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

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Abstract

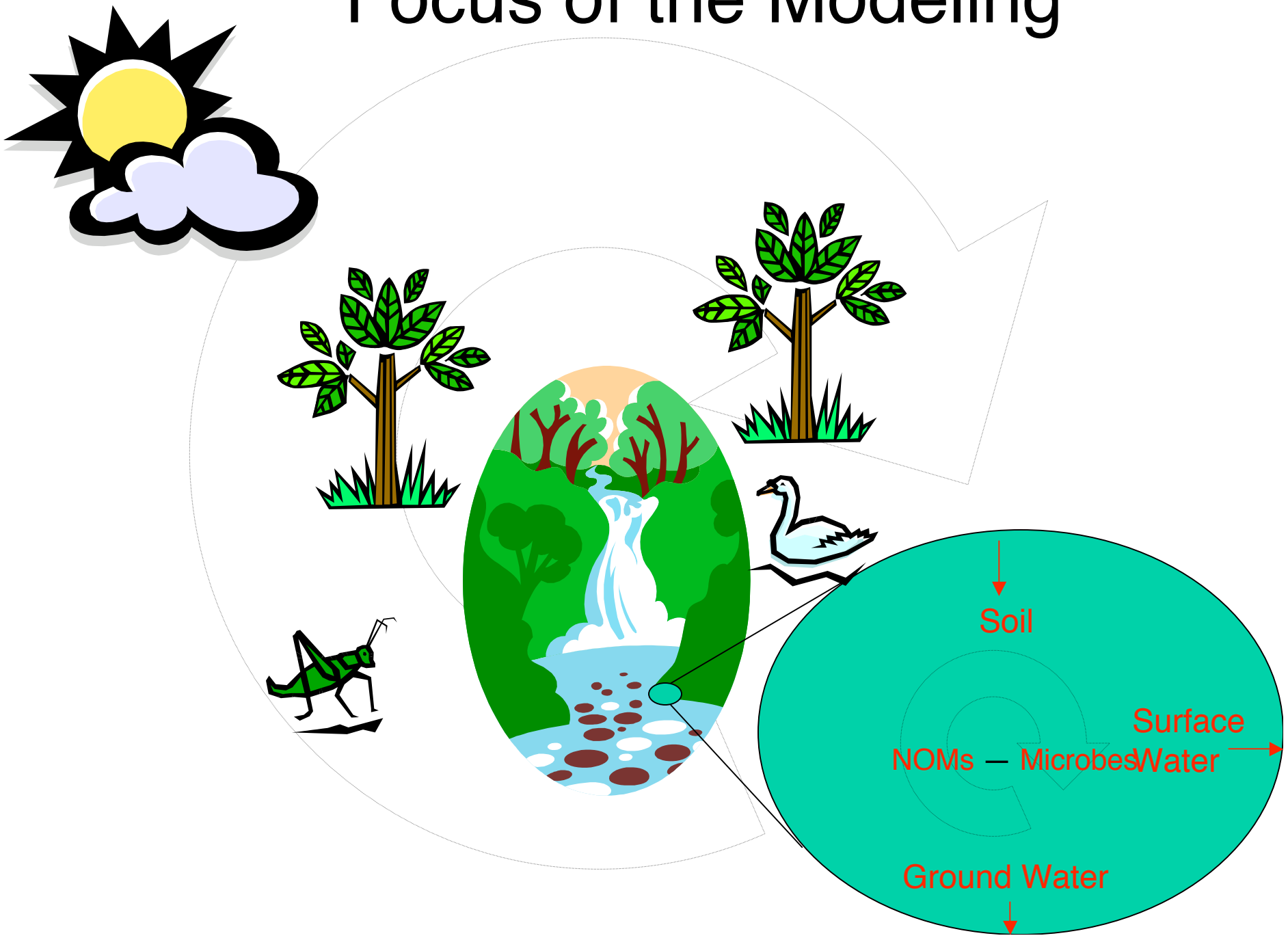
We describe an application of infrastructure, query Optimization, data warehousing and data mining technologies in support of the simulation of Natural Organic Matter (NOM) in the soil.

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.

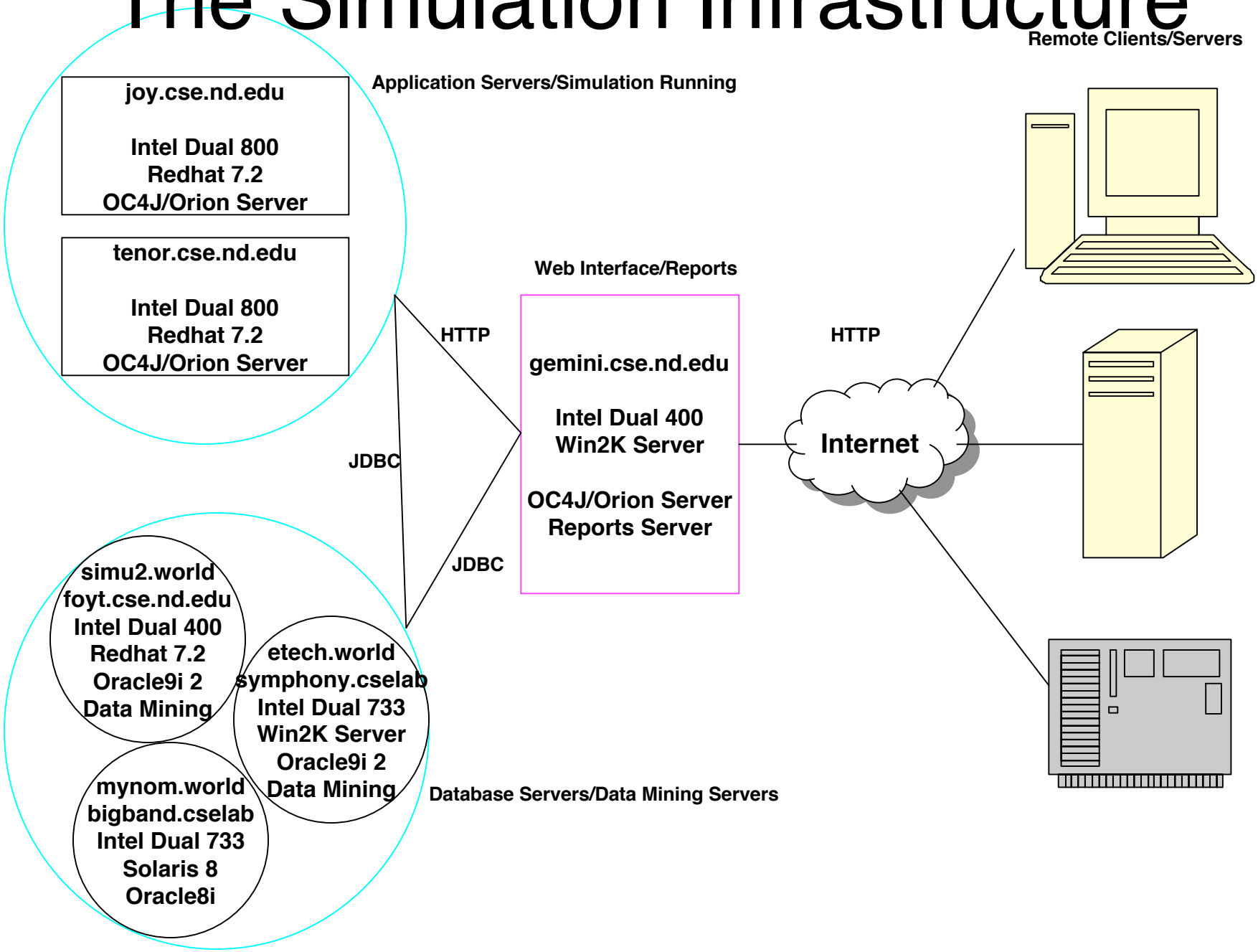
Natural Organic Matter

- 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



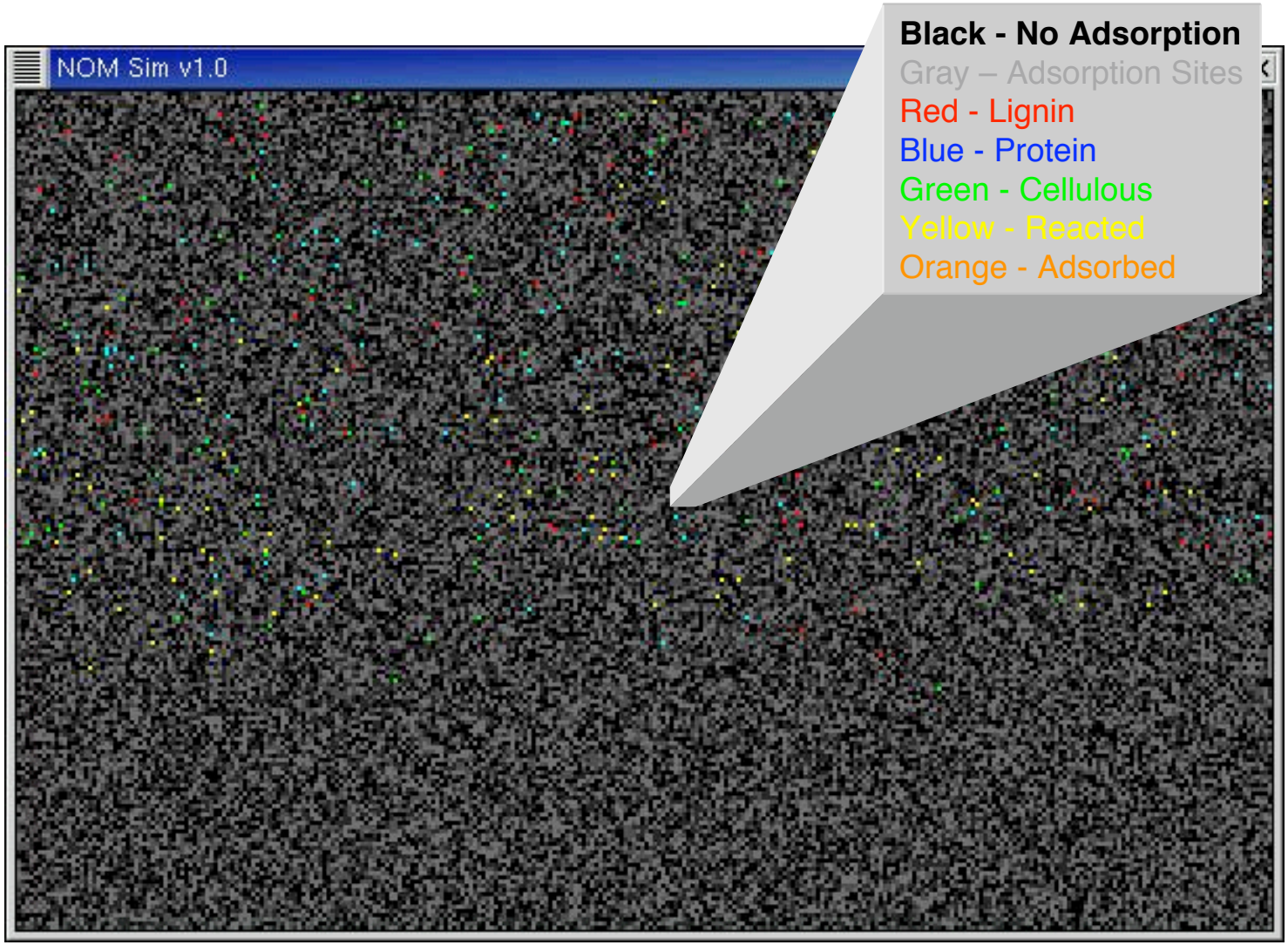
NOM 1.0

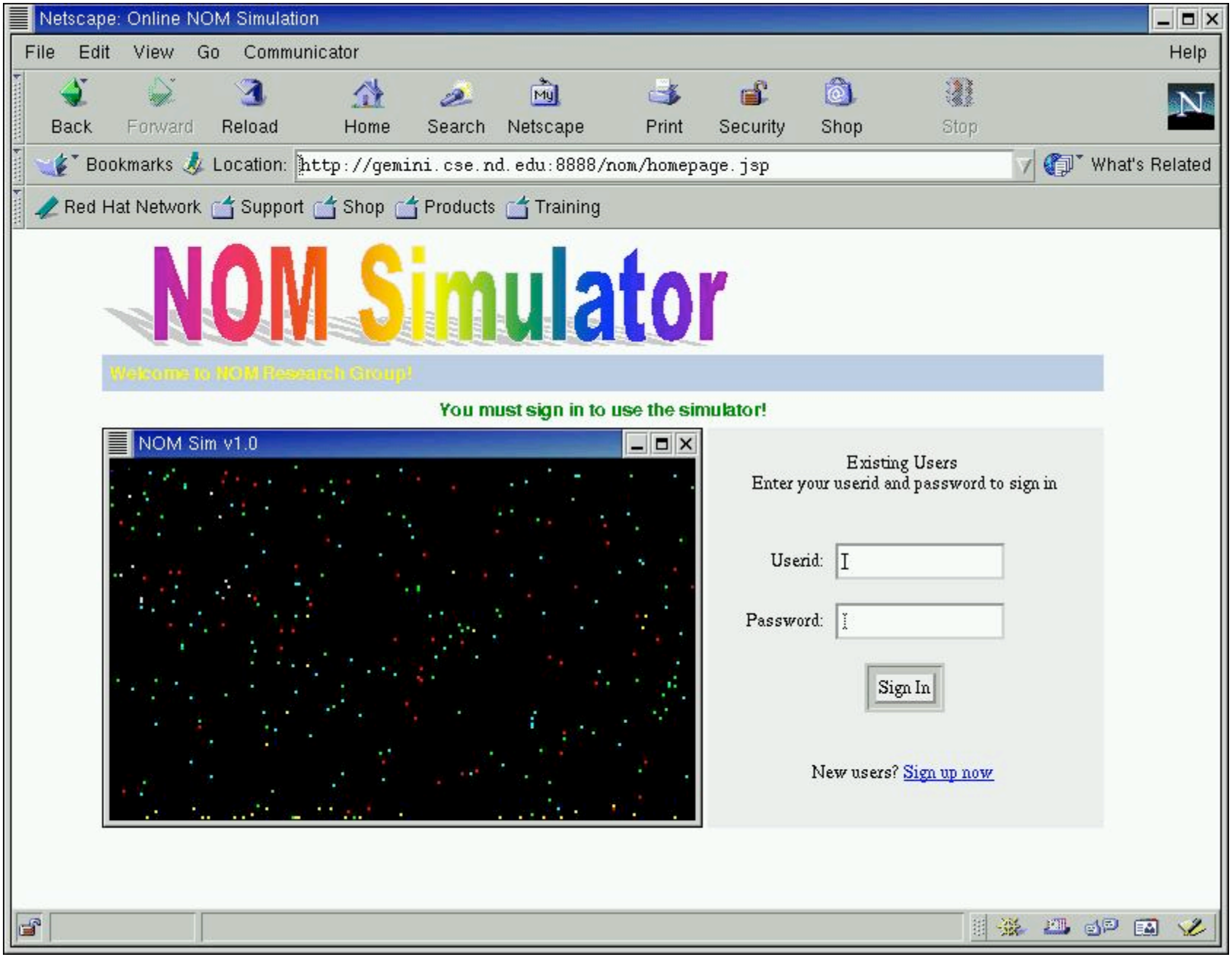
- Distributed systems
  - 2 Application servers (Orion Servers)
  - 3 Database servers (Oracle)
  - Reports server (OC4J Server/Reports Server)
- Load balancing (round robin based on computational needs)
  - application servers & database servers
- Fail over
  - application servers & database servers
- 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

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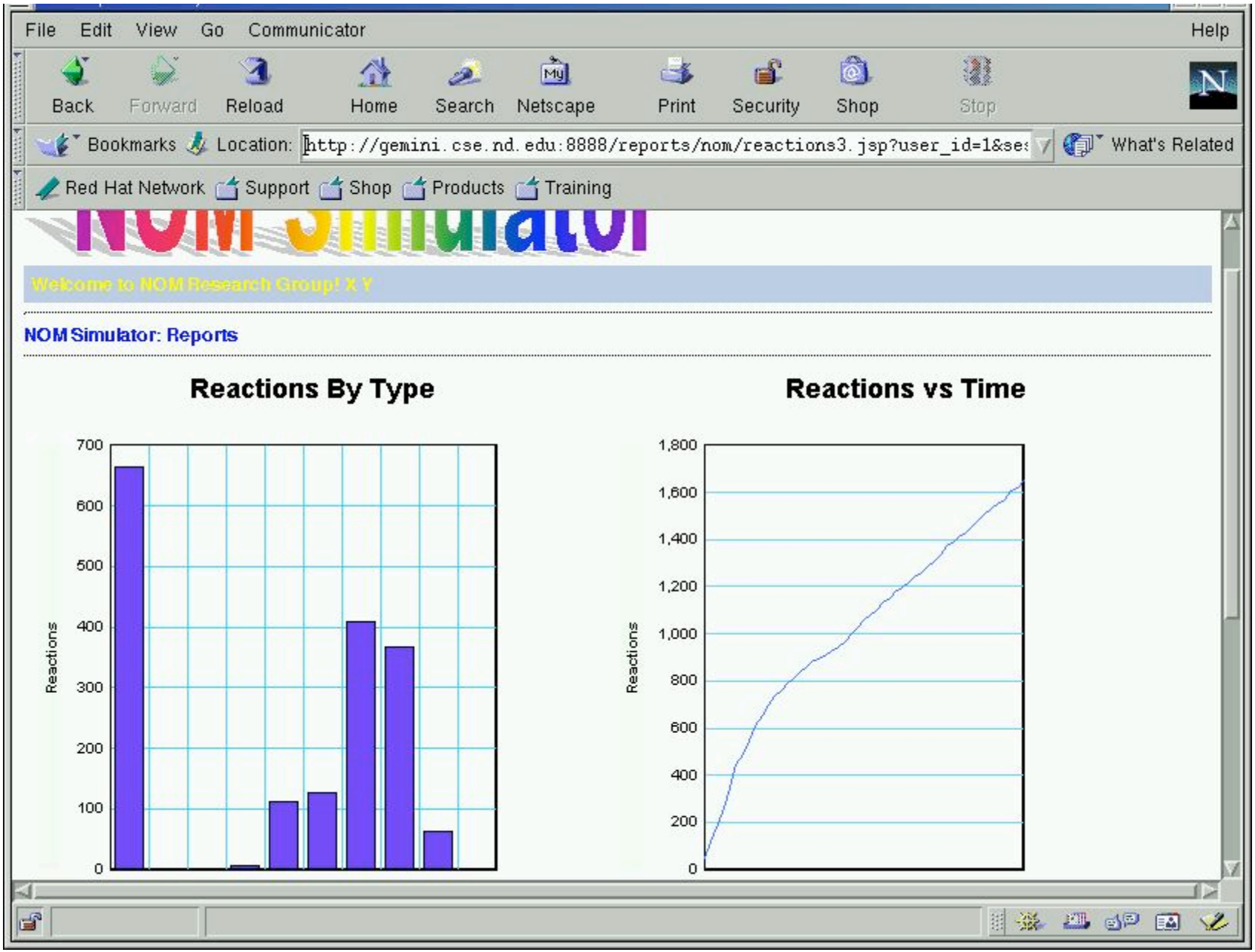
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NOM Simulator: Reports
Reactions By Type
Reactions
700
600
500
400
300
200
100
0
Reactions vs Time
Reactions
1,800
1,600
1,400
1,200
1,000
800
600
400
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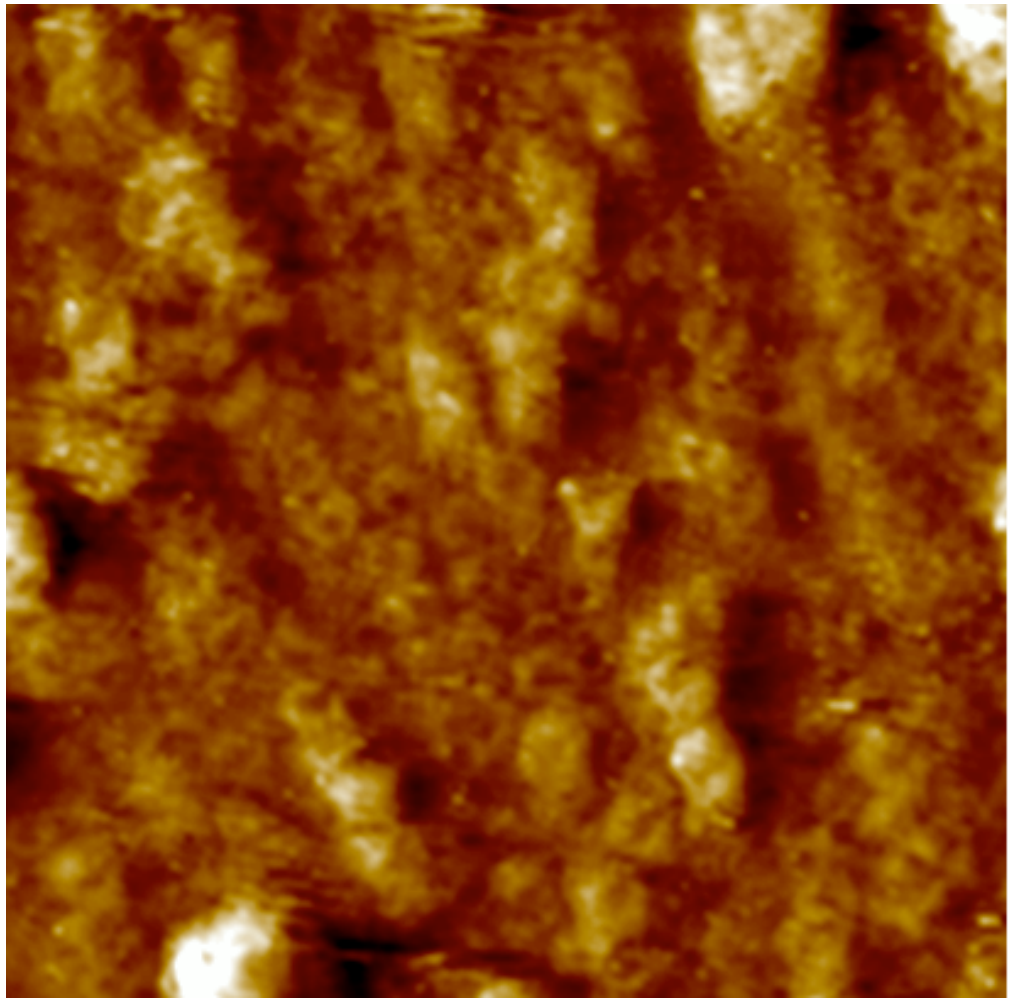
Insertion and Query Performance Comparison

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
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