Introduction to Modeling and Simulation, Particle Methods

Monte Carlo Methods I: Percolation

Martin Z. Bazant

Department of Mathematics, MIT

Figure removed for copyright reasons.

(Bunde & Havlin)

Statistical (Monte Carlo) Methods

- Continuum fields represent average properties, but sometimes you care about fluctuations and/or microscopic details
- “Monte Carlo method”: model and simulate a complex system by a statistical ensemble of *random* realizations
- MC methods are less accurate, but much simpler and more efficient, than detailed models of interacting particles (“molecular dynamics”)
- Examples:
  - Lec 3: Random-walk simulations of diffusion
  - Lec MC2: Sticky random-walk simulations of fractal pattern formation (electrodeposits, bacteria colonies, snowflakes,…)
  - Lec MC3: Simulations of random packings (glasses, granular flow,…)
  - Lec MC1: Simulations of connectivity in random environments…

percolation

Percolation

- Flory (1941): polymers, Broadbent and Hammersley (1958): porous media

- Randomly color the vertices (or bonds) of a graph and study connected "clusters" of the same color.

- Vary the concentration of each color….

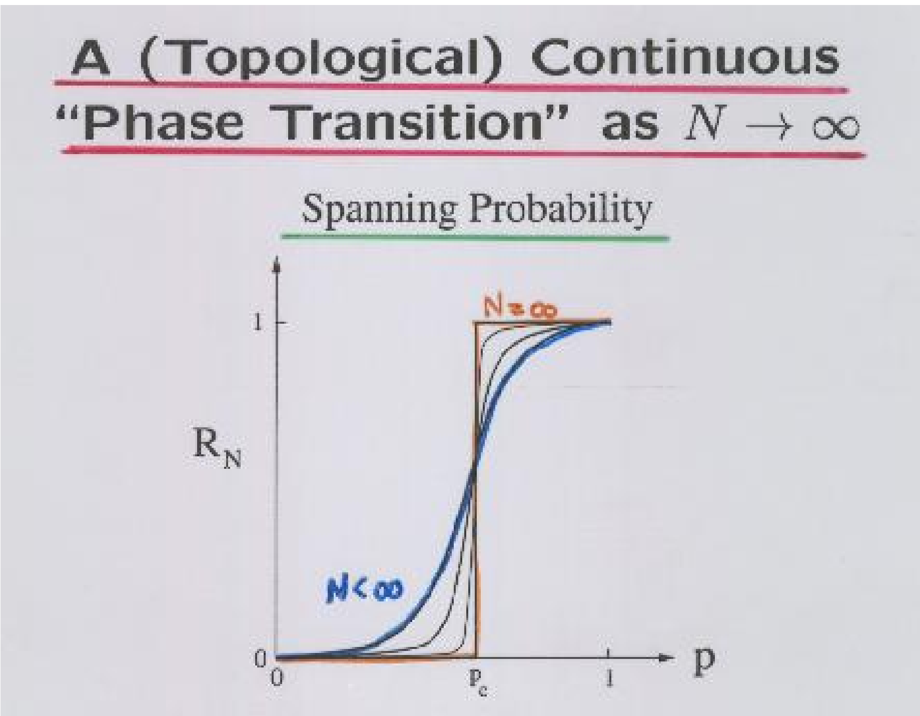
Figure removed for copyright reasons.

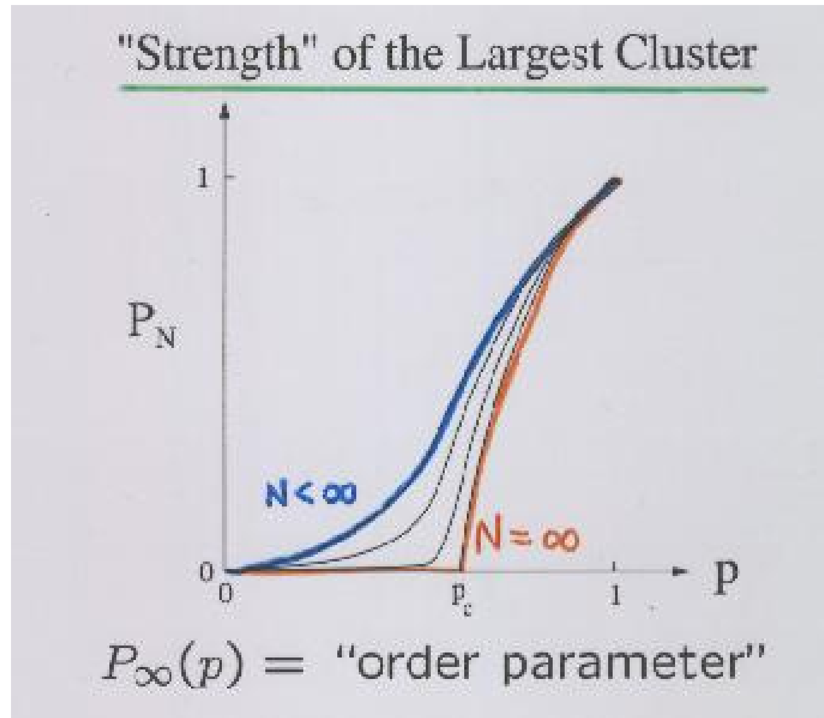
Try demo by
Bob Sumner
(Mod/Sim 2001):
perc

Figure removed for coyright reasons.
See: Bunde, A., and S. Havlin, eds. *Fractals and Disordered Systems*. New York, NY: Springer, 1996.

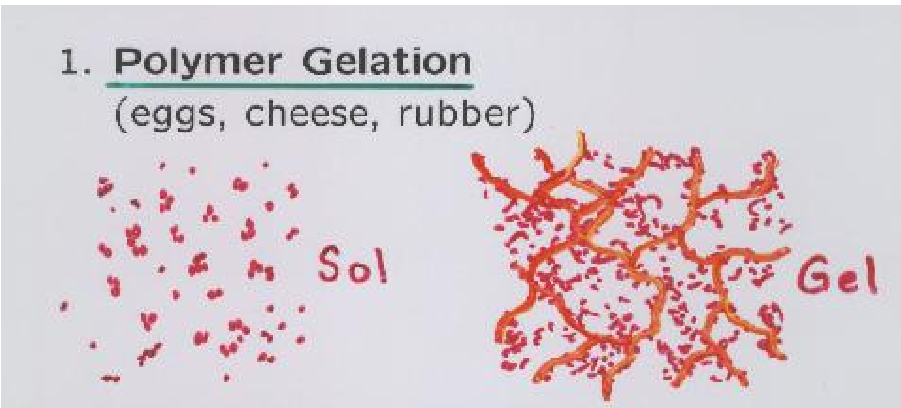
(Bunde & Havlin)

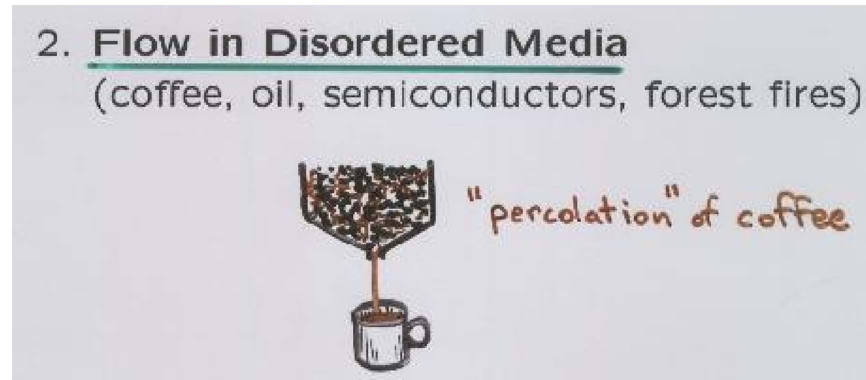
The Percolation Transition

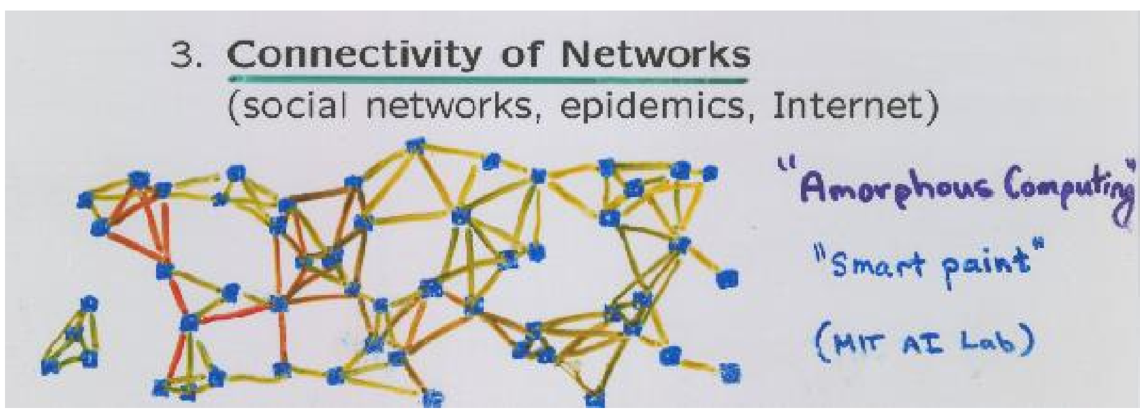




Some Applications of Percolation







Leath Algorithm

"Grows" a single percolation cluster recursively
(like the spreading of an epidemic or forest fire)

```
void grow(int i0, int j0)
{
  for each virgin neighbor [i,j] of [i0,j0] inside the boundary {
    if(random_number < p) {
      cluster[i,j] = 1;
      grow(i,j);
    }
    else {
      cluster[i,j] = 0;
    }
  }
}
```

Nice Java applet: http://theorie.physik.uni-wuerzburg.de/~reents/ComputationalPhysics/percgr.html

What is the critical probability?

• Depends on lattice and dimension:
= 1 in one dimension
= 1/2 for square bond lattice (d=2)
= 0.5927… for square site lattice (d=2)
= 0.312… for cubic lattice (d=3)
= 1/(z-1) Cayley tree with z branches/node (“d=infinity”)

• Can approximate by “renormalization group” analysis