

# Complex Systems Simulation Models

Prof Ken Hawick  
Massey University  
December 2012

# Discrete Lattice Models on meshes

- Ising
- Potts
- Sznajd
- Axelrod
- Conway Game of Life
- Wolfram CA
- Rock-Paper-Scissors-Lizard-Spock
- Invasion Percolation

# (Regular) Field Models on meshes

- Cahn-Hilliard-Cook
- Time-Dependent Ginzburg-Landau
- Coupled Oscillators
- Lotka-Volterra & Variants
- Navier-Stokes & Variants
- Heisenberg

# Particle Models in real-space (x,y,z)

- Gravitational Forces (Planets)
- Lennard-Jones Molecular Dynamics Forces
- Electromagnetic Forces (Plasma)
- Hard Disk/Sphere Collisions
- Variants - Hybrids; Mixtures; Repel/Attract
- Rule-based Systems - Boids

# d-dimensions & geometry

- 1d - line
- 2d - plane (square, triangular, hexagonal)
- 3d - cubic or variants
- 4d and above - hyper-cubic

# Neighbourhoods

- Nearest-Neighbour
- Next-Nearest-Neighbour
- Both = Moore neighbourhood
- Radial proximity - all within radial distance  $r$
- Non-trivial counts in different dimensions

# State-Space

- Can be finite
  - from discrete number of values on each site
  - eg  $2^N$  for Ising on N-site lattice
- Nearly always too big to enumerate exactly
- Importance sampling
- Trajectory sampling

# Initialisation

- Random uniform often used
- Nearly always not a likely state for the particular parameter combination being explored
- System relaxes towards a more likely state



# Parameters

- Usually interested in some sort of macroscopic behaviour
  - eg order or disorder
  - Size of biggest cluster
  - Number of clusters
- Varies with microscopic parameters
- Or sometimes varies with Temperature

# Time-Evolution

- Microscopic rule to update each site
- Explicit if-then-else rule
- Time-integration like finite difference
- Usually scheme is local - the inputs are:
  - The value of the cell itself
  - The value of its local neighbouring cells
- Sometimes all-to-all eg N-body particles

# The Experiments

- Usually:
  - Initialise randomly (hot start)
  - Time-evolve (timestep or integrate)
  - Once equilibrated (transients died out)
  - Measure something that characterises the finalised or equilibrated system
- 
- Do this lots of times to get average independent of any pathologies from the particular starting values
  - Do all over for different parameter values

# Phase Transitions

- Often Find that there is some abrupt or unexpected change in the measured property ( eg order parameter) even when control parameter is changed smoothly and slowly
- *eg Magnetization(Temperature)* in Ising
- *Largest-Cluster-Size(traits)* in Axelrod

# Finite-Size effects

- Often find the location of the transition is affected by how big the system is
- Hopefully a weak but systemic effect
- Also usually find the location and nature of the phase transition varies with dimension and sometimes with lattice and geometry too.

# How do we Simulate?

- Ideally want to be able to build software that:
  - Is Independent of dimension, geometry etc
  - Reuses hard-to-debug measurement code
  - Allows easy switch to a new & different model
  - Is Platform independent & portable
  - Is Reliable
  - Supports Graphical Visualisation
  - Is Very fast for batch runs and
  - Is Fast-enough for interactive runs (to debug & understand)

# Choice of Languages

- C/C++/D/OpenGL
  - Java/Swing
  - Ruby/Python
  - Sometimes must work with legacy eg Fortran
  - Declarative eg Lisp/Scala,...
- 
- Internal DSLs based on above
  - Standalone External DSL

# Libraries

- Sometimes language/System constrained by availability of a particular library
- eg scientific library code for
  - Matrix/linear algebra
  - BigInteger arbitrary precision
  - Rendering system
  - Arbitrary dimensionality - eg k-indexing
- Sometimes worth porting to desired platform



# Complex Networks

- Some models defined on networks
- Meshes is just a regular graph
- Can add
  - Distortions
  - Extra/less connectivity
  - Long range (small world) connectivity
- Spatial proximities generate a graph
- So does geographic map data
- Or Internet/Power grids/bio-nets/...
- Other specialist graph generation algorithms

# Static Properties

- Sometimes the static fixed properties of the graph itself are interesting
- Transitions or critical connectivities
- Sometimes focus on the model's dynamical properties
- Might behave different from mesh because of properties peculiar to the static graph

# Dynamical Graphs

- Adaptive Meshes
- The network or graph itself changes with time
- Some algorithm or procedure for adding or removing nodes or arcs
- Dynamical properties need to be tracked in time

# More Information

<http://complexity.massey.ac.nz>

[K.A.Hawick@massey.ac.nz](mailto:K.A.Hawick@massey.ac.nz)