Digging into Digital Soil

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NOM Research Group

Background

- What is NOM?
  - natural organic molecules
- What are we simulating?
  - Stochastic interactions of NOM
  - movement, reactions, sorption
- Who is sponsoring this?
  - National Science Foundation
- Why do they care?
  - controlling pollution, nuclear waste

Personnel

- Dr. Madey
  - you know…the professor for this class
  - supervisor
- Yingping Huang
  - half-TA-half-student for this class
  - databases, sys admin, web interaction
- Xiaorong Xiang
  - TA for this class
  - web interaction, core simulation
- Eric Chanowich
  - the guy giving this chalk talk
  - core simulation
- Dr. Cabaniss, Dr. Maurice, and other scientists

NOM 101

- Examples of NOM
  - protein, lignin, cellulose
- Types of actions
  - movement - move around in environment
  - reaction - first or second order
  - sorption - sticking or unsticking

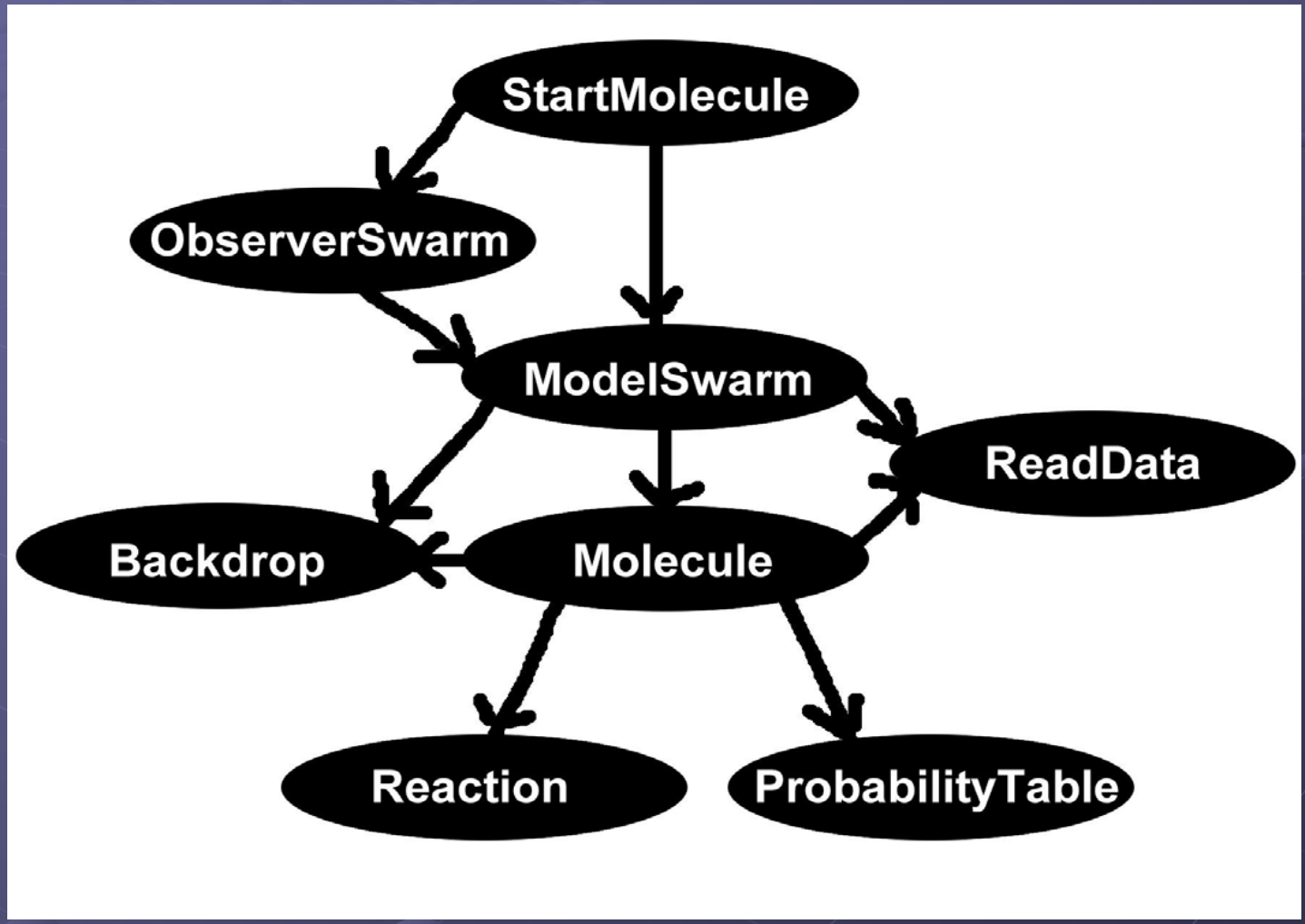
Technologies

- Java
  - chosen for GUI capabilities
  - Swarm is available for Java
- Swarm
  - open-source Java package
  - agent-based simulation tools
  - used for GUIs and robust random numbers
  - http://www.swarm.org
- Oracle

Representing NOM

- Molecular Attributes
  - empirical formula
  - counts of functional groups
    - alcohols, esters, ethers, phenols, etc.
- Environment
  - discrete two-dimensional grid
  - molecules enter at top and flow out bottom
  - adsorption sites

Class Hierarchy



Simulation Access

- Local
  - GUI interface
  - simulated set up and started by probes
  - primarily used for debugging
- Remote
  - web interface
  - simulation set up and started by web pages
  - primarily used by scientists