Introduction to N-Body Simulations

Background: Discrete Models
Molecular Dynamics

Discrete Models
- The course introduction slides mentioned two types of models used in CSE
  - Continuous
    - uses numeric methods to solve differential equations
    - “top-down” approach
    - example: computational fluid dynamics
  - Discrete
    - aka ab initio models
    - simulation of objects from the domain of study
    - example: n-body methods

Population Models
- An example of both approaches to understanding a complex system: population models in ecology
  - Classic method: Lotka-Volterra equations to describe predator-prey interactions
    - see: http://www.math.duke.edu/education/ccp/materials/diffeq/predprey/pred1.html
  - Goal: a set of equations to predict the sizes of two interacting populations over time
    - example: Canadian lynx and showshoe hare

Reading
- Molecular Dynamics: An Introduction
  - Lloyd Fosdick, Univ of Colorado
  - PDF on-line: MolecularDynamics.pdf
Predator-Prey Model

- Let \( x(t) \) be the size of the prey population at time \( t \)
- \( y(t) \) is the size of the predator population at \( t \)
- Without predation, prey population will grow continuously
  - the change in population depends on the current size of the population:
    \[
    \frac{dx}{dt} = ax
    \]
    where \( a \) is a parameter that determines growth rate
  - when there are predators, the size of the prey population decreases by a factor that depends on the interaction of the two populations:
    \[
    \frac{dx}{dt} = ax - bxy
    \]

Predator-Prey Model (cont’d)

- The predator population will decrease steadily when there is no food:
  \[
  \frac{dy}{dt} = -cy
  \]
- The predator population increases by a factor that depends on interaction with prey:
  \[
  \frac{dy}{dt} = -cy + pxy
  \]
- The final model is a dynamic system that does not have an analytical solution:
  \[
  \frac{dx}{dt} = ax - bxy
  \]
  \[
  \frac{dy}{dt} = -cy + pxy
  \]

Modeling Packages

- There are several software packages that allow users to define equations, set initial conditions, plot results
  - From Dan Udovic’s lab: JavaDemography
    http://darkwing.uoregon.edu/~bsl
  - A commercial package: Stella (http://www.hps-inc.com)

Individual Based Modeling

- The discrete approach to population simulation is known as individual-based modeling
  - create a set of objects representing individuals
  - define rules for interactions between individuals and their environment
    - a time-stepped simulator computes the next state of the system as a function of the current state
  - Familiar example: Conway’s “Game of Life”
    - cellular automaton
    - object survives if \( n \ldots m \) neighboring cells have objects
IBM for Lynx and Hare

- A cellular automaton can simulate the lynx/hare model
- Define a territory as a rectangular grid
- A cell can hold zero or more animals of each type
- Rules for population size
  - probability of reproduction
  - probability of dying
- Rules for movement
  - direction
  - max cell occupancy
  - attraction/repulsion

IBM for Lynx and Hare (cont’d)

- Initialize the system with a random distribution of “objects” from each population
- Run the model for some number of time steps
- At each time step:
  - compute interactions in each cell (i.e. predation)
  - add new objects (“births”)
  - move objects (migration)

Aside: Boundary Conditions

- How should the model treat events at the boundaries?
- A common situation in scientific models
- One solution: periodic boundaries
- The simulated system is a small patch of a larger system
  - in lynx/hare: wraparound
  - animal moving off one edge reappears on the other side

Aside: Hexagonal Grids

- How should movement be defined?
- If an animal can only move to neighboring cells, a diagonal move requires two time steps
- But the center of a diagonal neighbor is further than the center of an orthogonal neighbor, so diagonal moves should not be as frequent
- One solution: hexagonal grids
- See: Discrete Global Grids (http://www.sou.edu/cs/sahr/dgg)
IBM vs DS

IBMs have advantages and disadvantages

**Pro:**
- flexibility in modeling variation (age, sex, health, etc)
- interactions with environment (terrain, other conditions)
- expands to multiple species

**Con:**
- requires quantifying, modeling many different attributes, behaviors
- lack of formalism -- what do the results mean?
- difficulty of verifying, analyzing model

Molecular Dynamics

Molecular Dynamics (MD) is important application area for N-body methods
- molecular biology: protein-protein and protein-DNA interactions

**Typical model is for a conservative system**
- no external forces
- all motion is determined by internal interactions

**Forces are additive**
- sum over pairwise interactions, e.g. electrostatic forces
- sum over different types of forces

**Force field:** collection of forces acting on a body at a point in space

Energy

For many systems there is a formula for energy

In a conservative system, force is defined by the energy gradient:

\[ f(r) = -\nabla \phi(r) \]

**Notation:**
- \( r \) position (coordinate)
- \( \phi(r) \) potential energy
- \( f(r) \) force

2D and 3D Models

Many forces are a function of the distance between two bodies
- Examples: electrostatic force, gravity

In 2D and 3D models, the distance between two bodies is the norm of the difference of their positions

\[ d = ||r|| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \]
**Hooke’s Law**

- Use Hooke’s law to model a system in which two bodies are connected.
- When the system is at an equilibrium (distance = \( x_e \)) there is no energy.
- Moving the bodies closer or further apart increases potential energy.
- Force attracts (\( f < 0 \)) or repels (\( f > 0 \)) bodies.
- Example:
  - atoms connected by a chemical bond

\[
\phi(x) = \frac{k}{2} (x - x_e)^2 \\
\quad f(x) = -k(x - x_e)
\]

**Lennard-Jones Potential**

- The Lennard-Jones potential function was originally used to model atoms in an argon gas.
- Atoms are not connected by bonds.
- When distance is above a threshold there is a weak attraction.
- When atoms are too close their electron orbits overlap and there is a very strong repulsion.

\[
\phi(d) = \left( \frac{1}{d^{12}} - \frac{1}{d^6} \right)
\]

**Hard Sphere Model**

- In a hard sphere (“billiard ball”) model there is no interaction between bodies until they collide.
- Model elastic collisions:
  - same total kinetic energy before collision and after collision
  - no deformation
  - no spin
- Collisions modify the velocity vectors of the bodies.
- Used to model gases, liquids.

**Dreiding Force Field**

- One of the papers on the class web site describes an algorithm to compute the potential energy in a DNA molecule.
- Dreiding force field: sum of seven energy terms (next slide)
  - use in energy minimization studies
  - find the “best” (least energetic) configuration of atom
  - alternative to X-ray crystallography
- 455/555 project in 1994
  - Tom Rush: grad student in Peticolas lab at
  - implemented in MPL (data-parallel dialect of C) on SIMD MasPar-1
  - published in CS conference (HICSS)
Dreiding Force Field (cont’d)

- Bond energy
  - difference from equilibrium bond length
  \[ \sum \frac{1}{2} k_b (R - R_0)^2 \]

- Angle energy
  - same, but for divergence from equilibrium angle
  \[ \sum \frac{1}{2} k_a (\theta - \theta_0)^2 \]

- Torsion energy
  - “twist” in central bond connecting group of 4
  \[ \sum \sum \frac{1}{2} k_t \left[ 1 - d \cos(n \phi) \right] \]

- Inversion energy
  - base of pyramid is angle deviation in height of fourth atom
  \[ \sum \frac{1}{2} C \left( \cos \omega - \cos \omega_0 \right)^2 \]

N-Body Project

- Next project this term:
  - simple n-body simulation
  - only force is gravity
  - compute pairwise interactions of body with every other body
  - sum of forces determines update to velocity, position

- Details next lecture
  - equations of motion
  - time-stepped implementation
  - parallel algorithms

Dreiding Force Field (cont’d)

- Coulombic attraction
  - non-bonded interaction based on static charge on each atom
  \[ \sum \frac{Q_i Q_j}{4 \pi \varepsilon_0 R_{ij}^2} \]

- van der Waals attraction
  - a version of the Lennard-Jones force
  \[ \sum D_{6} \left[ \left( \frac{R_0}{R_{ij}} \right)^{12} - 2 \left( \frac{R_0}{R_{ij}} \right)^6 \right] \]

- Hydrogen bond interaction
  - a quantum level interaction
  - single electron in H attracted toward C in CH bond, altering static charge of H
  \[ \sum D_{6} \left[ 5 \left( \frac{R_0}{R_{ij}} \right)^{12} - 6 \left( \frac{R_0}{R_{ij}} \right)^6 \right] \cos^4 \theta_{ij} \]