# An Online Environmental Research Portal

Xiaorong Xiang  Yingping Huang  Greg Madey
Department of Computer Science and Engineering
University of Notre Dame

Steve Cabaniss
Department of Chemistry
University of New Mexico

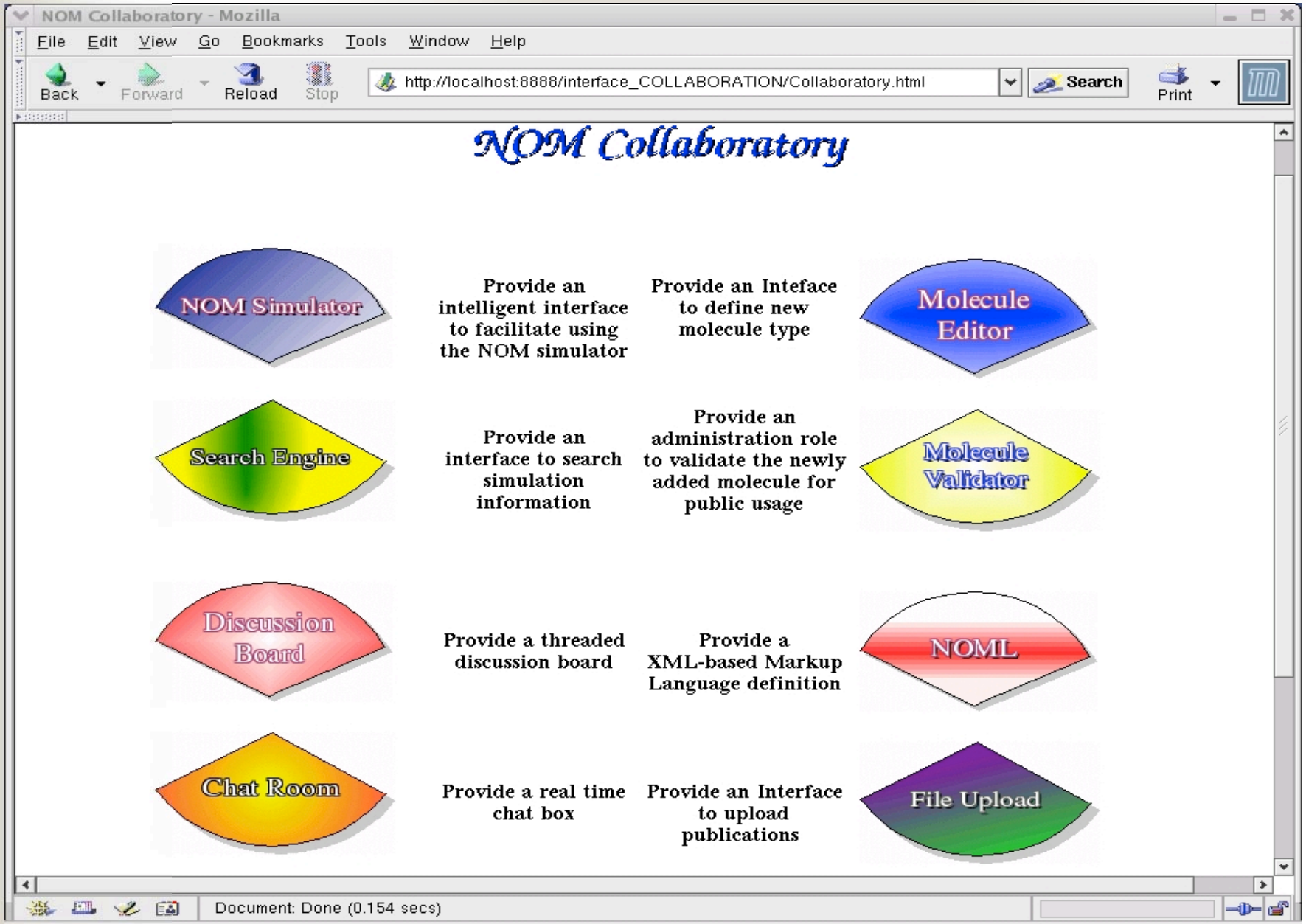
NDEER 2003 – 11/12/2003
*This research was supported in part by NSF ITR Grant No. 0112820*

# Introduction

- Interdisciplinary project
  - Supporting research on Natural Organic Matter (NOM)
  - Understanding NOM behavior is an important environmental research area
  - Simulations of NOM in the soil and groundwater
- Objectives
  - Information and model sharing
  - Data repository and analysis support tools
  - Electronic communication tools
- No installation or maintenance of computation resources needed by the environmental scientists

# NOM Portal Components

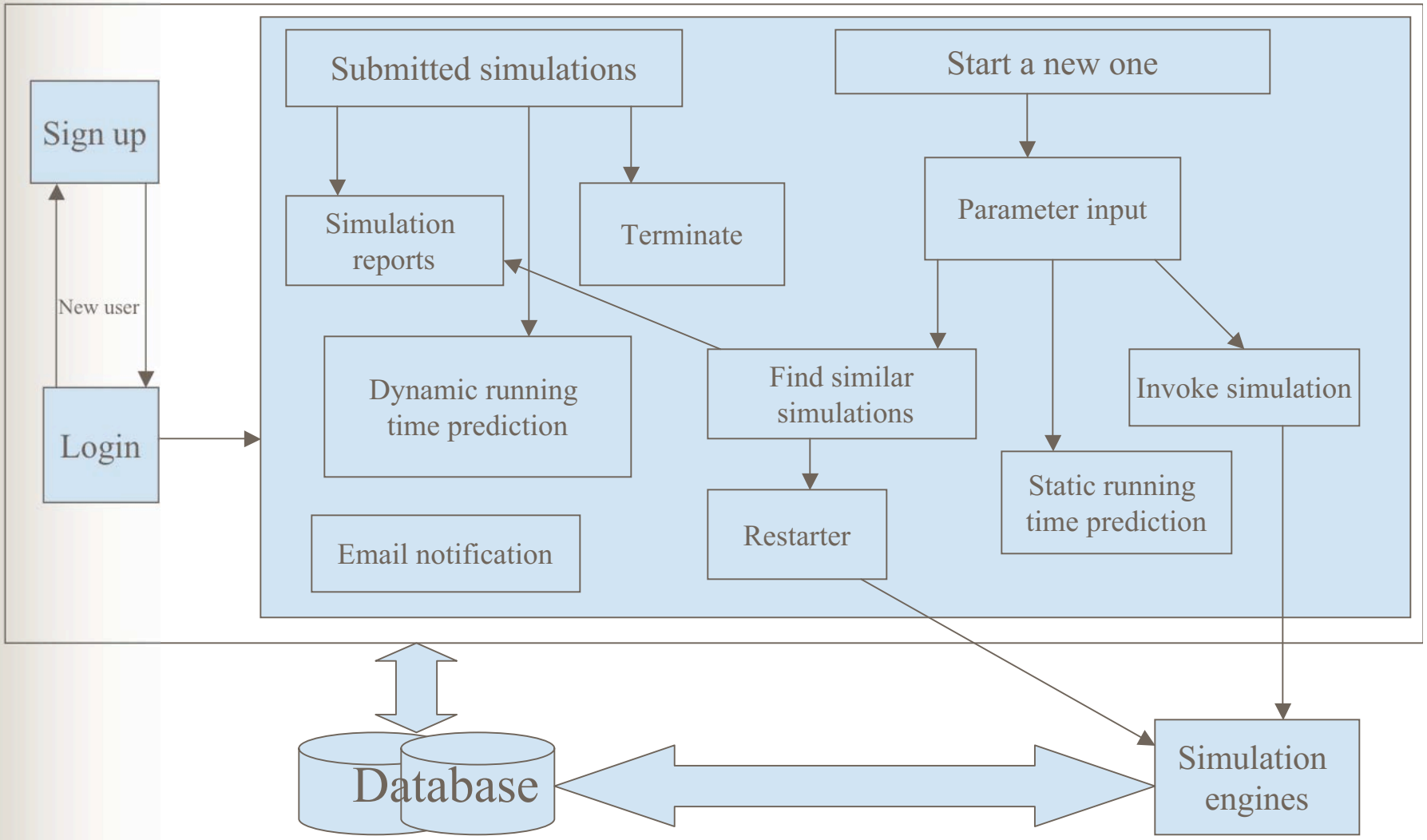
- NOM simulators
- Search engine
- NOML upload
- Molecule editor
- Molecule validation
- Simulation finder
- Automatic restart
- Completion predictor
- Data Analysis
  - Graphical reports
  - XML reports
  - Data mining
- Communication Tools
  - Discussion board
  - Chat room
  - File sharing


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)

# Web Technologies

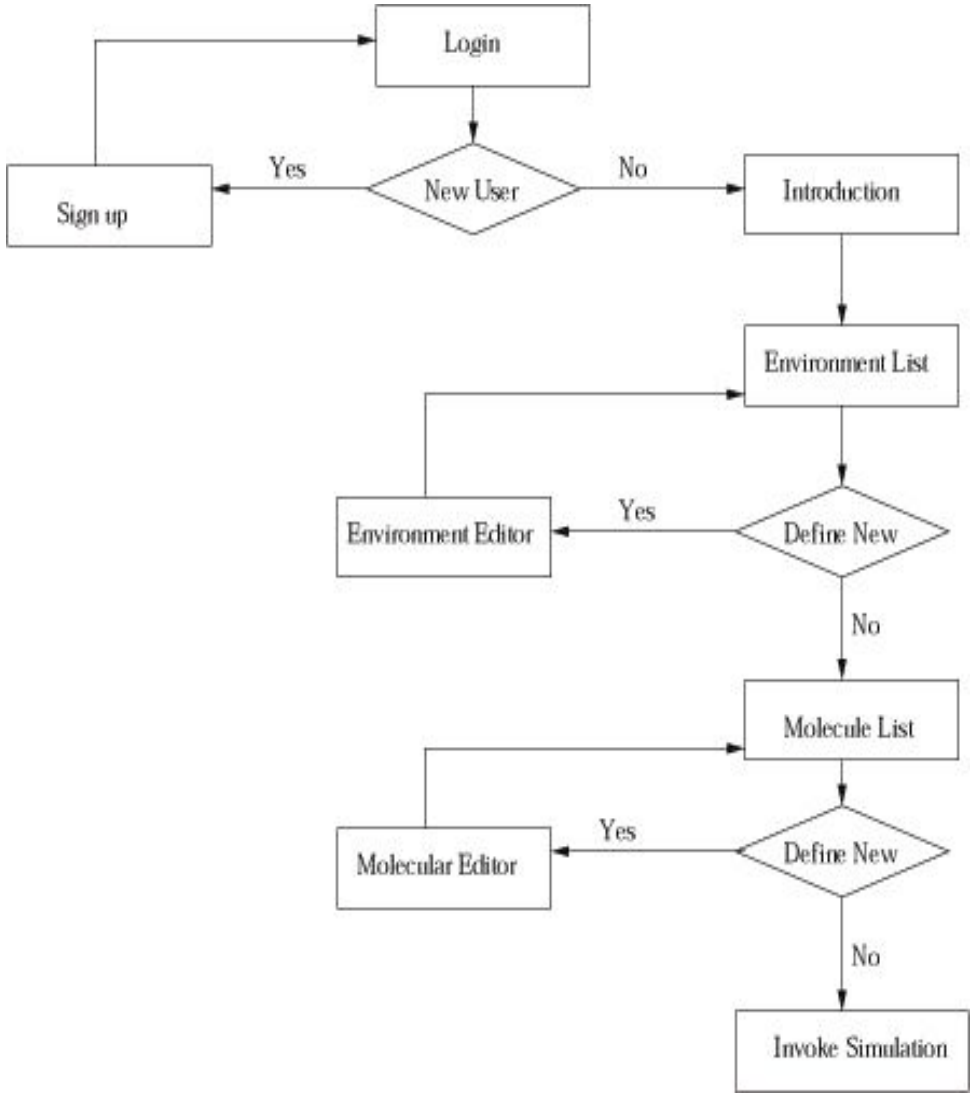
- Sun Java 2 Enterprise Edition (J2EE)
  - Java Servlets, Java Server Pages (JSP)
  - Enterprise Java Beans (EJB)
  - Java Transaction Service/API (JTS/JTA)
- RDBMS (Oracle):
  - Java DataBase Connectivity (JDBC)
  - Data analysis packages
  - Data mining technologies
- XML
  - NOML
  - XSQL

# Web-based Interface



# Web-based Interface Logic

- Input the simulation parameters
- Invoke the simulation
- Stop the simulation
- View the real-time simulation results



# Example of Interface


**Welcome to NOM Research Group!** **Leilani Arthurs**

(*Required fields)

**Molecule Name*** 3ficFA

☐ **Make it available to public**

**Atoms of the molecule**
Each field must be a non-negative integer.
**Default value is 0.**

| (Atom) C | (Atom) H | (Atom) N |
|---|---|---|
| 66 | 64 | 0 |
| **(Atom) O** | **(Atom) S** | **(Atom) P** |
| 38 | 0 | 0 |

**Functional groups of the molecule**
Each field must be a non-negative integer.**Default value is 0.**

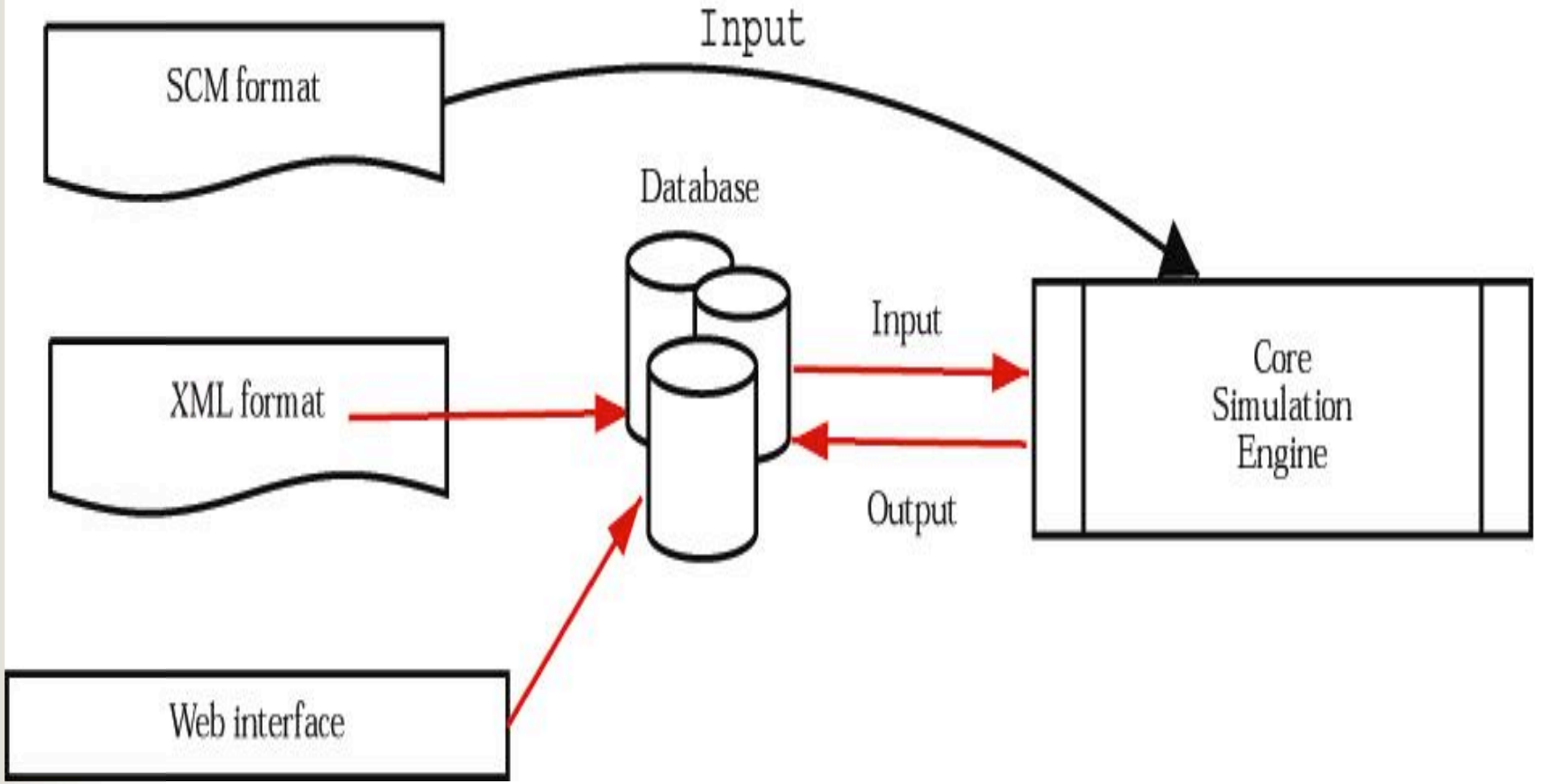
| DoubleBond | Rings | Phenyl | Alcohols | Phenols |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| **Ethers** | **Esters** | **Ketones** | **Aldehydes** | **Acids** |
| 0 | 0 | 0 | 0 | 0 |
| **Arylacids** | **Amines** | **RingN** | **Amides** | **Thioethers** |
| 0 | 0 | 0 | 0 | 0 |
| **Thiols** | **Phosphoesters** | **HPhosphoesters** | **Phosphates** | |
| 0 | 0 | 0 | 0 | |

Create New Molecule Type

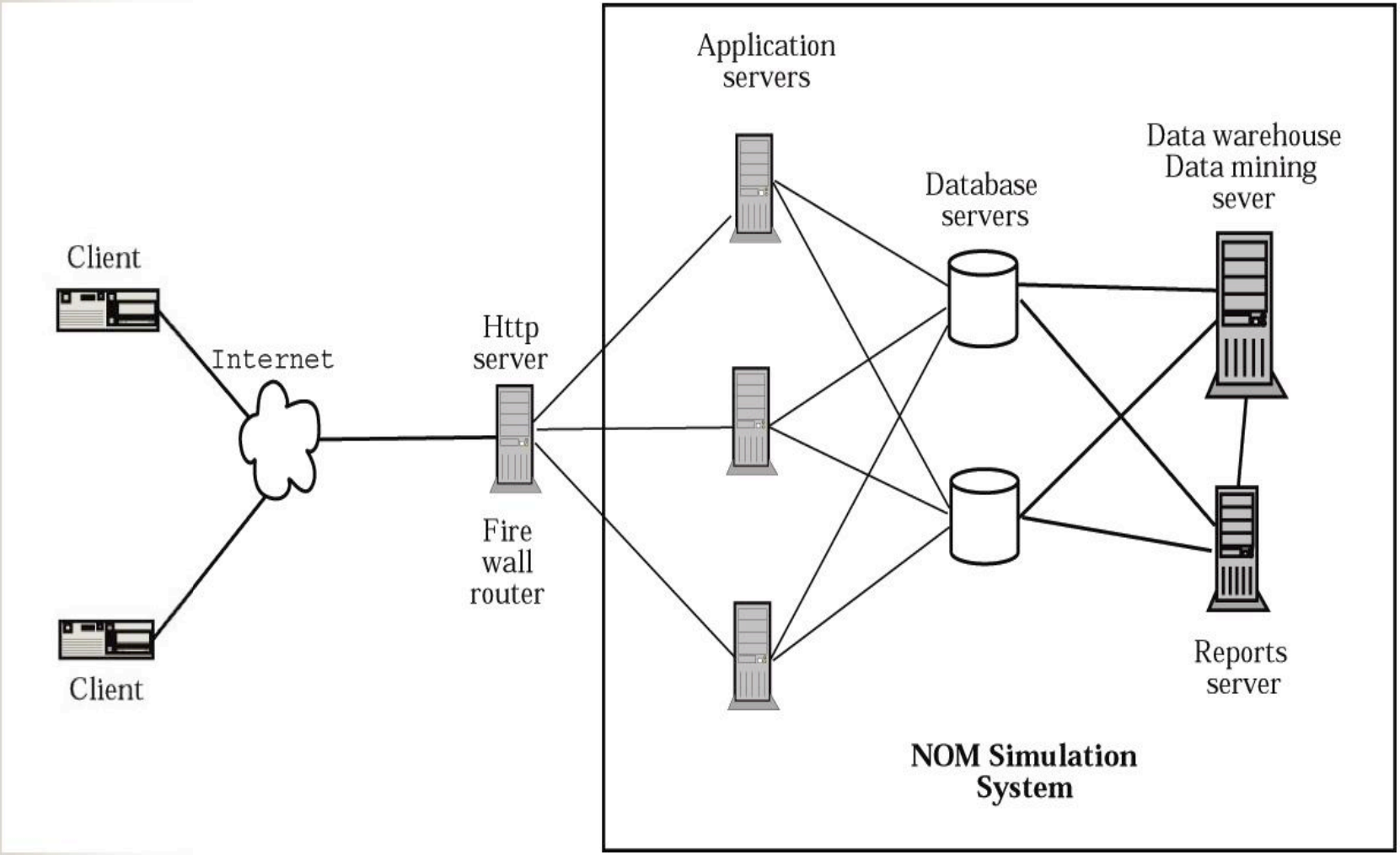
# XML-based NOM Markup Language

- NOML:
  - Standard data format
  - Environment.dtd, Molecules.dtd, Setup.dtd
  - Environment.xml, Molecules.xml, Setup.xml
- Facilitates communication
  - User ==== User
  - Application ==== Application
  - User ==== Application
- Extensions planned

# Data Input Options

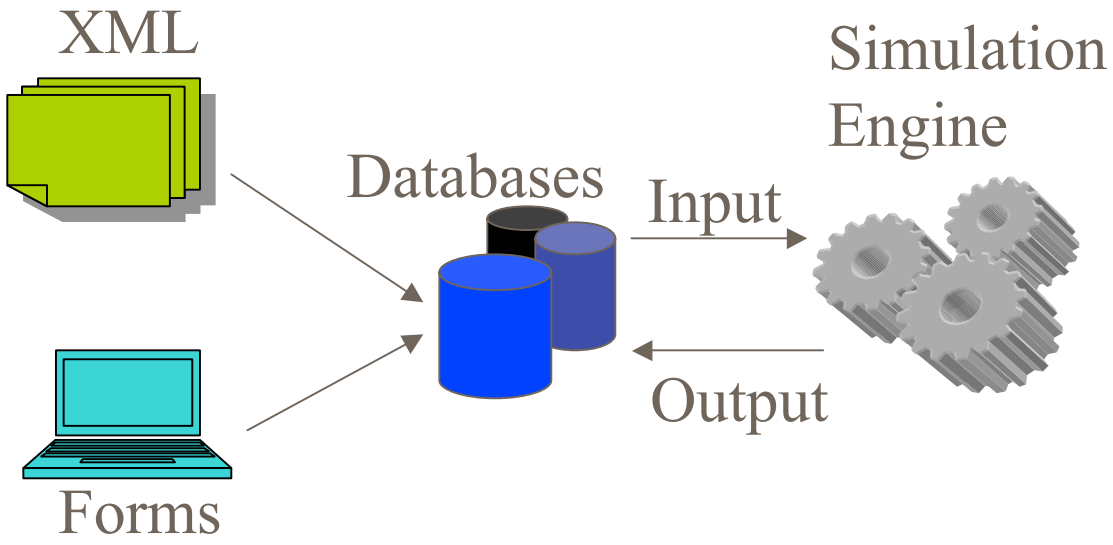


# Architecture

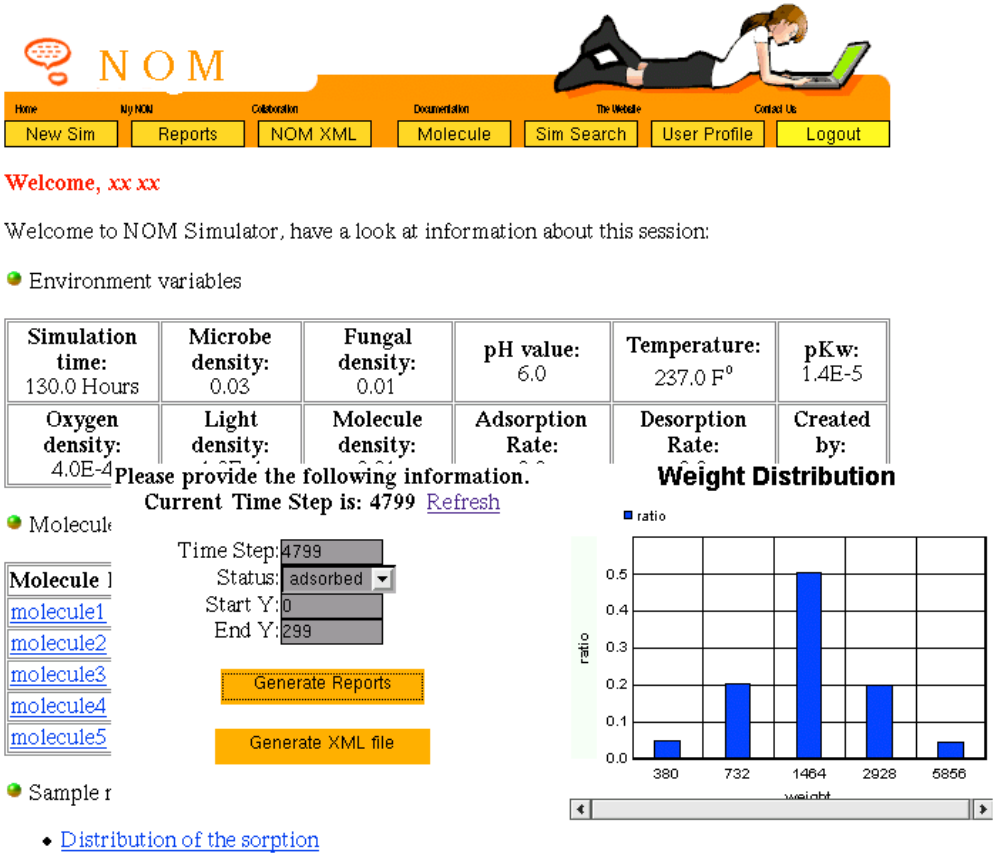


# NOM Simulation Engine

- Design
  - Agent-based
  - Stochastic
  - Discrete event
- Packages
  - Swarm
  - RePast
- Languages
  - Java
  - SQL & PL/SQL



# Report Example



# Conclusion

- Web-based Collaboratory
- A Web-based simulation architecture (multiple simulation servers, database servers, and data mining technologies)
- A Web-based configuration interface
- NOML data upload