A Stochastic Simulation of Natural Organic Matter and Microbes in the Environment

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Objectives

- New approach for NOM modeling
  - Agent-based modeling
- E-Science on the Web
- Intelligent interface
- The NOM Collaboratory

Outline

- **Introduction**
- **Modeling**
- **Core simulation engine**
- **Intelligent Web-based interface**
- **The NOM collaboratory**
- **Conclusion**
- **Future work**

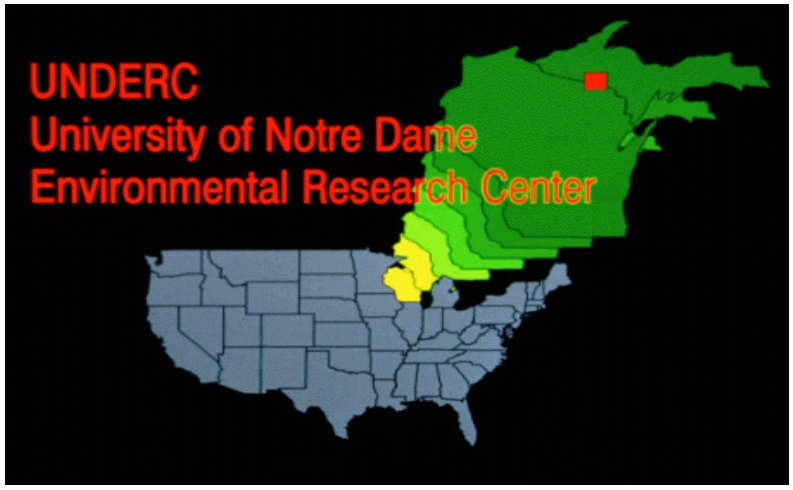
Introduction

- What is Natural Organic Matter (NOM)?
- Role of NOM in various science disciplines
  - Mobility and transport of pollutants
  - Availability of nutrients for microorganisms and plant communities
  - Affects quality of drinking water
- Need to understand the evolution and heterogeneous structure of NOM

Forest Service Bog [DOC] 7 MW 2200

Twomile Creek [DOC] 17 MW 1500

Nelson Creek [DOC] 79 MW 900

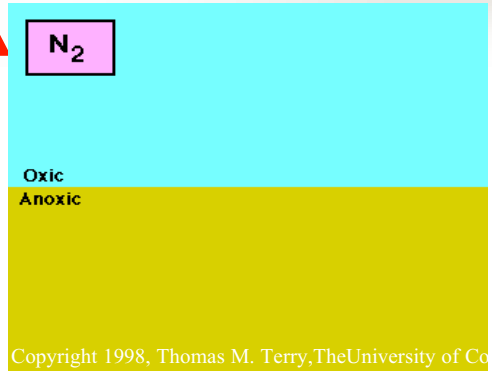


Previous models

- Two examples:
  - Daisy (S. Hansen, H. E. Jensen, and N. E. Nielsen 1990-present)：a soil plant atmosphere system model
  - StochSim (C. J. Morton-Firth 1998-present): Stochastic simulation of cell signaling pathways

large

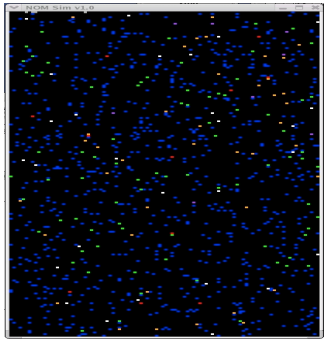
(Large ecosystem) (Years)



Elemental Cycling

Daisy

NOM 1.x

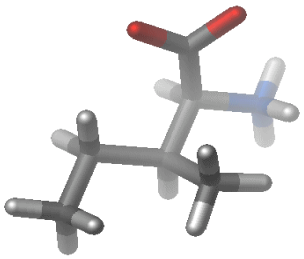


Scale

(size, temporal)

StochSim

Connectivity Maps



(One molecule) (nanoseconds)

small

low

(Atoms number Percentage)

Detail

(structure)

high

(Forces between atoms Electron density)

Our model

- Agent-based modeling (Individual-based modeling)
  - Agent-based model
    - Reynolds (1987): Flocks, herds, and schools: A distributed behavioral model. *Computer Graphics*
  - Each molecule as an individual object with spatial properties
  - Bottom-up approach
  - Stochastic model
  - Trace changes of the system → Database and data mining technologies

Our model (cont.)

- Web-based simulation model
  - Serve as an example for E-Science
    - G. Fox (2002): E-science meets computational science and information technology. *Computing & Engineering*
    - R. M. Jakobovits, J. F. Brinkley, C. Rosse, and E.Weinberger (1998): Enabling clinicians, researchers, and eductors to build custom Web-based biomedical information system
  - Support the collaborations, data and information sharing between scientists
  - No installation, expensive computation resources needed by scientists

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Modeling

- A complex system
  - Consists of a large number of objects
    - Molecules, Microbes
      - **Heterogeneous properties**
      - **Individual behaviors**
      - **Interaction between each other**
      - **Objects behavior and interaction are stochastically determined by:**
        - **Attributes** (intrinsic parameters)
        - **Reactions rates**
        - **Environment condition** (extrinsic parameters)
  - No central control
  - Emergent properties

Modeling (cont.)

- Agent Attributes
  - More specific than “percent carbon” but less detailed than a molecular connectivity map
  - Elemental composition
    - (C, H, O, N, S, P)
  - Functional groups
    - (double bonds, ring structure, alcohols …)
  - The origin of objects
    - spatial position in the system
    - Precursor type of molecule
  - Probability table of physical and chemical reactions
  - Molecule weight

Modeling (cont.)

- Agent Behaviors (reactions and processes):
  - Transport through soil pores by water (spatial mobility)
  - Adsorb onto or desorbed from mineral surfaces
  - Chemical reactions
    - Total 10 types in current model
    - First order
    - Second order
  - Stochastically determined
- Space:
  - 2-D grid

Modeling(cont.)

- Environmental parameters
  - Temperature
  - pH
  - Light intensity
  - Microbe density
  - Water flow rate
  - …

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Core simulation engine

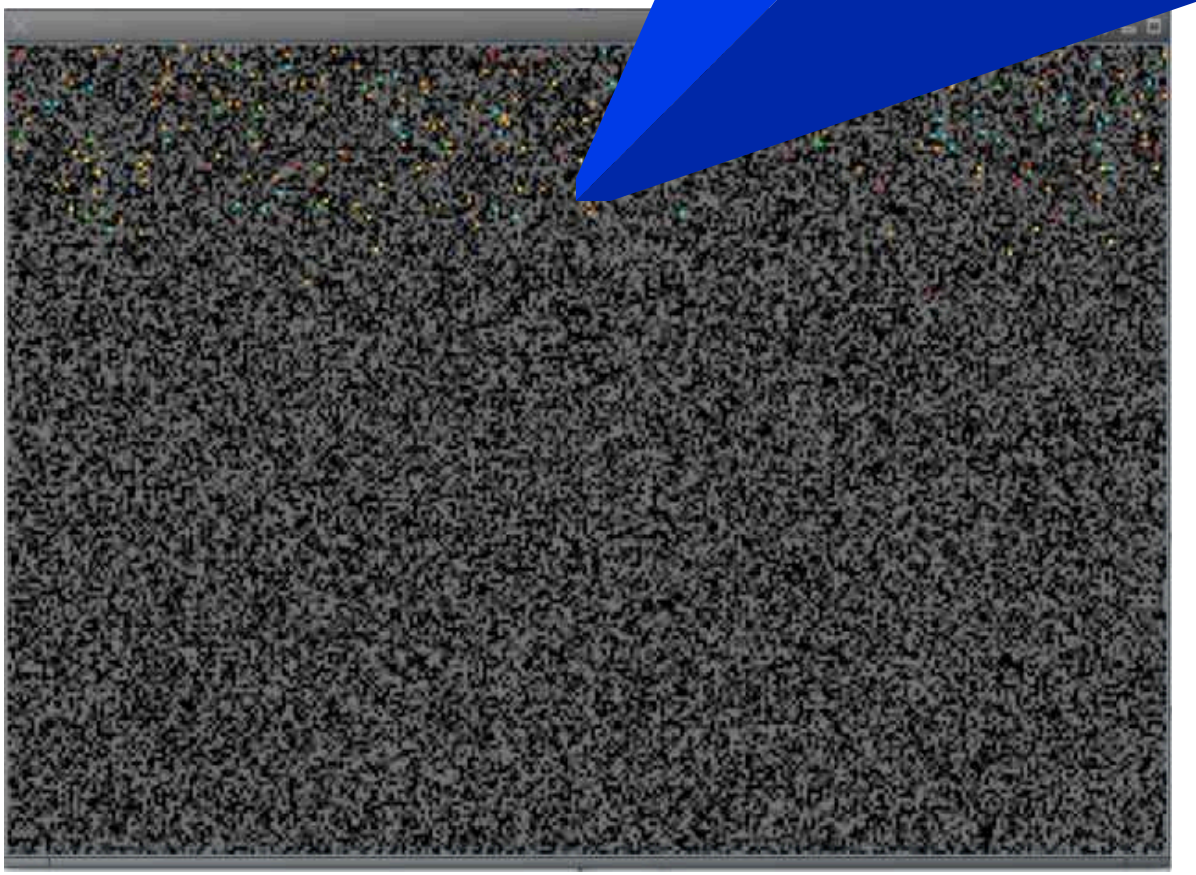
- Implementation
  - Swarm toolkit (Santa Fe Institute)
  - Java programming language (Sun JDK 1.4.1_01)
- GUI version
  - View the animation of molecules
  - Easy for debugging and modeling
- Web-based version

Core simulation engine (cont.)

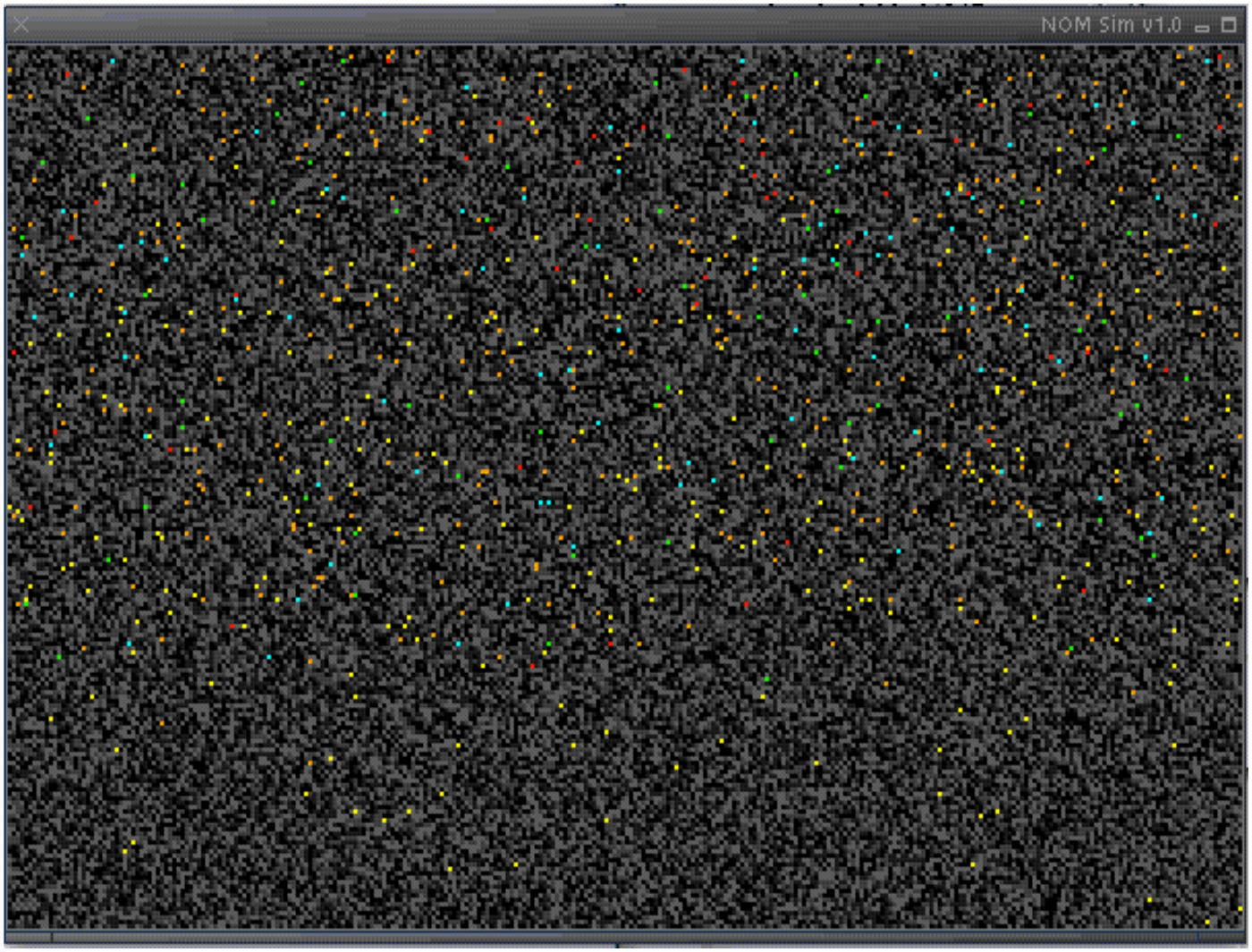
- Read simulation parameter from the database (JDBC)
  - Environmental parameters (pH, temperature, light intensity, and so on)
  - Molecule types and distributions
- User defined time has been separated to a large number of equal size time steps
- Write relevant data into the database every time step (JDBC)
  - Trace the dynamic properties of individuals and the system over time

Visualization

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



Visualizations – NOM molecules in solution and adsorption



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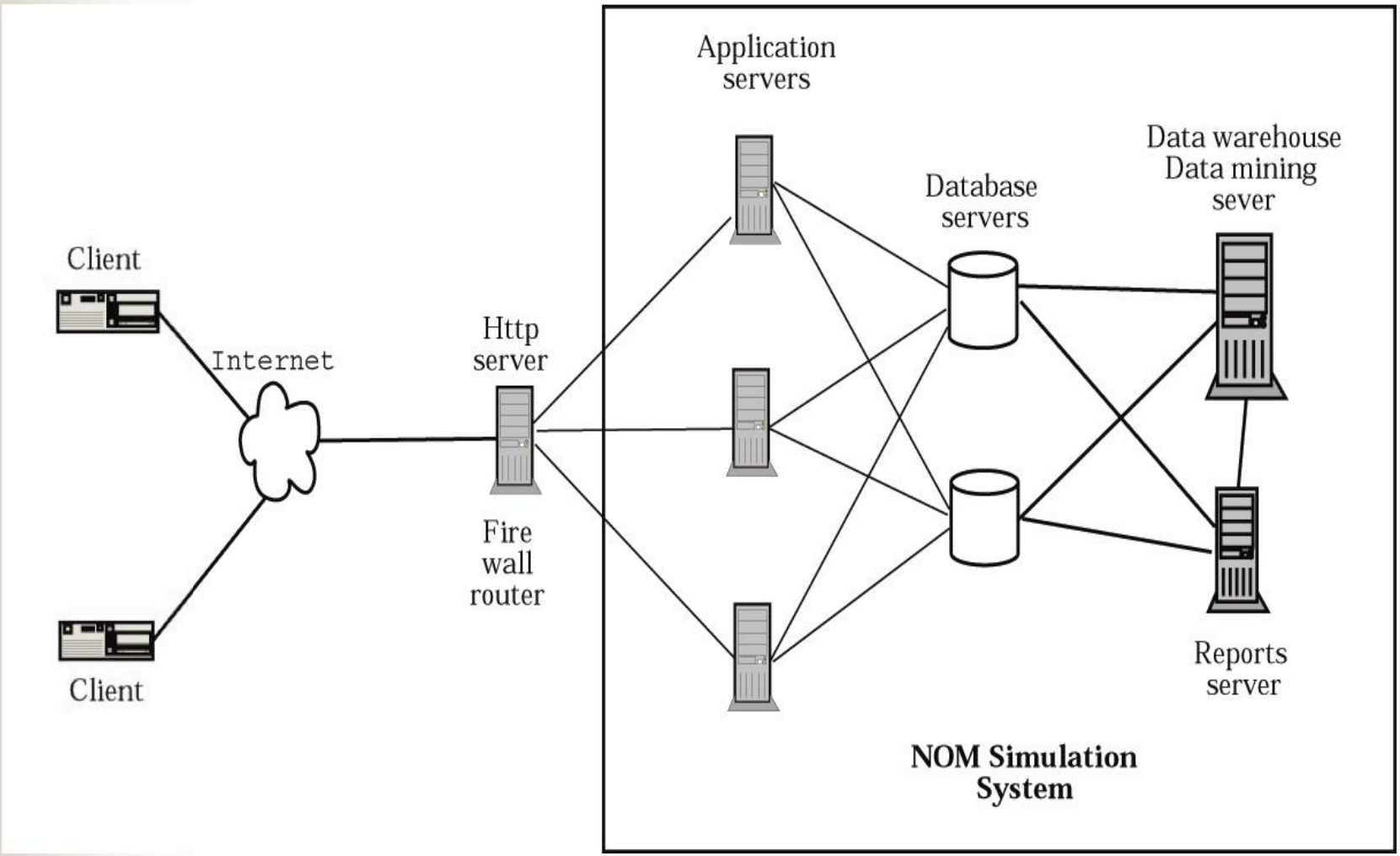
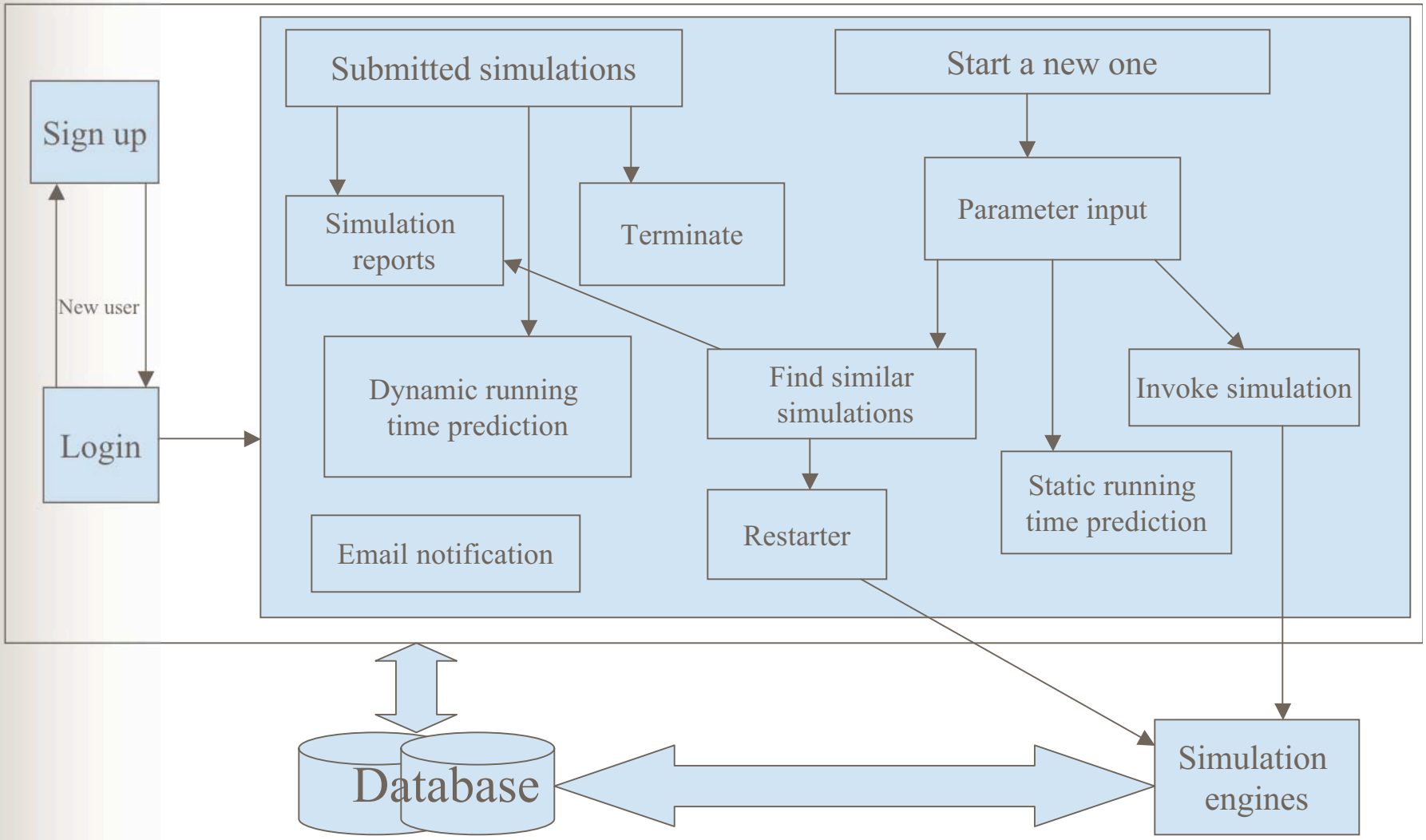
Web-based model

- Distributed, Web-based scientific application model
- Based on Sun Java 2 Enterprise Edition (J2EE)
  - Standard HTML Forms / JSP
  - Java Servlets, Java Beans
  - JDBC - Oracle
  - Oracle Database, Oracle Forms, and Reports
- Three parts:
  - Intelligent Web-based interface
  - Core simulation engine
  - Data analysis packages, Data mining technologies

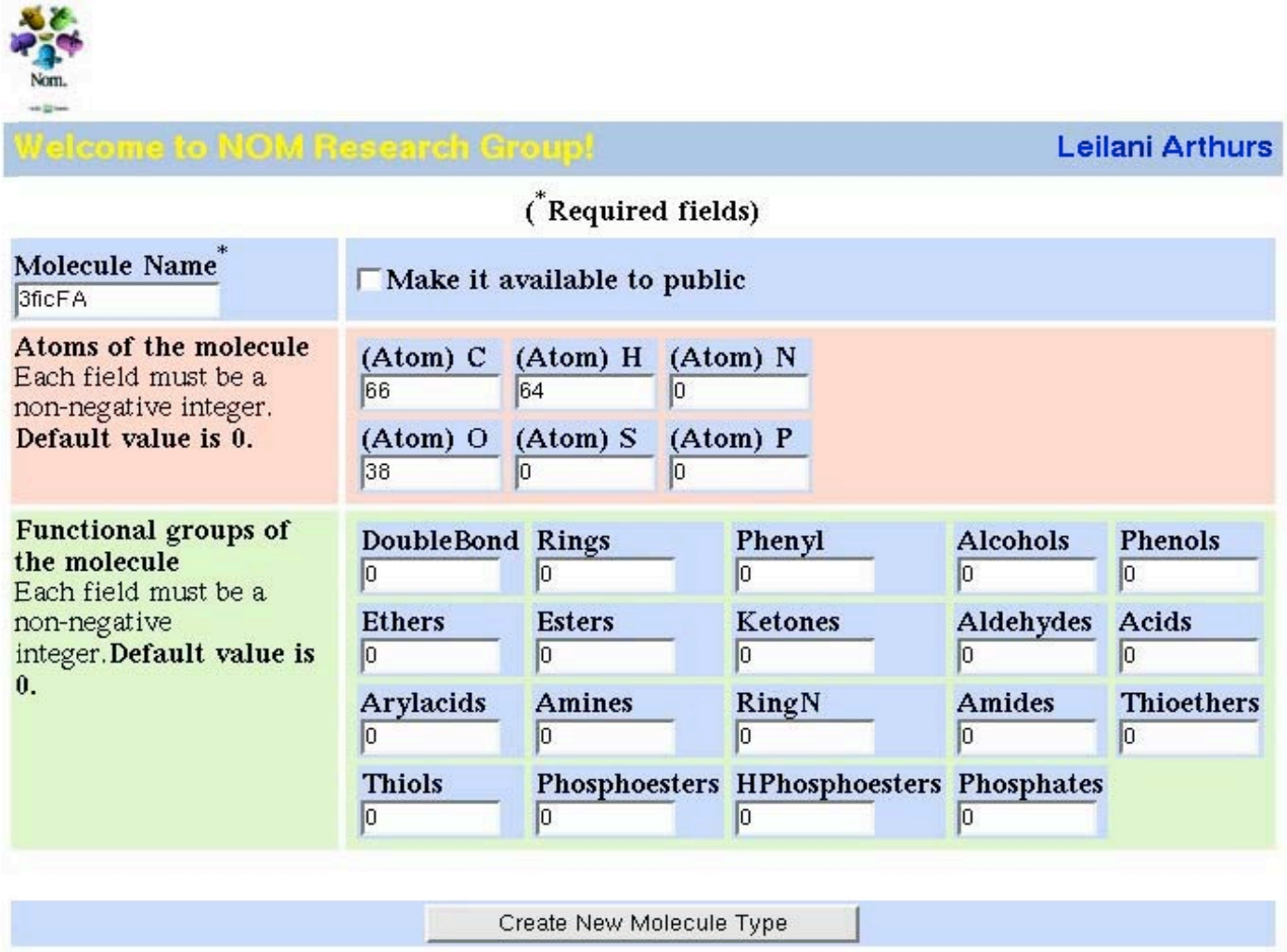
Access NOM simulation from Web



Web-based interface



Example of Interface



Report example

Please provide the following information.

Current Time Step is: 1969 Refresh

Time Step: 1969

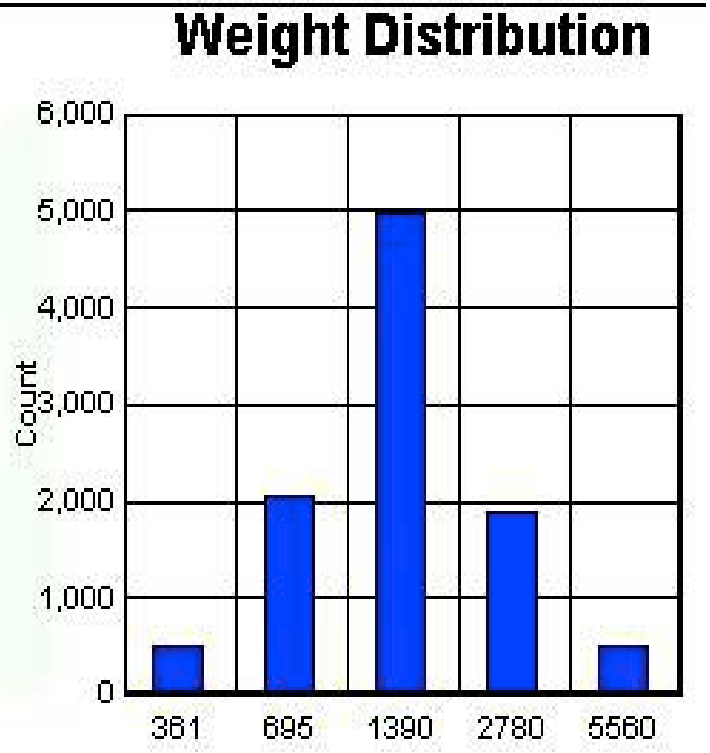
Status: adsorbed

Start Y: 0

End Y: 299

Generate Reports

Generate XML file



Intelligent interface components

- Email notification
- Running time prediction
  - Static
    - number of molecules
    - number of time steps
  - Dynamic
    - current time step
    - current wall clock time

Intelligent interface components (cont.)

- Find similar simulations
  - Environment parameters
  - Molecule types and distributions
  - Retrieve the data sets from database
  - Points on a high dimension space
  - Euclidean distance
  - Ordered list
  - Review the simulation results or restart

Intelligent interface components (cont.)

- Automatic restarter
  - Save the state of each objects in the system to database every check point
  - Load the state to the core simulation engine

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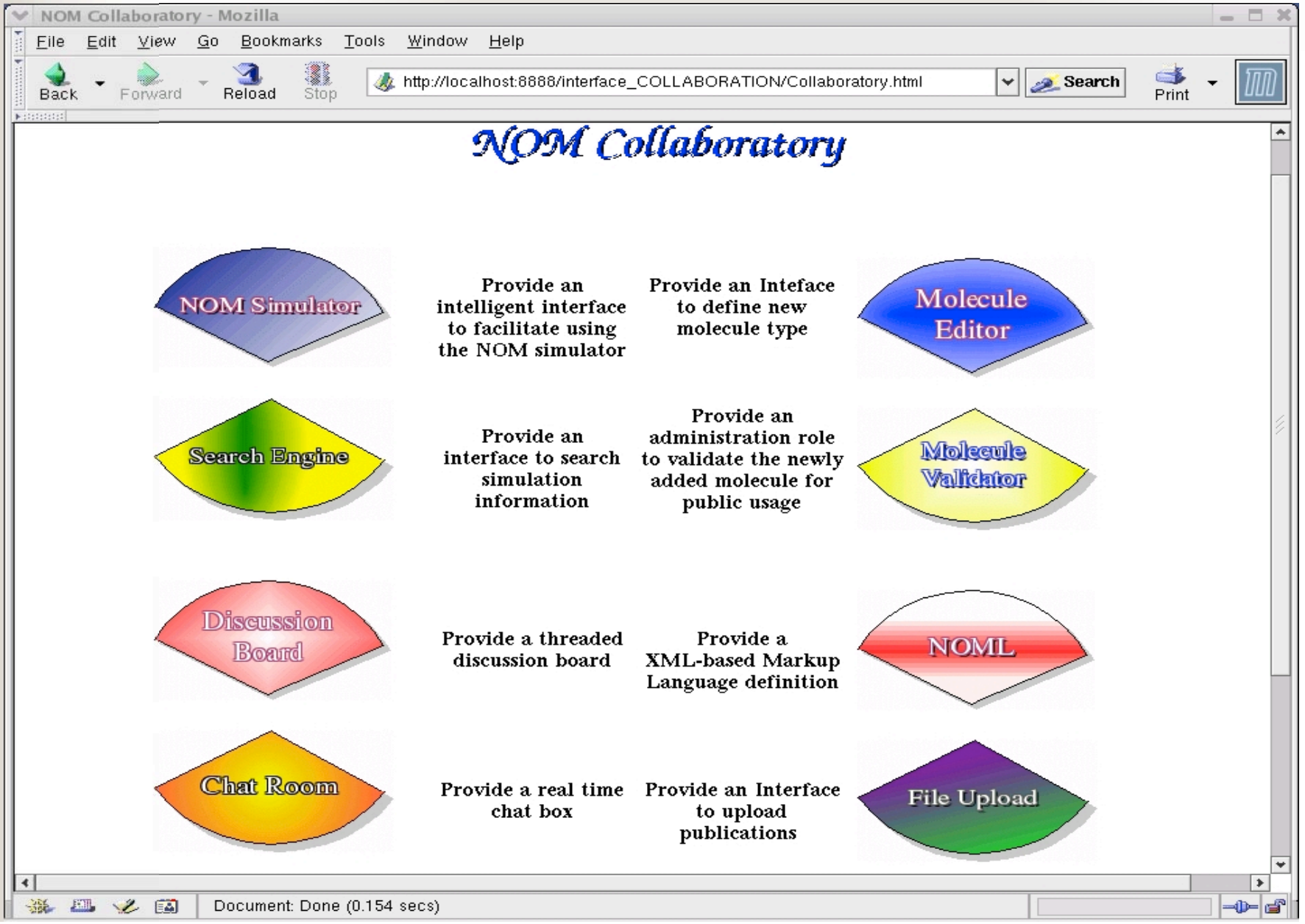
Previous work

- Combination of words “collaboration” and “laboratory” first coined by William Wulf (1996):
  Richard T. Kouzes, James D. Myers, and William A. Wulf. Collaboratories: Doing science on the internet. *IEEE Computer, 1996*
- Diesel Collaboratory: C. M. Pancerella, L. A. Rahn, and C. L. Yang: The diesel combustion collaboratory: combustion researchers collaborating over the internet. In *Proceedings of the 1999 ACM/IEEE conference on Supercomputing*
- BioCoRE: *http://ks.uiuc.edu/Research/biocore*
- EMSL Collaboratory: *http://www.emsl.pnl.gov:2080/docs/collab*

The NOM Collaboratory

- Interdisciplinary project
  - Chemists
  - Biologists
  - Ecologists
  - Computer Scientists
- Build and integrate software using J2EE
  - NOM modeling & simulation software
  - XML-based standard data format definitions
  - Data querying and manipulation tools
  - Electronic communication tools


NOM Collaboratory - Mozilla
File Edit View Go Bookmarks Tools Window Help
Back Forward Reload Stop
http://localhost:8888/interface_COLLABORATION/Collaboratory.html
Search
Print
NOM Collaboratory
NOM Simulator
Provide an intelligent interface to facilitate using the NOM simulator
Provide an Inteface to define new molecule type
Molecule Editor
Search Engine
Provide an interface to search simulation information
Provide an administration role to validate the newly added molecule for public usage
Molecule Validator
Discussion Board
Provide a threaded discussion board
Provide a XML-based Markup Language definition
NOML
Chat Room
Provide a real time chat box
Provide an Interface to upload publications
File Upload
Document: Done (0.154 secs)

XML-based NOM Markup Language (NOML)

- NOML:
  - Standard data format
    - Environment.dtd, Molecules.dtd, Setup.dtd
- Facilitate communication
  - User ===== User
  - Application ===== Application
- Extension

Other tools

- Molecule editor
  - Define new molecule type
- Molecule validator
  - Authorized persons (Chemists) to validate data
  - Share the molecule type
- Search engine
  - Ad-hoc query
  - View results of the completed simulations
  - Restart some simulations

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Conclusion

- Agent-based stochastic model for simulating the NOM evolution with discrete temporal and spatial properties
- A Web-based simulation architecture (multiple simulation servers, database servers, and data mining technologies)
- Database technologies
- A Web-based intelligent configuration interface
- The NOM collaboratory

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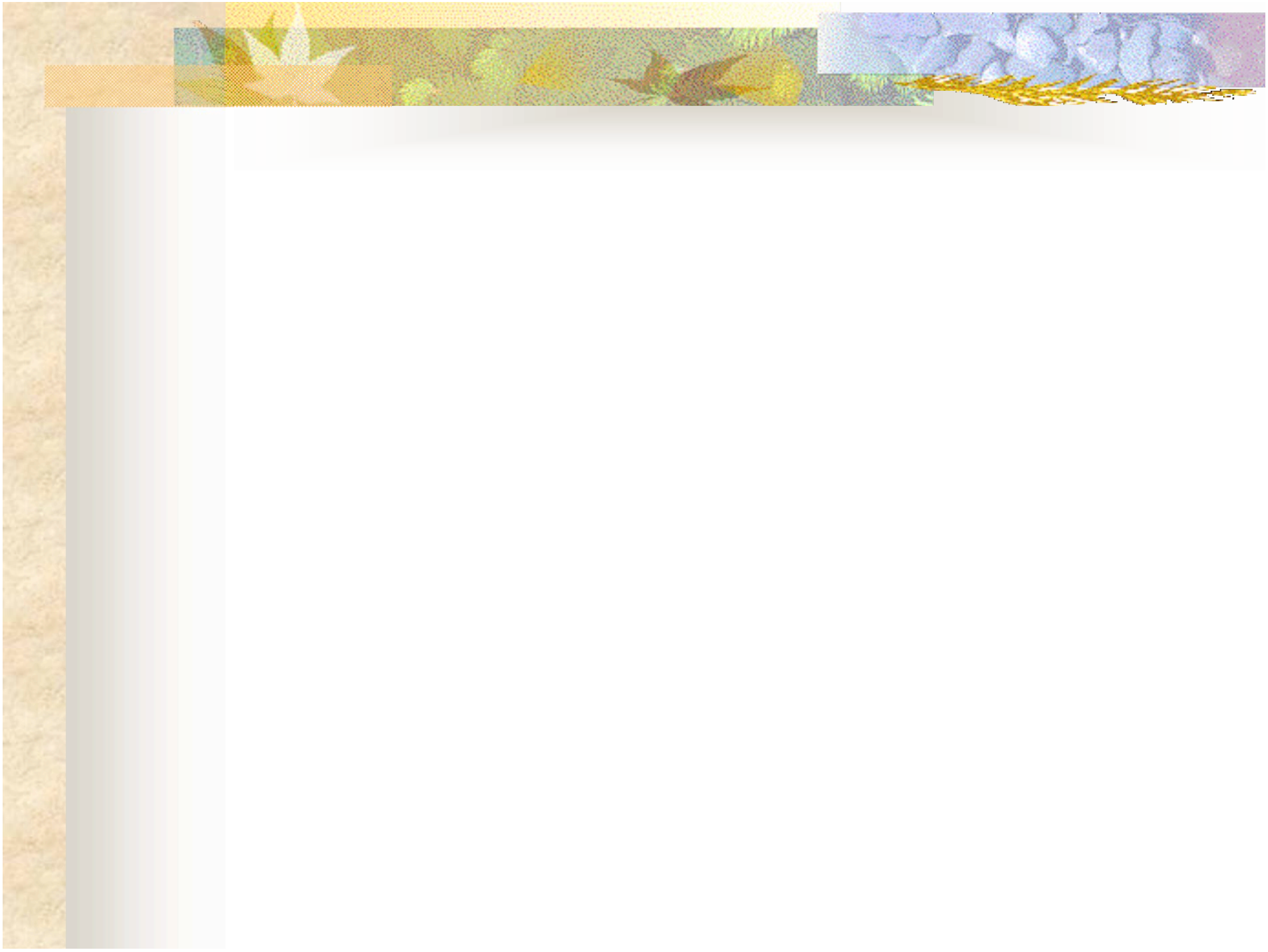
Future work

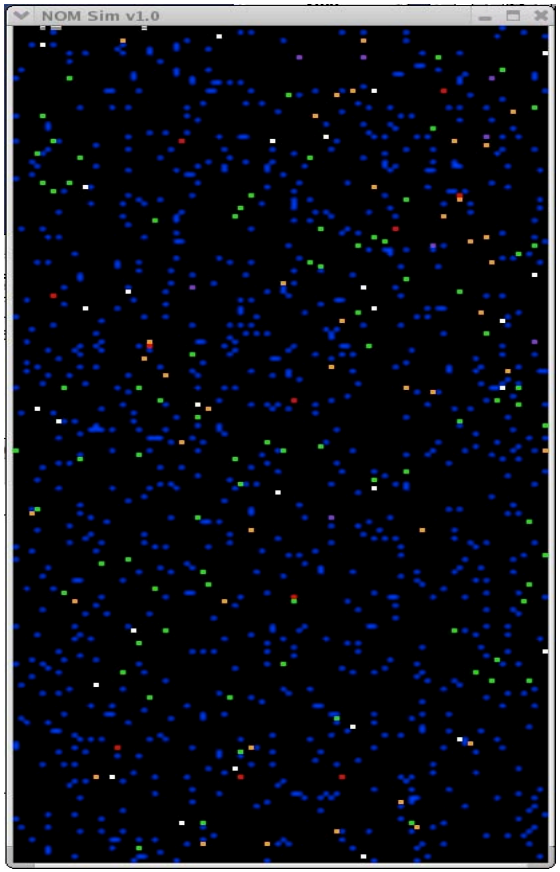
- Model testing (this summer)
  - Testing of the sorption process
  - More features need to be added into the core simulation engine
- Model validation (this summer)
- Collaboratory:
  - More communication tools
  - More simulation models for NOM study
  - NOML extension

Thank You !

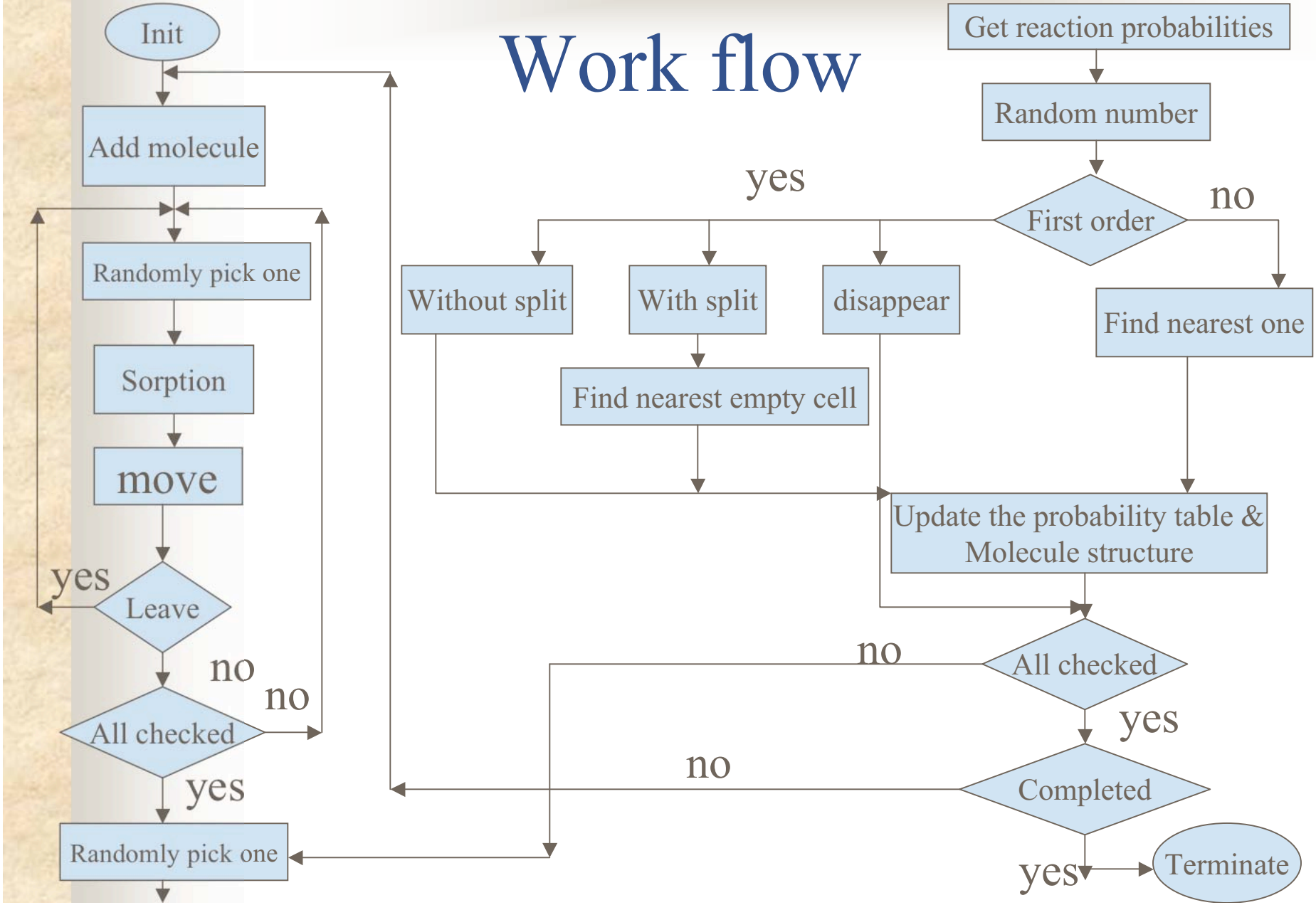
Questions?



GUI version



Work flow


Init
Add molecule
Randomly pick one
Sorption
move
yes
Leave
no
All checked
no
yes
Randomly pick one
Get reaction probabilities
Random number
yes
First order
no
Without split
With split
disappear
Find nearest one
Find nearest empty cell
Update the probability table &
Molecule structure
no
All checked
yes
no
Completed
yes
Terminate