simulator (downloadable and online) by Steve Cabaniss next!