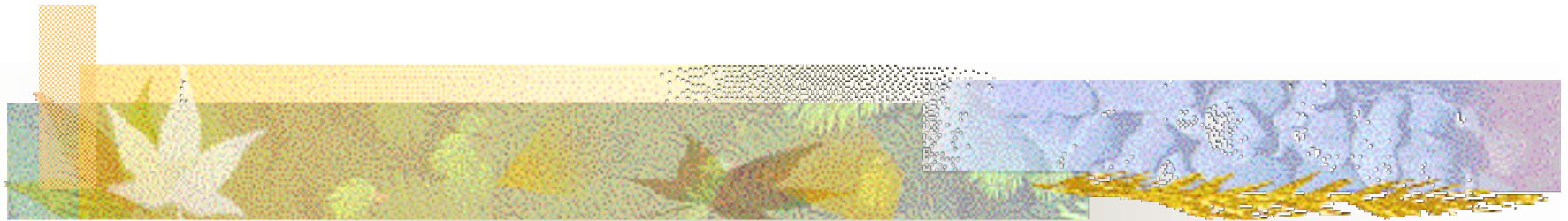


# An Online Environmental Research Portal



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# 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](http://localhost:8888/interface_COLLABORATION/Collaboratory.html) Search Print

# NOM Collaboratory

	Provide an intelligent interface to facilitate using the NOM simulator	Provide an Interface to define new molecule type	
	Provide an interface to search simulation information	Provide an administration role to validate the newly added molecule for public usage	
	Provide a threaded discussion board	Provide a XML-based Markup Language definition	
	Provide a real time chat box	Provide an Interface to upload publications	

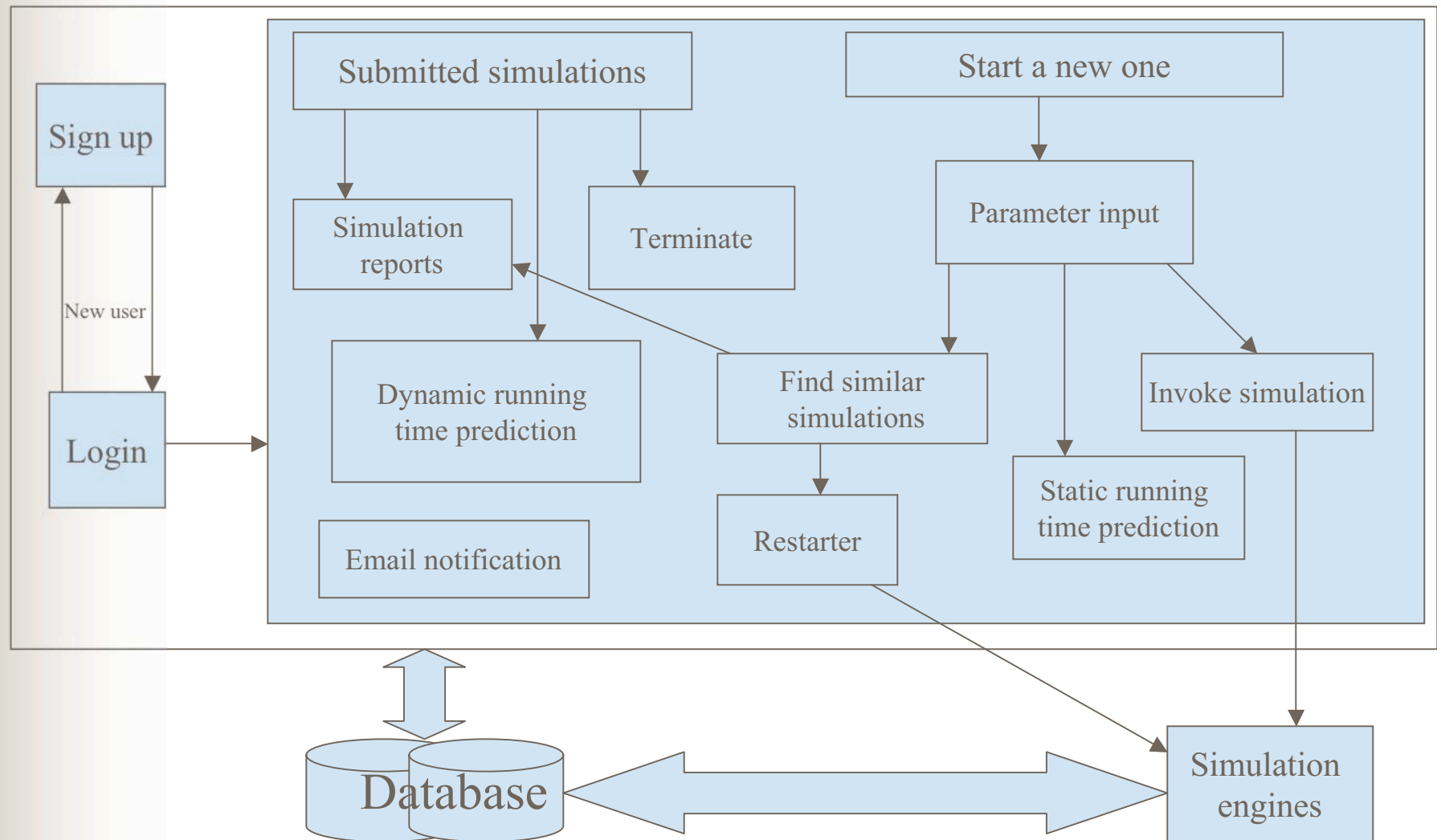
Document: Done (0.154 secs)



# Web Technologies

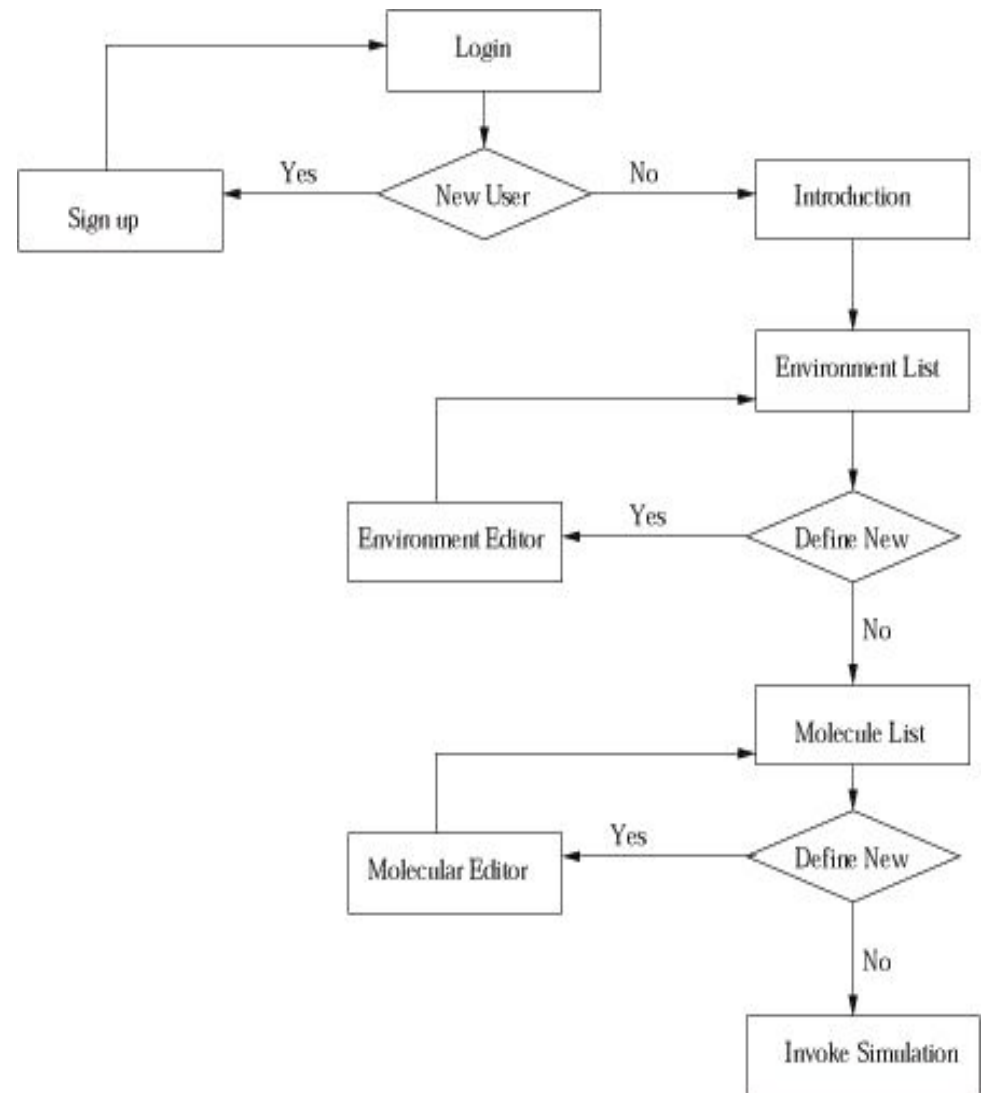
- Sun Java 2 Enterprise Edition (J2EE)
  - Java Servlets, Java Server Pages (JSP)
  - Enterprise Java Beans (EJB)
  - Java Transaction Service/API (JTS/JTA)
- RDBMS (Oracle):
  - Java DataBase Connectivity (JDBC)
  - Data analysis packages
  - Data mining technologies
- XML
  - NOML
  - XSQL

# 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)

<b>Molecule Name*</b> 3ficFA	<input type="checkbox"/> Make it available to public				
<b>Atoms of the molecule</b> Each field must be a non-negative integer. Default value is 0.	<b>(Atom) C</b> 66	<b>(Atom) H</b> 64	<b>(Atom) N</b> 0		
	<b>(Atom) O</b> 38	<b>(Atom) S</b> 0	<b>(Atom) P</b> 0		
<b>Functional groups of the molecule</b> Each field must be a non-negative integer. Default value is 0.	<b>DoubleBond</b> 0	<b>Rings</b> 0	<b>Phenyl</b> 0	<b>Alcohols</b> 0	<b>Phenols</b> 0
	<b>Ethers</b> 0	<b>Esters</b> 0	<b>Ketones</b> 0	<b>Aldehydes</b> 0	<b>Acids</b> 0
	<b>Arylacids</b> 0	<b>Amines</b> 0	<b>RingN</b> 0	<b>Amides</b> 0	<b>Thioethers</b> 0
	<b>Thiols</b> 0	<b>Phosphoesters</b> 0	<b>HPhosphoesters</b> 0	<b>Phosphates</b> 0	

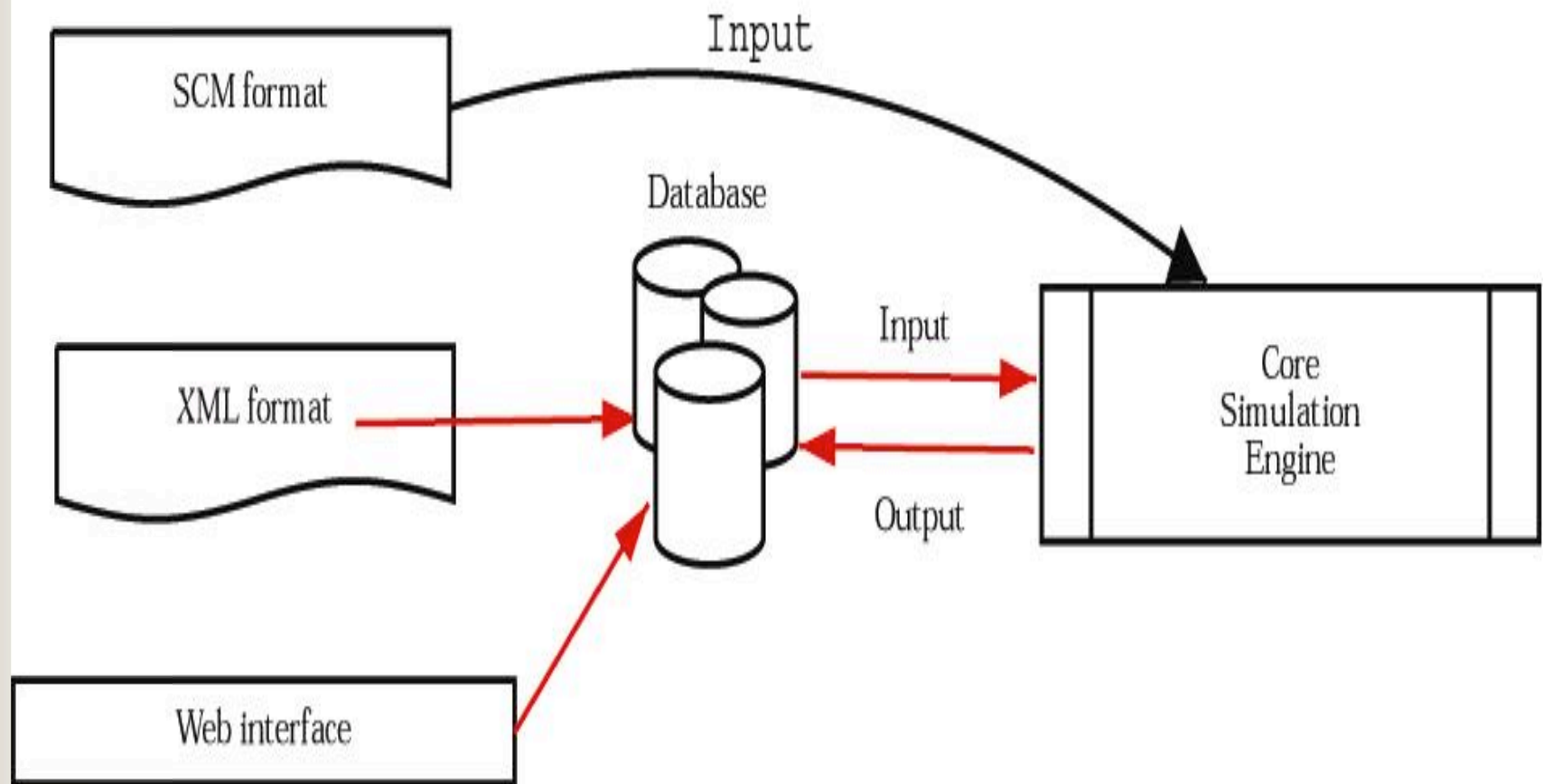
Create New Molecule Type



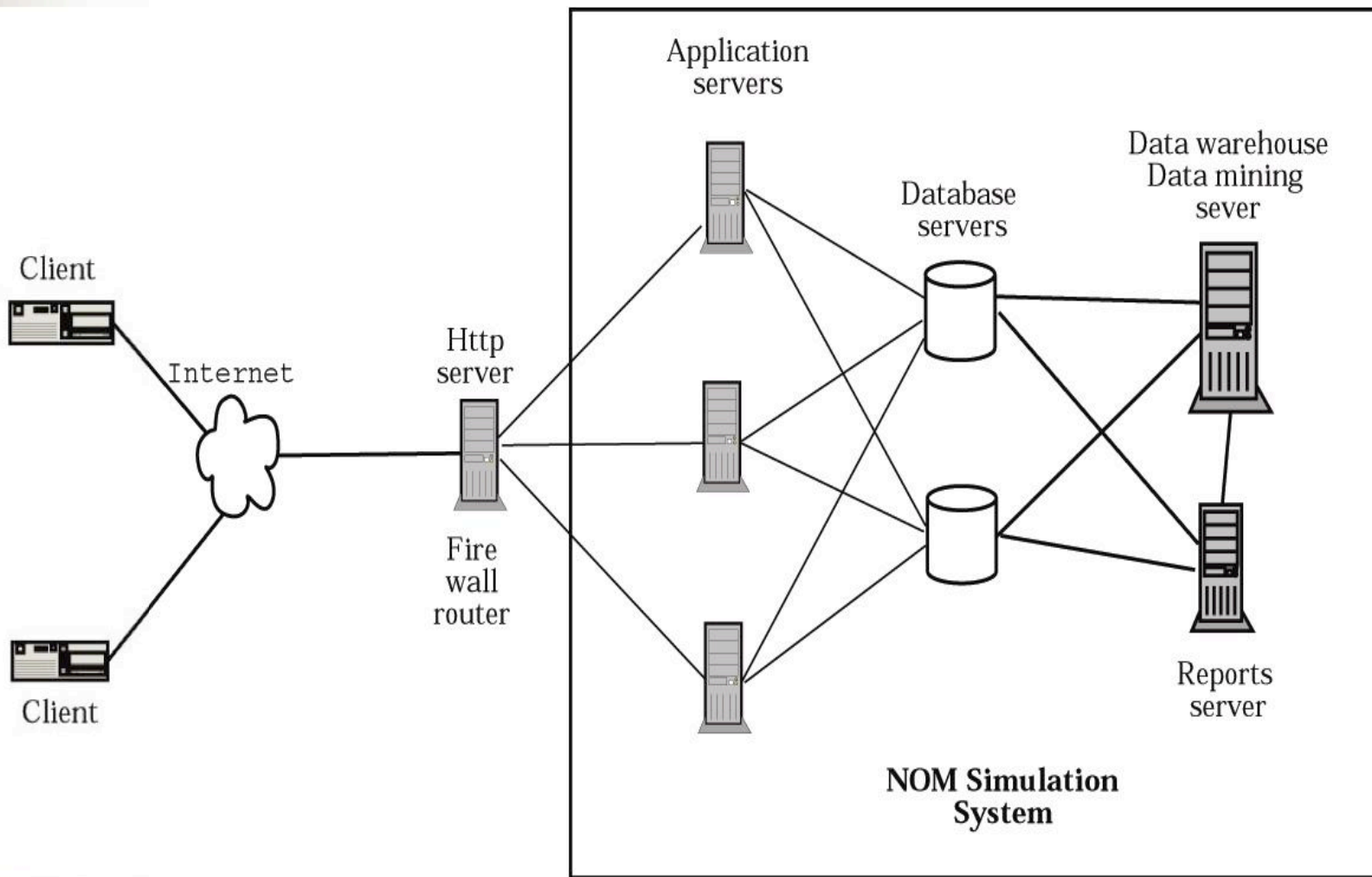
# XML-based NOM Markup Language

- 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

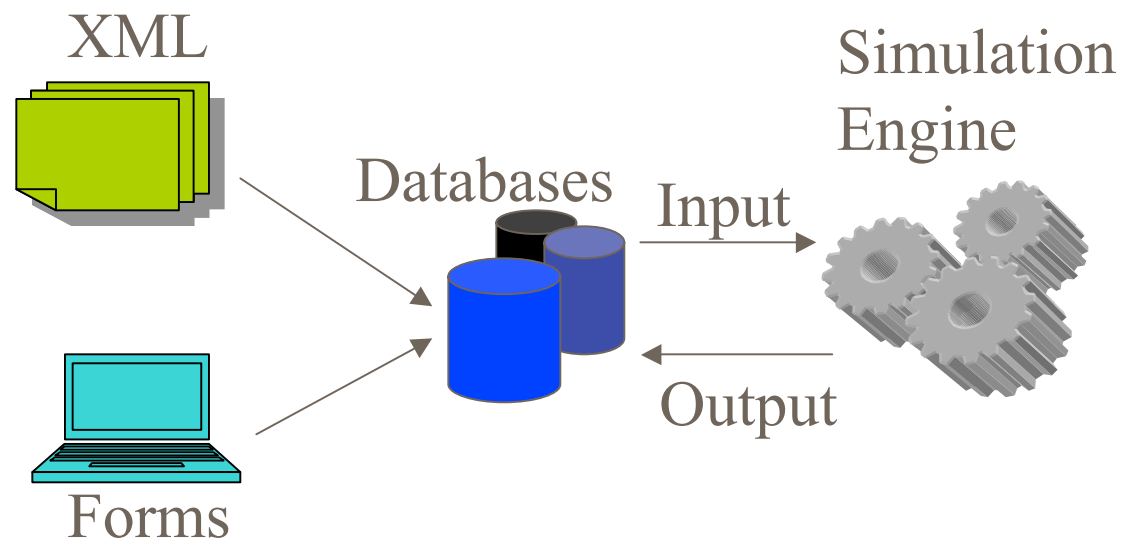
- Agent-based
- Stochastic
- Discrete event

- Packages

- Swarm
- RePast

- Languages

- Java
- SQL & PL/SQL



# Report Example



- Home
- My NOM
- Collaboration
- Documentation
- The Website
- Contact Us
- New Sim
- Reports
- NOM XML
- Molecule
- Sim Search
- User Profile
- Logout

Welcome, xx xx

Welcome to NOM Simulator, have a look at information about this session:

- Environment variables

<b>Simulation time:</b> 130.0 Hours	<b>Microbe density:</b> 0.03	<b>Fungal density:</b> 0.01	<b>pH value:</b> 6.0	<b>Temperature:</b> 237.0 F <sup>o</sup>	<b>pKw:</b> 1.4E-5
<b>Oxygen density:</b> 4.0E-4	<b>Light density:</b> 0.0001	<b>Molecule density:</b> 0.0001	<b>Adsorption Rate:</b> 0.0001	<b>Desorption Rate:</b> 0.0001	<b>Created by:</b> xx xx

Please provide the following information.  
Current Time Step is: 4799 [Refresh](#)

- Molecule

- Molecule 1
- [molecule1](#)
- [molecule2](#)
- [molecule3](#)
- [molecule4](#)
- [molecule5](#)

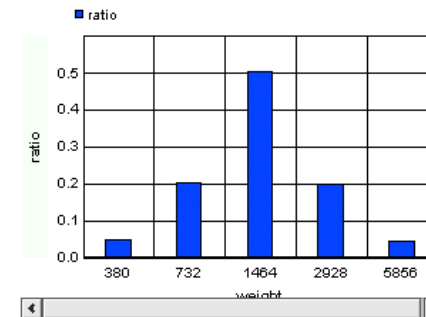
Time Step:   
 Status:   
 Start Y:   
 End Y:

- 
- 

- Sample r

- [Distribution of the sorption](#)

**Weight Distribution**





# 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