

# Information Technology in Support of the Simulation of Natural Organic Matter (NOM) in the Soil

Yingping Huang

Eric Chanowich

Xiaorong Xiang

Gregory Madey

Computer Science & Engineering  
University of Notre Dame

# Abstract

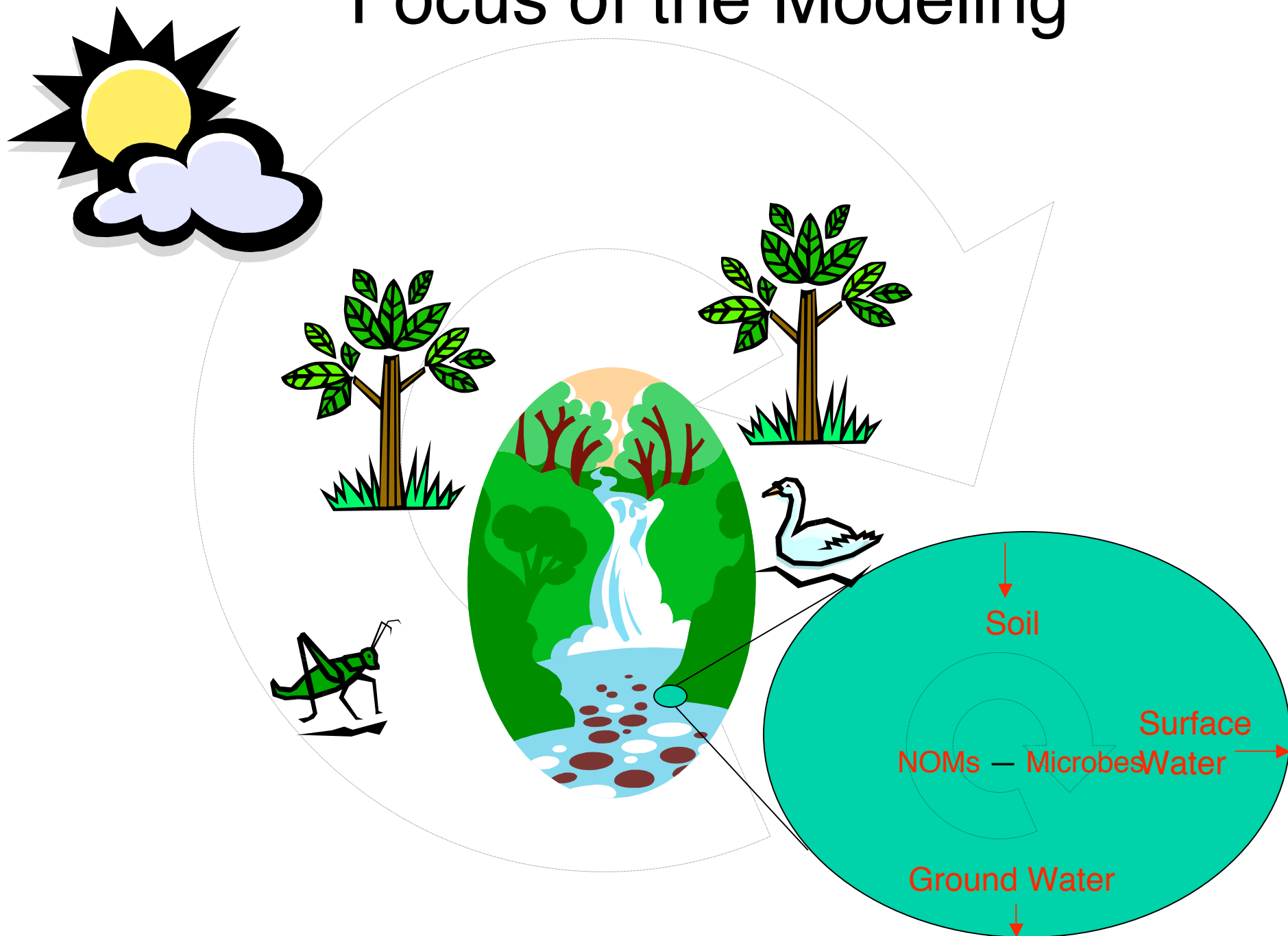
We describe an application of infrastructure, query Optimization, data warehousing and data mining technologies in support of the simulation of Natural Organic Matter (NOM) in the soil.

We present an agent-based stochastic simulation of NOM transformations. It employs advanced information technologies such as J2EE, Oracle, data warehousing and data mining to improve the reliability and scalability of the stochastic simulations and to facilitate analysis of the resulting large datasets.

# Natural Organic Matter

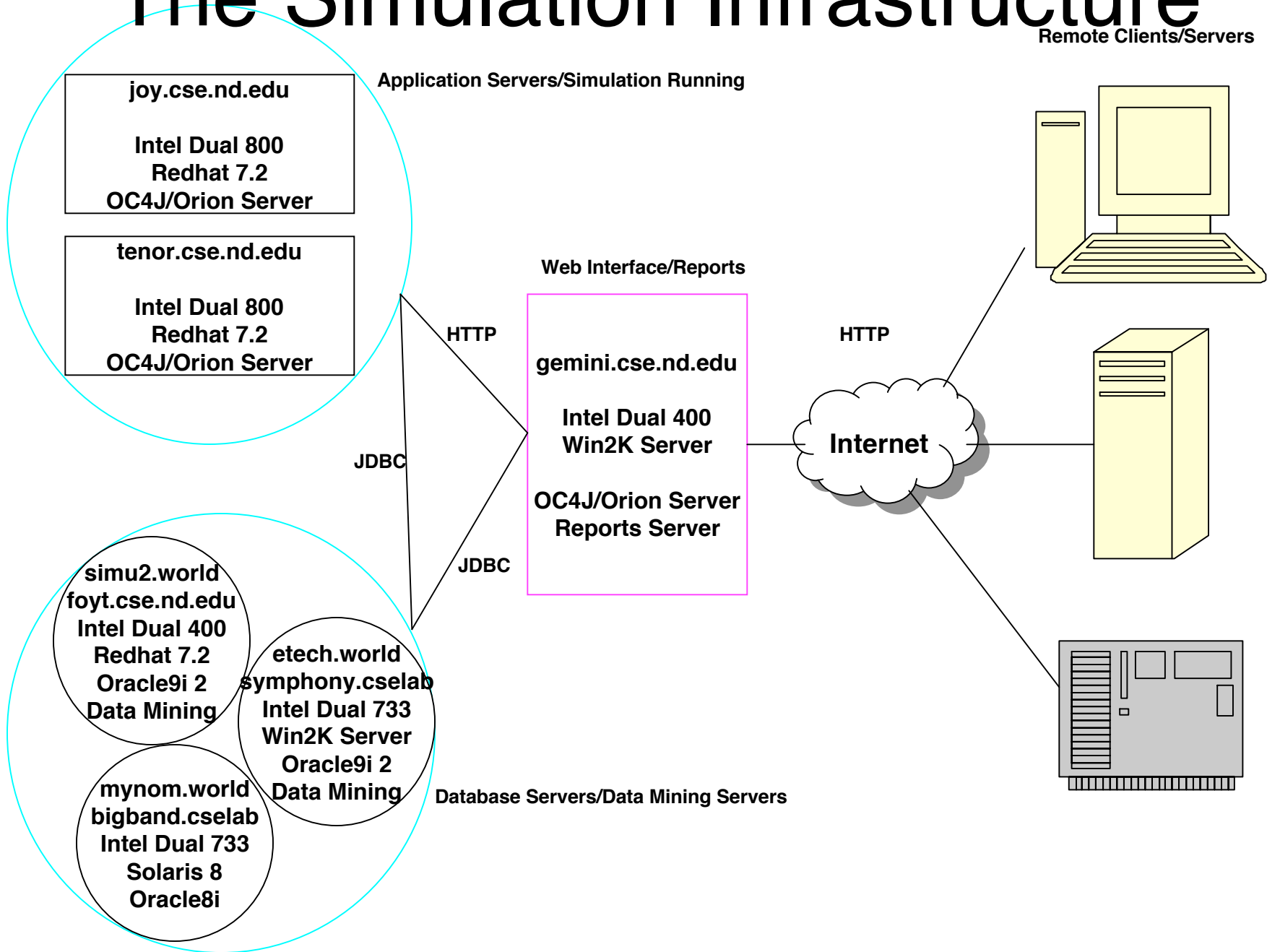
- NOM is ubiquitous in terrestrial, aquatic and marine ecosystems
  - Results from breakdown of animal & plant material in the environment
- Important role in processes such as
  - compositional evolution and fertility of soil
  - mobility and transport of pollutants
  - availability of nutrients for microorganisms and plant communities
  - growth and dissolution of minerals
- Important to drinking water systems
  - Impacts drinking water treatment
  - Impacts quality of well water

# Focus of the Modeling



# The Simulation Infrastructure

Remote Clients/Servers



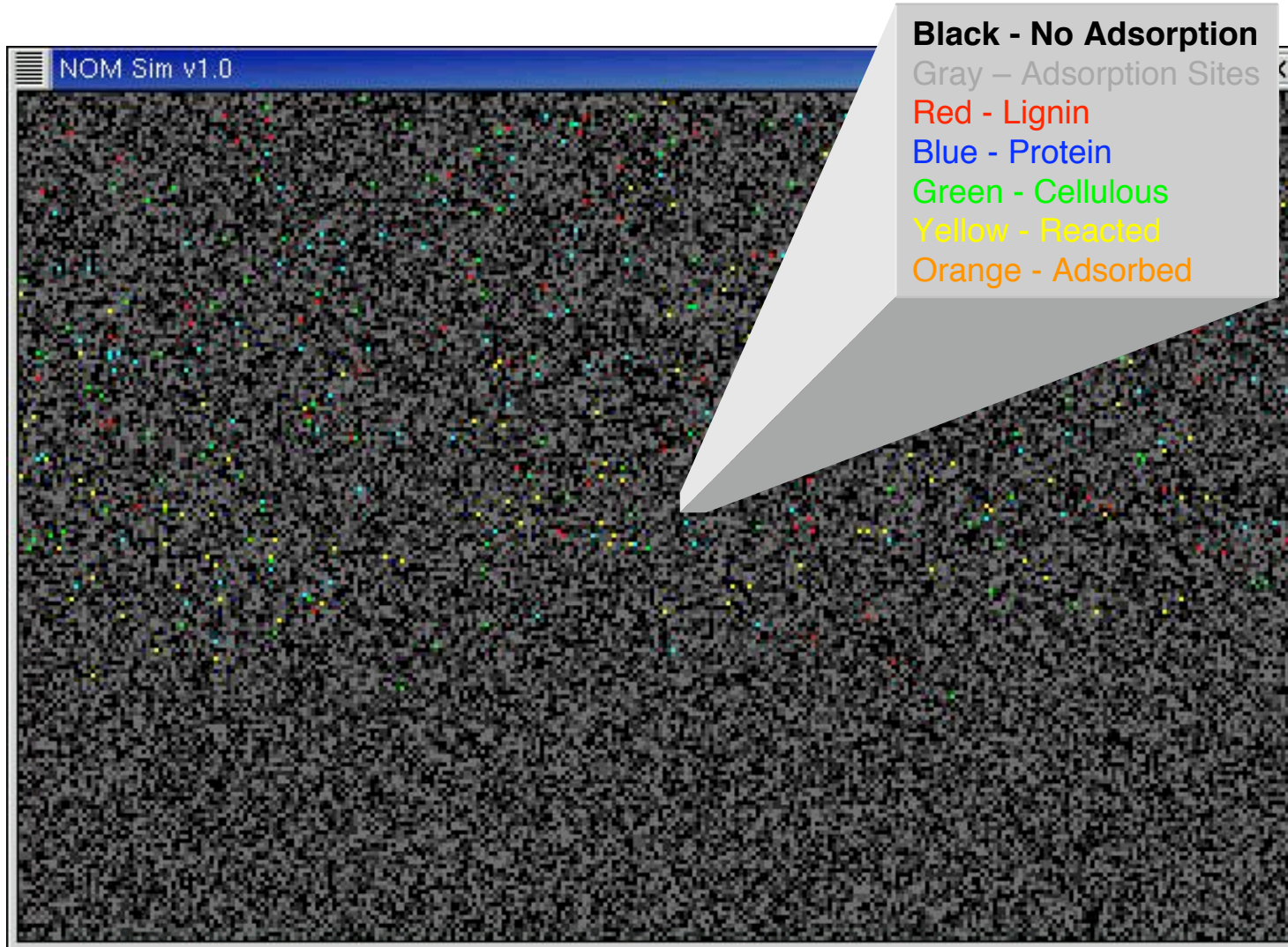
# NOM 1.0

- Distributed systems
  - 2 Application servers (Orion Servers)
  - 3 Database servers (Oracle)
  - Reports server (OC4J Server/Reports Server)
- Load balancing (round robin based on computational needs)
  - application servers & database servers
- Fail over
  - application servers & database servers
- Why fail-over (Assume down probability  $p$  for each machine)
  - No fail-over
    - **Simulation system down probability:  $1-(1-p)^2 = 2p-p^2$**
  - With fail-over
    - **Simulation system down probability:  $1-(1-p^2)(1-p^3) = p^2 + p^3 - p^5$**
  - Improvement:
    - **$2/p = 200$  if  $p=0.01$  (the smaller  $p$ , the larger improvement)**

# The Simulation Model

- Agent-based stochastic simulation
- GUI version - stand alone
  - Animation of molecules
- Web-based version
  - Using OC4J server & Oracle Reports
  - Oracle database servers
- Load-balancing & fail-over
  - Goal: efficiency, availability & reliability
- Data warehousing & Data Mining
  - Goal: data/pattern analysis

# GUI Animation



Netscape: Online NOM Simulation

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Location: <http://gemini.cse.nd.edu:8888/nom/homepage.jsp> What's Related

Red Hat Network Support Shop Products Training

# NOM Simulator

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:

New users? [Sign up now](#)

Windows taskbar icons: Start, Network, Internet Explorer, Messenger, Outlook, Paint

File Edit View Go Communicator Help

Back Forward Reload Home Search Netscape Print Security Shop Stop

Location: [http://gemini.cse.nd.edu:8888/reports/nom/reactions3.jsp?user\\_id=1&se](http://gemini.cse.nd.edu:8888/reports/nom/reactions3.jsp?user_id=1&se) What's Related

Red Hat Network Support Shop Products Training

# NOM Simulator

Welcome to NOM Research Group! X Y

## NOM Simulator: Reports

---

### Reactions By Type

Reaction Type	Reactions
1	660
2	0
3	0
4	10
5	110
6	125
7	410
8	370
9	60

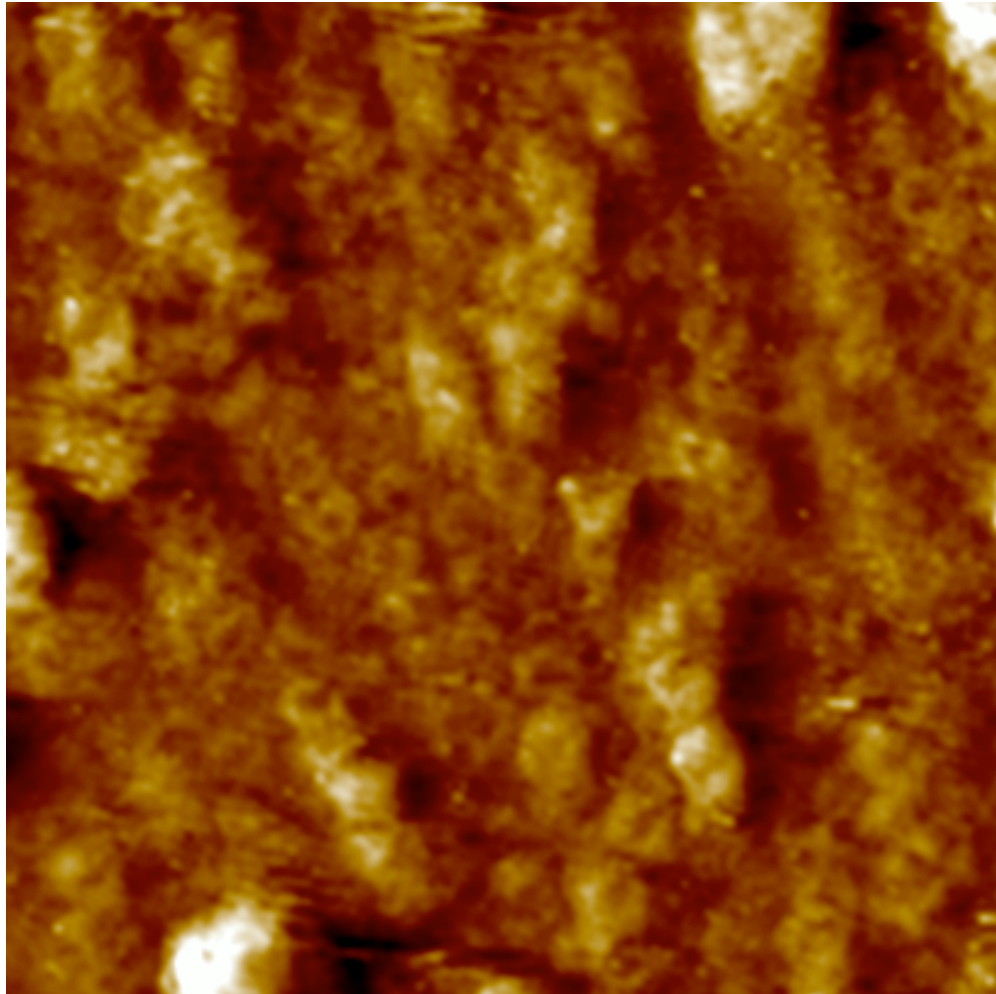
### Reactions vs Time

Time	Reactions
0	0
10	450
20	750
30	850
40	950
50	1100
60	1250
70	1400
80	1550
90	1650

# Insertion and Query Performance Comparison

Scenario (>16million)	Insertion (sec/row)	Query Time
No indexes No aggregation	0.0106	>1 hour
With indexes	0.0122	>0.5 hour
With aggregations	0.0107	5 seconds

# Data Mining & Micelle Formation



NOM  
Rings

Maurice, 1999

# Conclusion & Acknowledgement

- Contributions are
  - New model which treats NOM as a heterogeneous mixture
  - Simulation system with advanced web & database tools
  - System aspects of implementation of load-balancing and fail-over
  - Basic data mining features
- Acknowledgement
  - Steve Cabaniss, Chemistry, UNM
  - Patricia Maurice, CE/GEOS, UND