Statistical Physics

“The branch of physics that would remain true, even if all the laws of physics were different”

PHY 1090 Discovering Physics
10/23/2012

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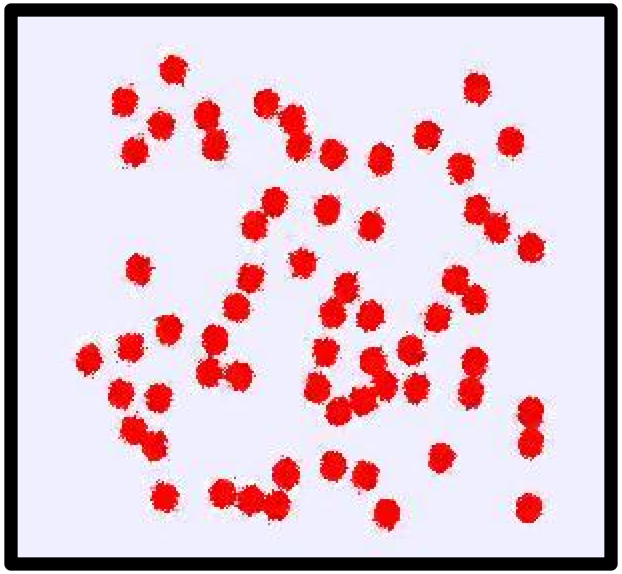
Prof. of Physics

What is Statistical Physics?

- The physics of systems that consist of ***large numbers*** of interacting "*particles*"
- The "particles" can be
  - **Nucleons**
  - **Atoms**
  - **Molecules**
  - **People or animals**
  - **Biological species**
  - **Computers**
  - **Web pages**
  - **Galaxies**
  - **……**



“Ideal Gas”

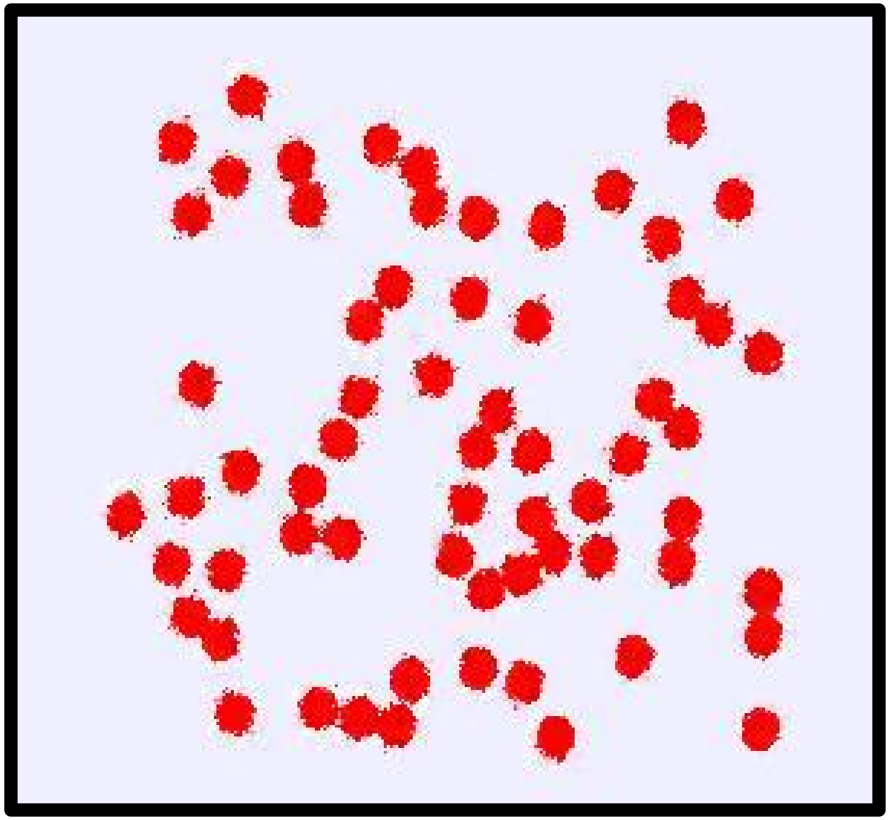
- The simplest statistical physics system is one consisting of *point particles that zip around in a box and collide with the walls*.
- This is a decent model for gases such as He or air, such as the atmosphere around us.
- *Each particle has its own velocity,* $\boldsymbol{v}_i$
- But there are ***too many*** of them to keep track of in detail! (And it wouldn’t be very interesting anyway.)

- So we instead describe the large-scale properties of the system by *macroscopic variables*.
- For the ideal gas of *N* “atoms”, these are:
- **Volume *V*:** Container volume
- **Pressure *P*:** Average *force per unit area*, due to atoms colliding with the walls.
- **Temperature *T*:** Average energy per particle
- Yield ***Ideal Gas Equation:***

$$PV = Nk_{\mathrm{B}}T$$

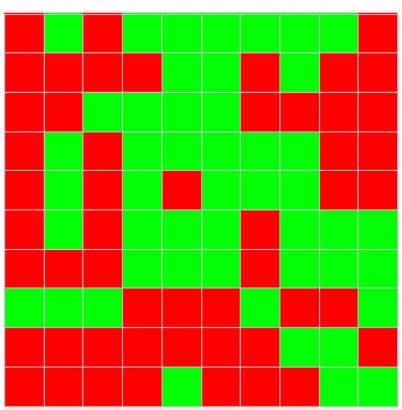
k_B is known as Boltzmann’s constant

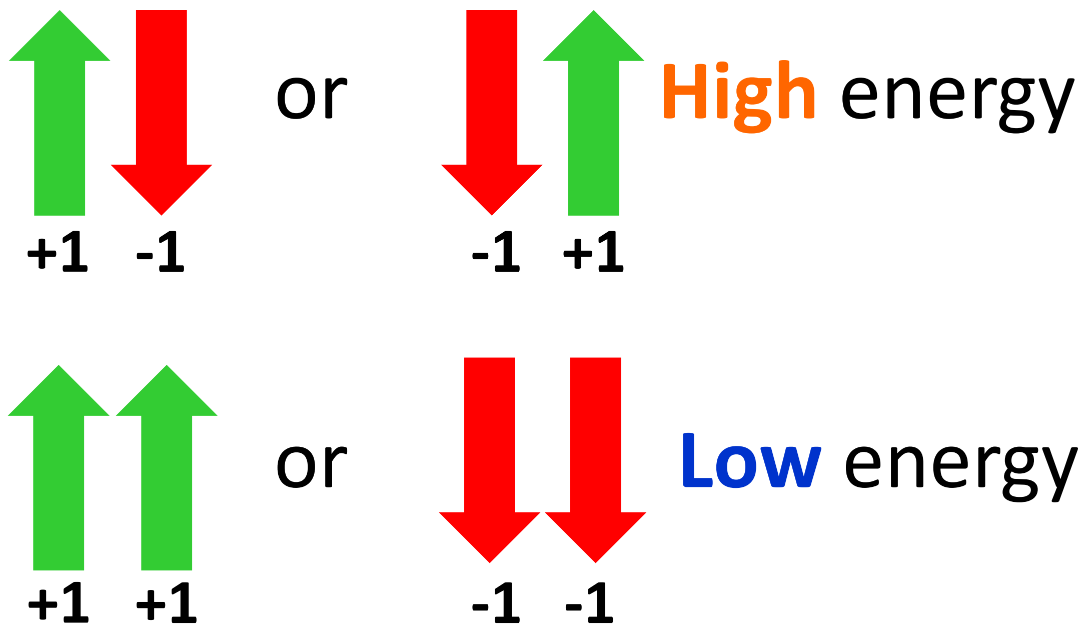
Java applet for ideal gas



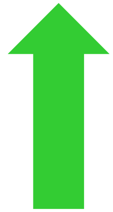
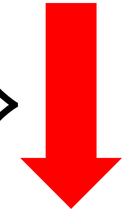
Interacting systems:
The Ising model

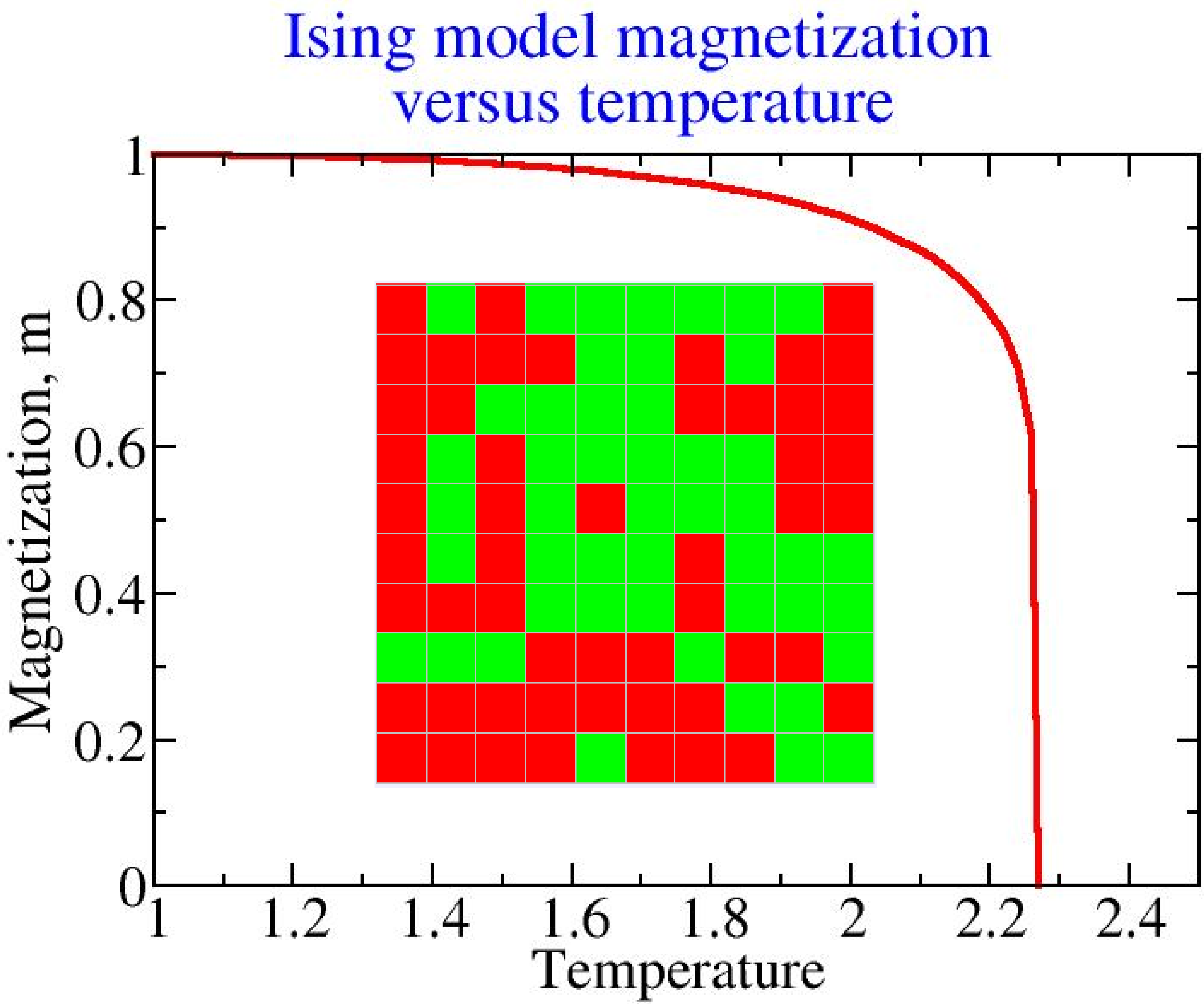
- This is a model for a magnet (or for gas molecules on a surface).
- Energy is given by *orientation of nearest-neighbor "spins"*:





Phase transition in Ising model

- Set ***s*** = **+1** ⇔  and ***s*** = **-1** ⇔ 
- We call the *average* of ***s*** over the whole system *the magnetization*, ***m***
  - ***m* = 0**: *half* the spins are **up** and *half* **down**
  - ***m* = +1**: *all* the spins are **up**
  - ***m* = -1**: *all* the spins are **down**


Ising model magnetization
versus temperature
Magnetization, m
1
0.8
0.6
0.4
0.2
0
1
1.2
1.4
1.6
1.8
2
2.2
2.4
Temperature

Monte Carlo simulation

- Monte Carlo simulation is a much used method in statistical physics.
- Algorithm:
  1. Choose a spin at random.
  2. Try to flip it.
     - Calculate the energy change ΔE that would occur
     - If $\Delta E < 0$, accept flip
     - If $\Delta E > 0$, accept flip with probability $\exp(-\Delta E/k_B T)$
  3. Return to 1

Let us try it on the Ising model!

http://stp.clarku.edu/simulations/ising/ising2d/index.html

Some other applications of statistical physics

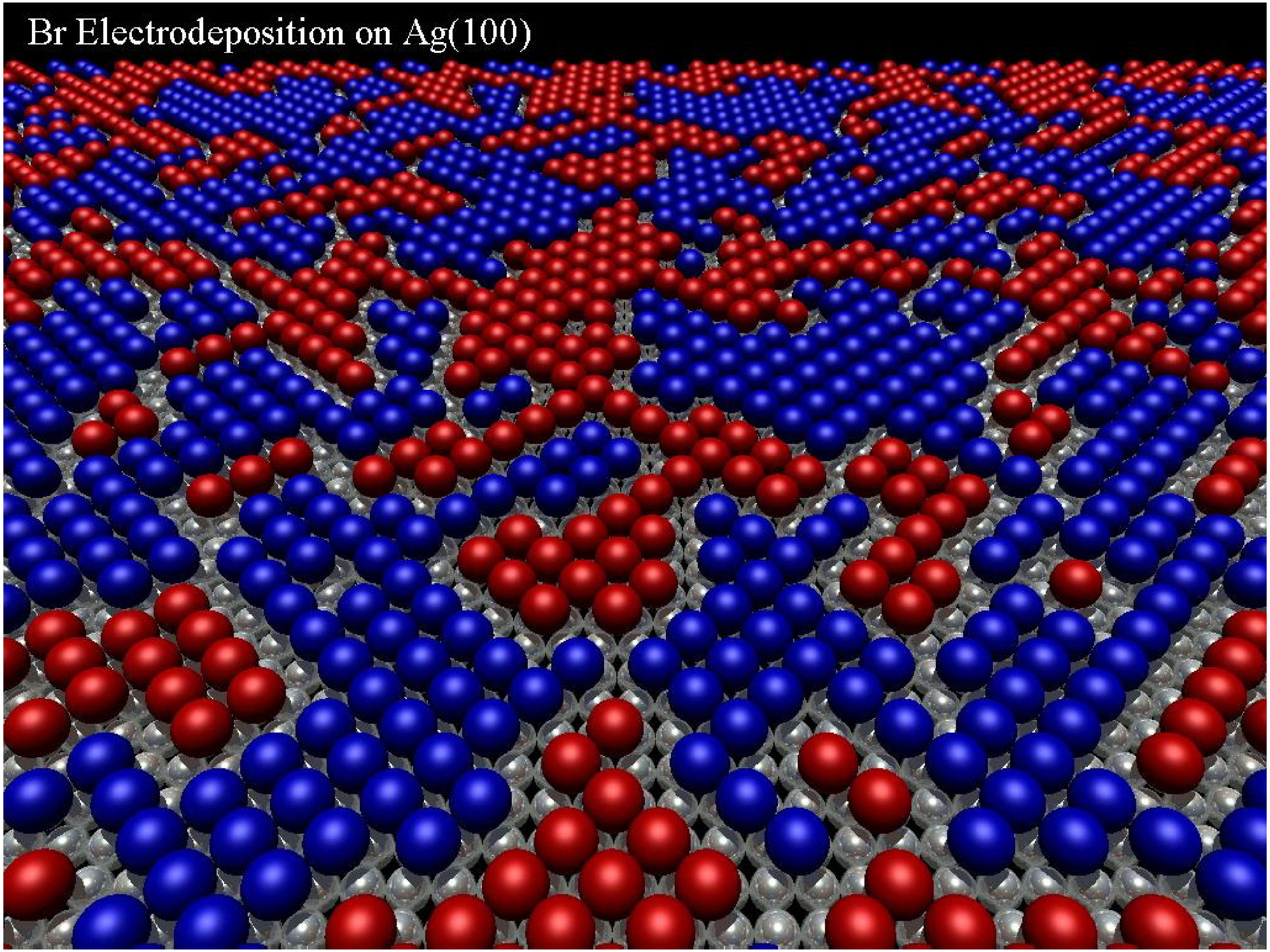
Surface Electrochemistry

- Important for the understanding of surface reactions, energy storage, and new methods to synthesize nanomaterials.

Electrosorption of bromine (Br) on silver (Ag)

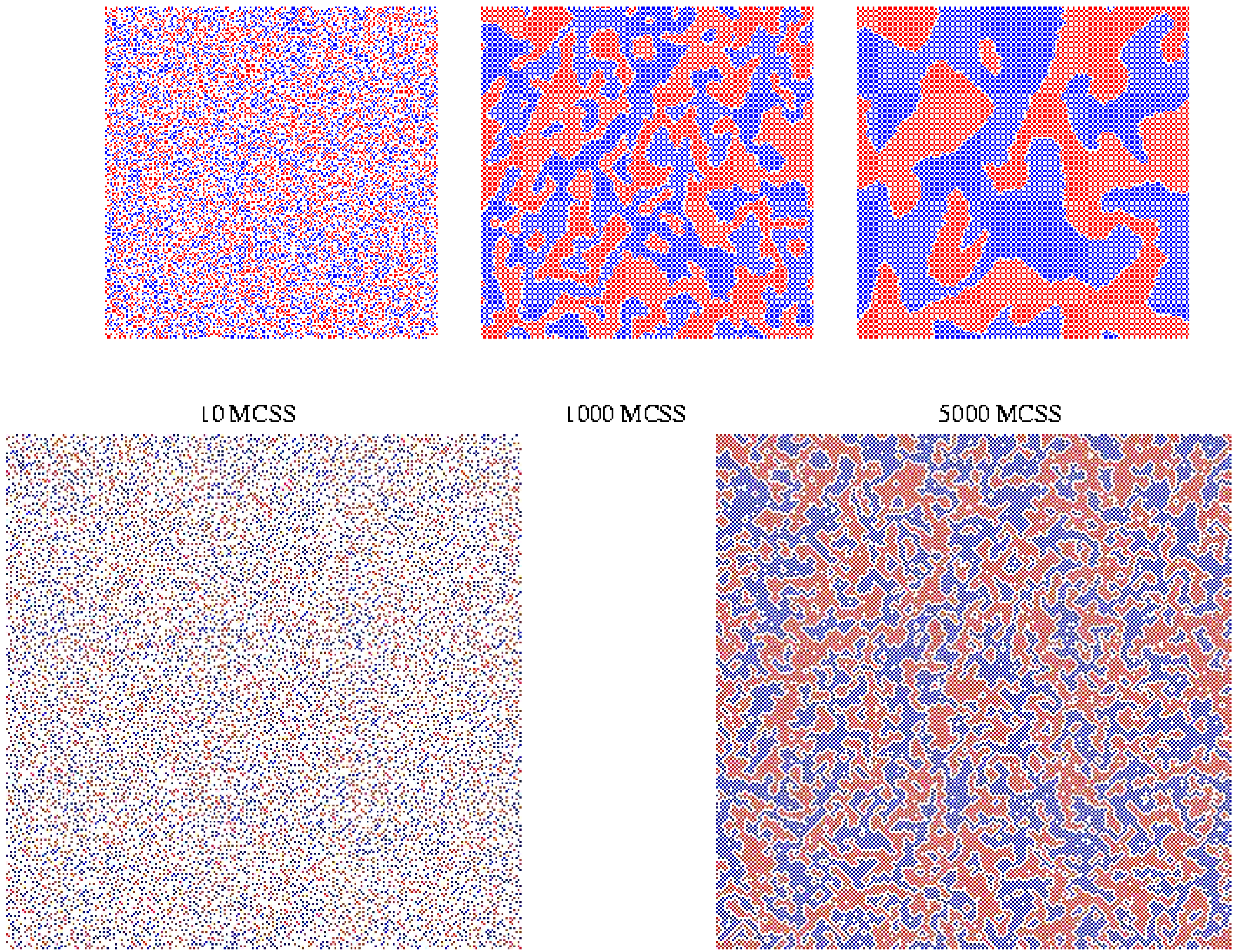
Using Ising lattice-gas models of the surface.

Configuration of Ordering System



Evolving system $L = 256$

Deep, positive-going potential step



A new charging method for Li-ion batteries, suggested by Molecular Dynamics simulations

Collaborators:
Dr. Ibrahim Abou Hamad, BP
Profs. M. A. Novotny and D. O. Wipf
Mississippi State U.

Li-ion batteries

- Popular energy sources for mobile applications (cell phones, cameras, laptops, cars, ...)

  + Rechargeable

  + High energy-to-weight ratio (> 10^2 Wh/kg)

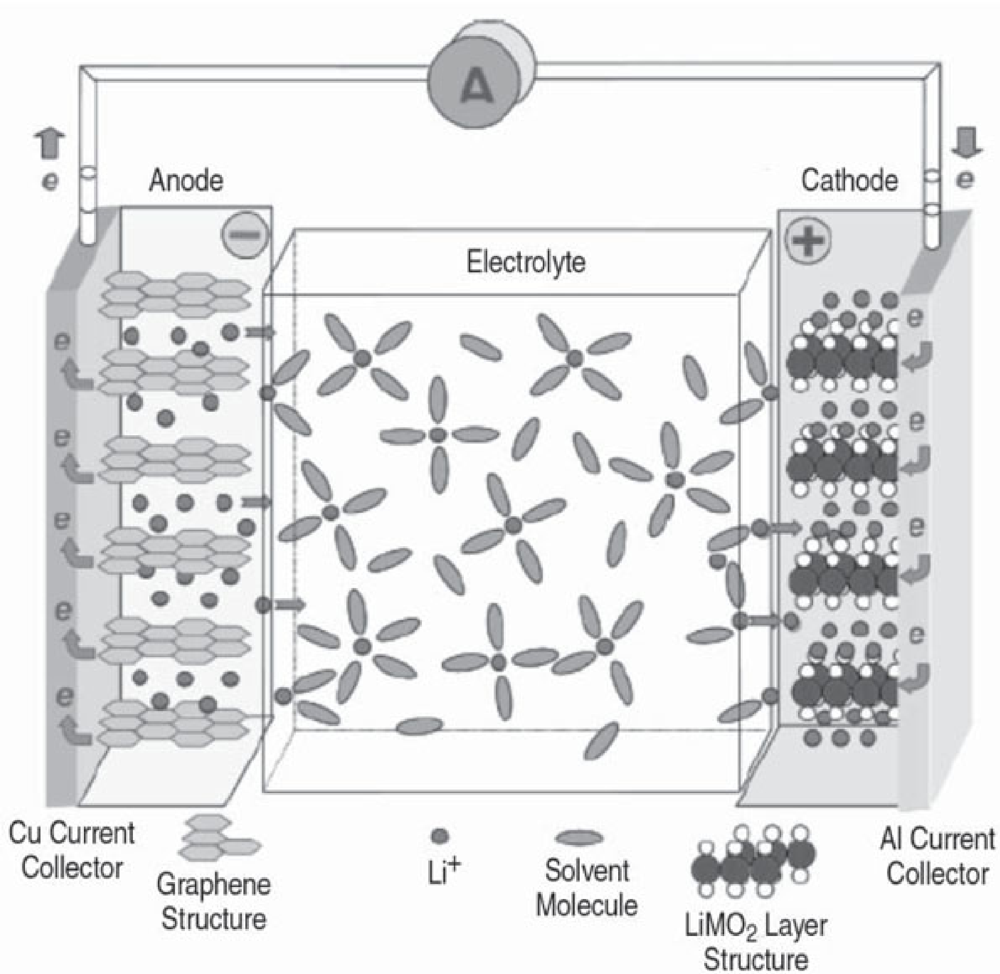
  + High voltage ($\approx$ 3.6 V)

  + Slow discharge when idle (< 10%/month)

  + Inexpensive raw materials (unlike fuel cells)

  - Lose capacity with time
  - High internal resistance
  - Safety concerns (fire, explosion)
  - **Slow recharge (> 5 hours)**

Structure of a Li-ion cell



Chemical reactions:

$LiCoO_2 + C_6$

Discharge ↑ ↓ Charge

$Li_{1-x}CoO_2 + C_6Li_x$

Claus Daniel: http://www.tms.org/pubs/journals/JOM/0809/Fig2.jpg

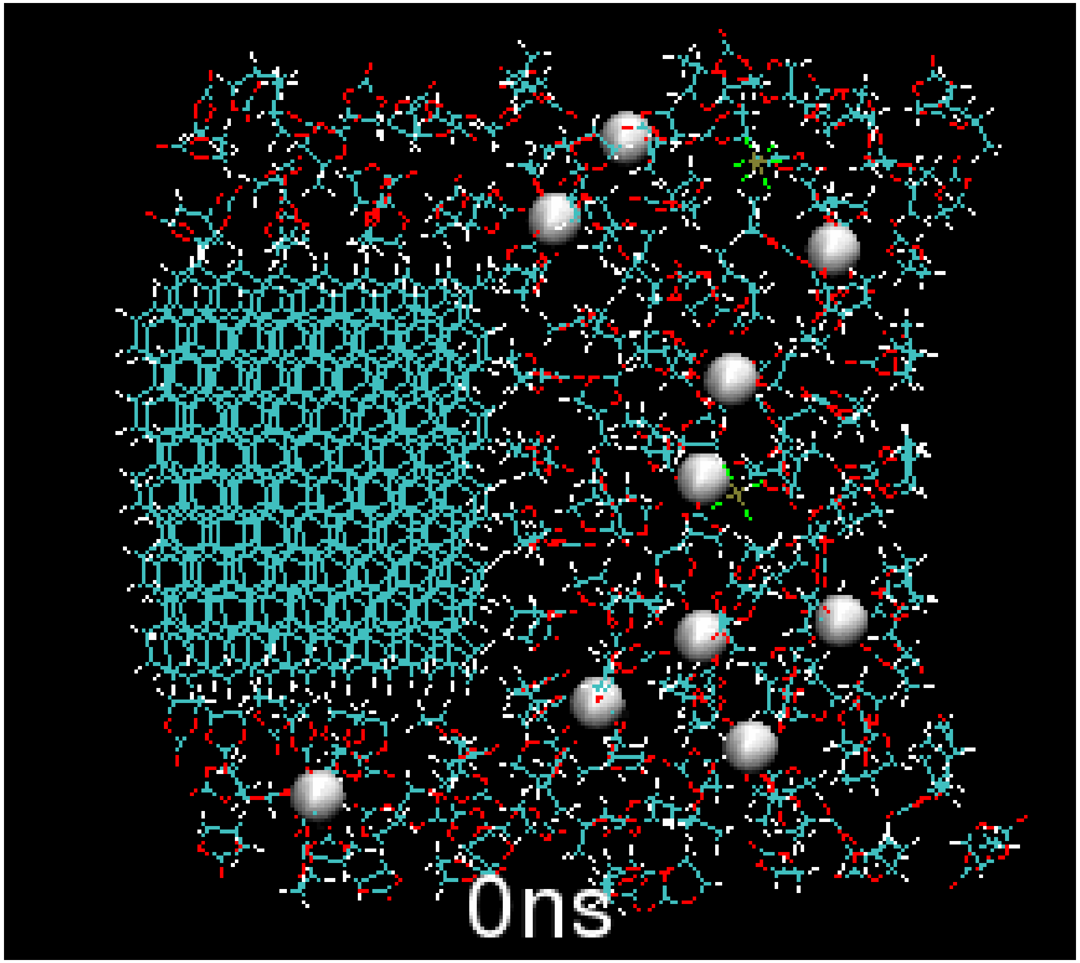
Simulation of charging process

- Large-scale molecular dynamics simulations to model environment near charged graphite sheets
- Model system:

  Graphite sheets, electrolyte,
  counter ions, Li^+ ions
- Software:
  SPARTAN (Hartree-Fock point charges)
  AMBER force fields for MD
  GAFF (generalized Amber force field)
  NAMD scalable MD package

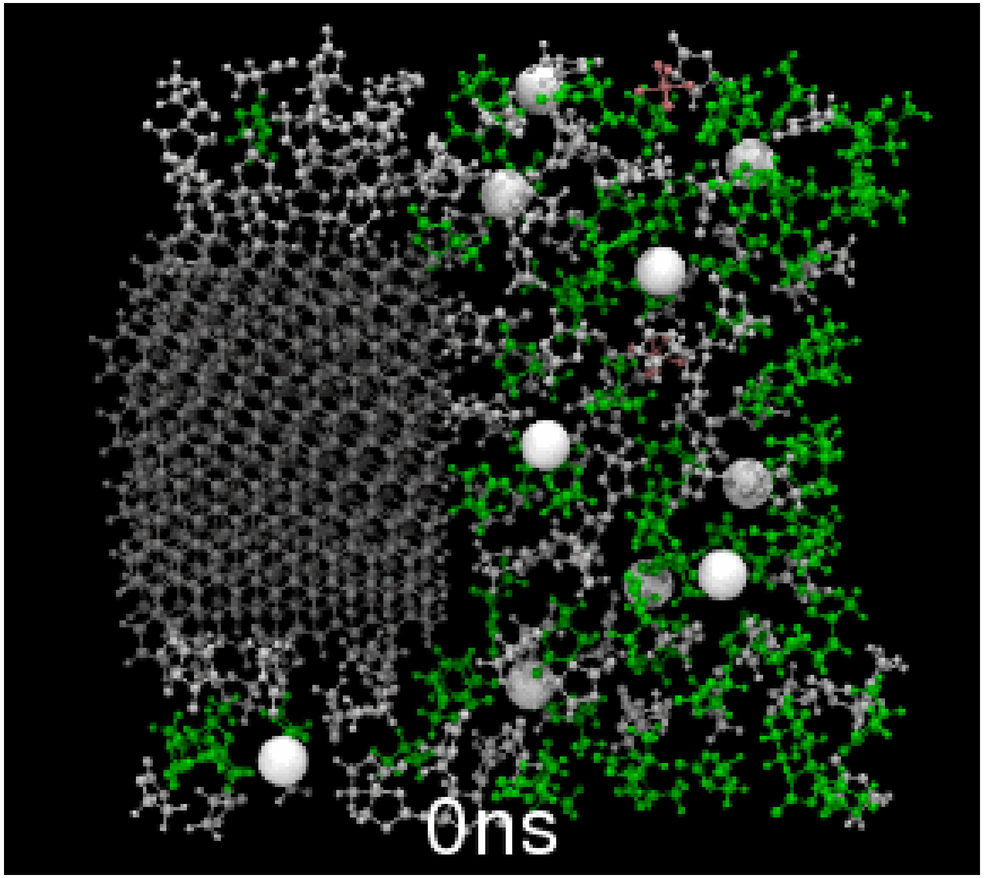
  VMD visualization

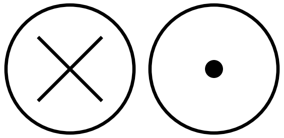
Animation: No External Field



Duration: 150 ns

Simulation with Applied Field



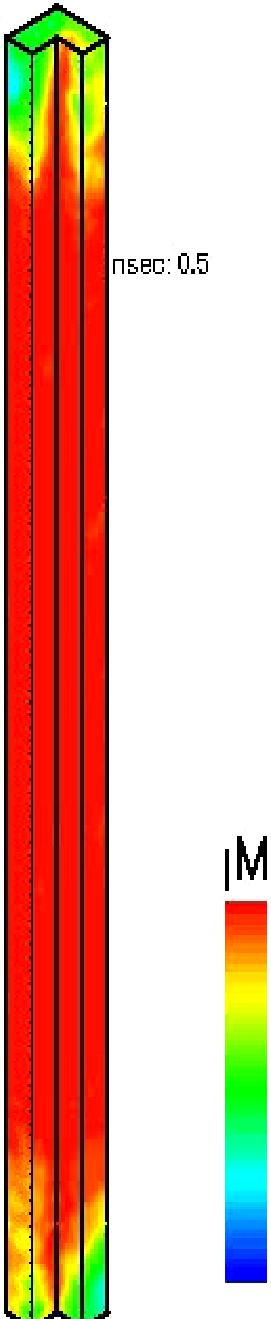


Duration 42 ns, intercalation at 39 ns

Nanomagnetism

- Important for the development of new ultrahigh-density recording media.
- Based on the physics of decay of metastable media (nonequilibrium statistical mechanics).

An example:
Simulated Nanomagnets



M_z

9 nm x 9 nm x 150 nm

Fe particle

H=800 Oe, *T*=20 K

Landau-Lifshitz-Gilbert

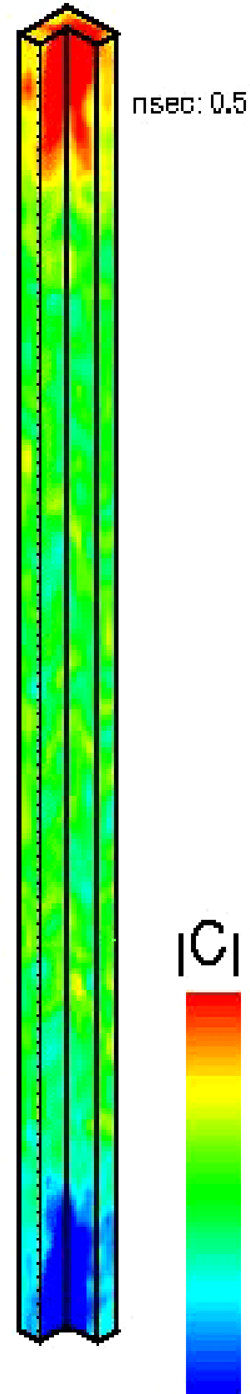
Langevin simulation

(micromagnetics)

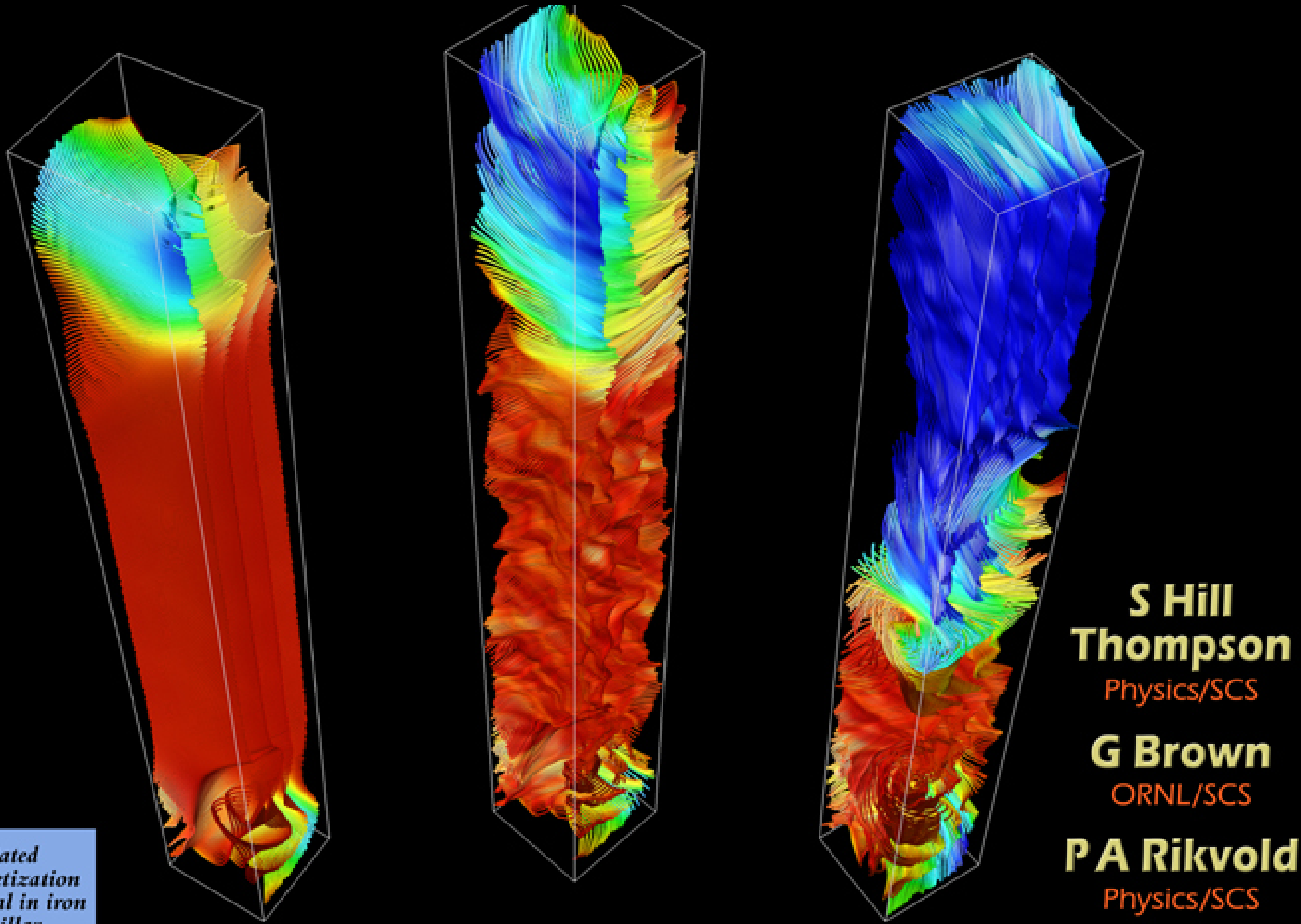
4949 lattice points

Time: 1.2 ns

Curl



Flux-line visualization



Simulated magnetization reversal in iron nanopillar

Statistical Physics of Evolution and Ecology

- Does evolution proceed uniformly or in fits and starts?
- Scarcity of intermediate forms (“missing links”) in the fossil record may suggest fits and starts.
- Fit-and-start evolution termed *punctuated equilibria* by Gould and Eldredge.
- Punctuated equilibria dynamics resemble *nucleation and growth in phase transformations* and *stick-slip motion in friction and earthquakes*.

Model

- Individuals of many species
  - Compete for resources
  - Interact directly (predator/prey, etc.)
- Individuals who get many resources and much food have larger probability of reproducing.
- Mutations that produce new species occur during reproduction.

Simulation Results

Diversity, $D(t)$

$N_{tot}(t)$, normalized

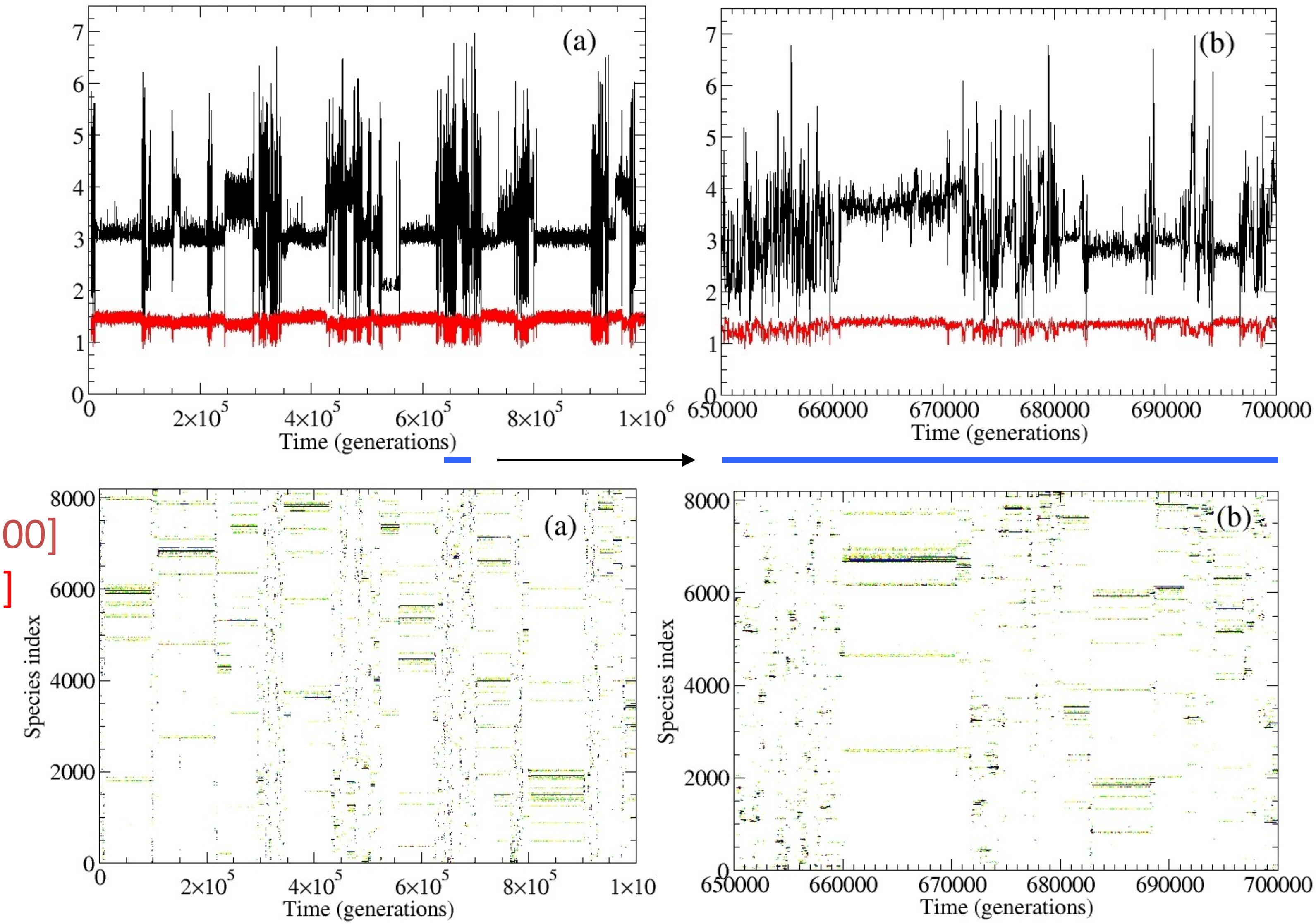
$n_I > 1000$

$n_I \in [101,1000]$

$n_I \in [11,100]$

$n_I \in [2,10]$

$n_I = 1$



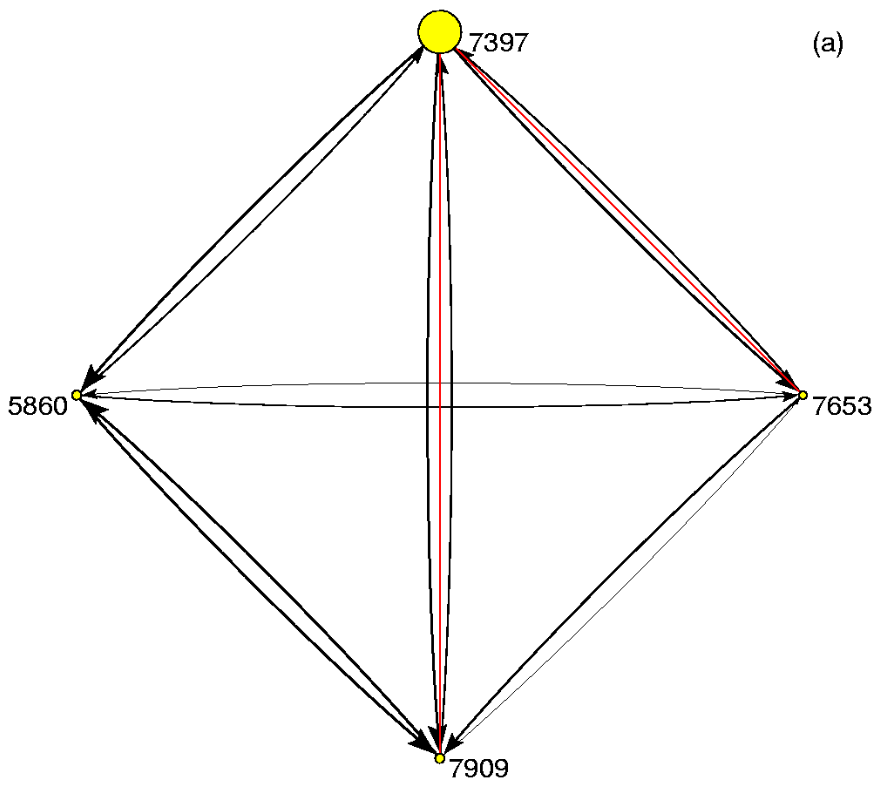
Quasi-steady states (QSS) punctuated by active periods. Self-similarity.

Typical community structures

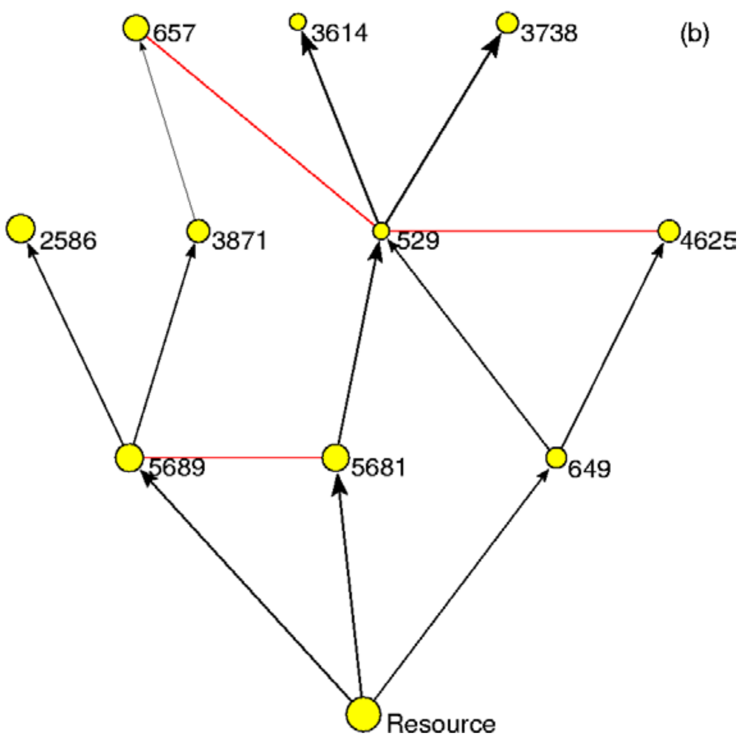
Networks

Model A

Model B



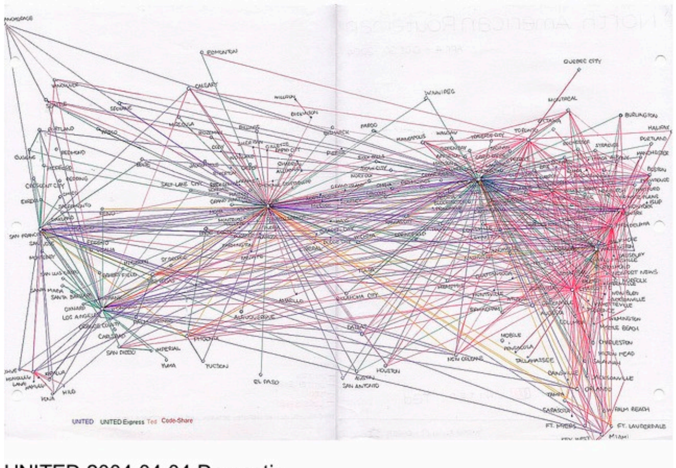
Mutualistic community



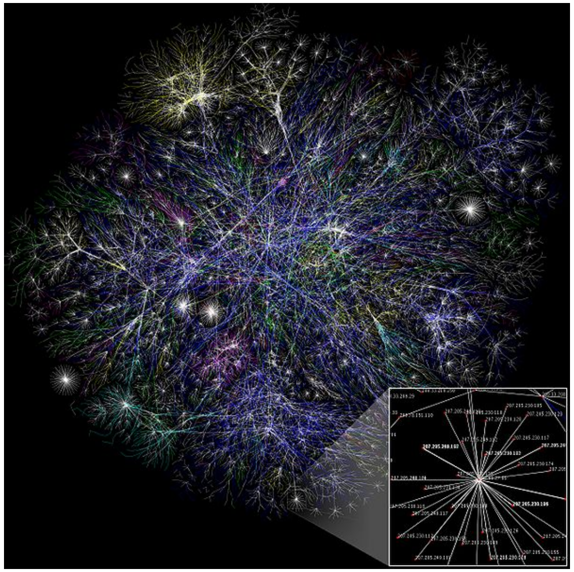
Predator-prey food web

Other network examples

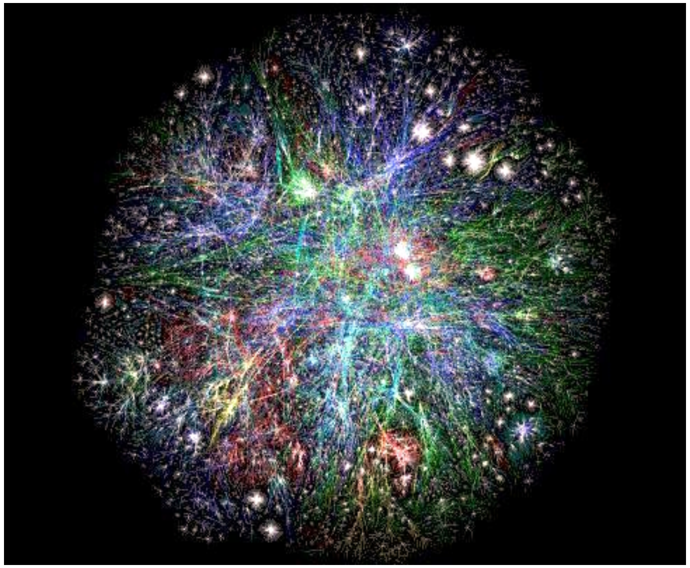
www.tokyometro.jp



UNITED 2004.04.04 Domestic
http://contrailscience.com/30-years-of-airline-travel/



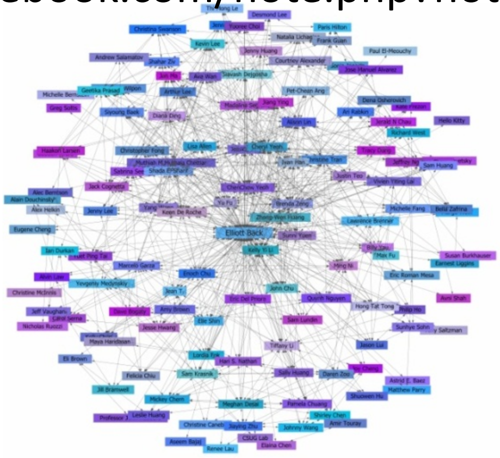
The Internet. From Wikipedia



World Wide Web. www.opte.org

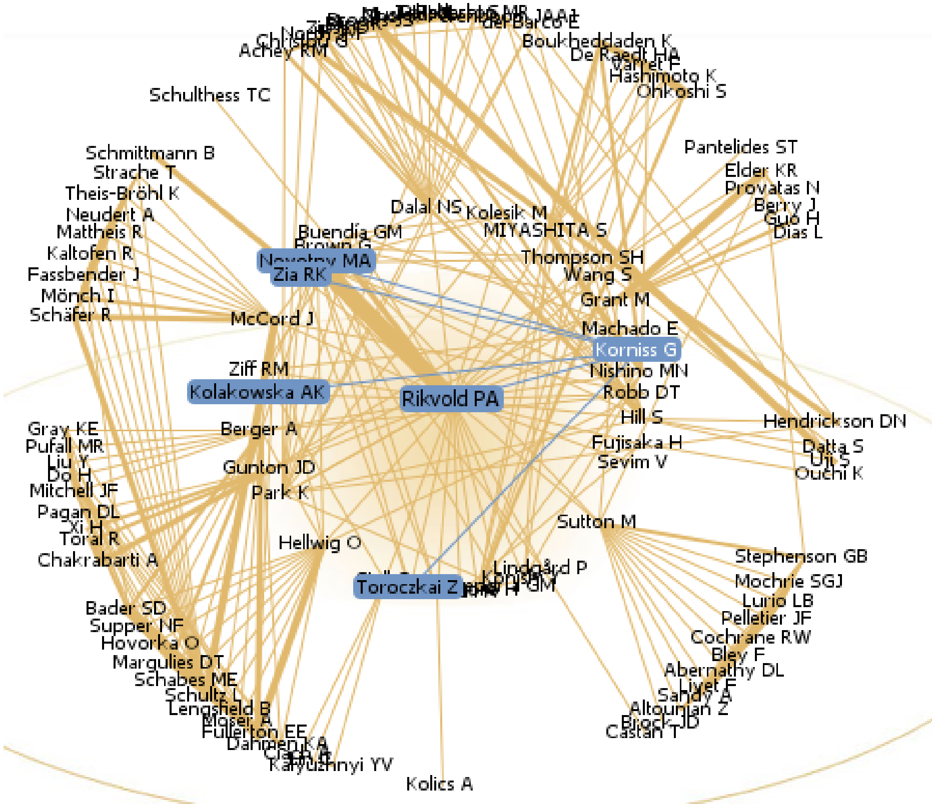
Social networks

http://www.facebook.com/note.php?note_id=469716398919



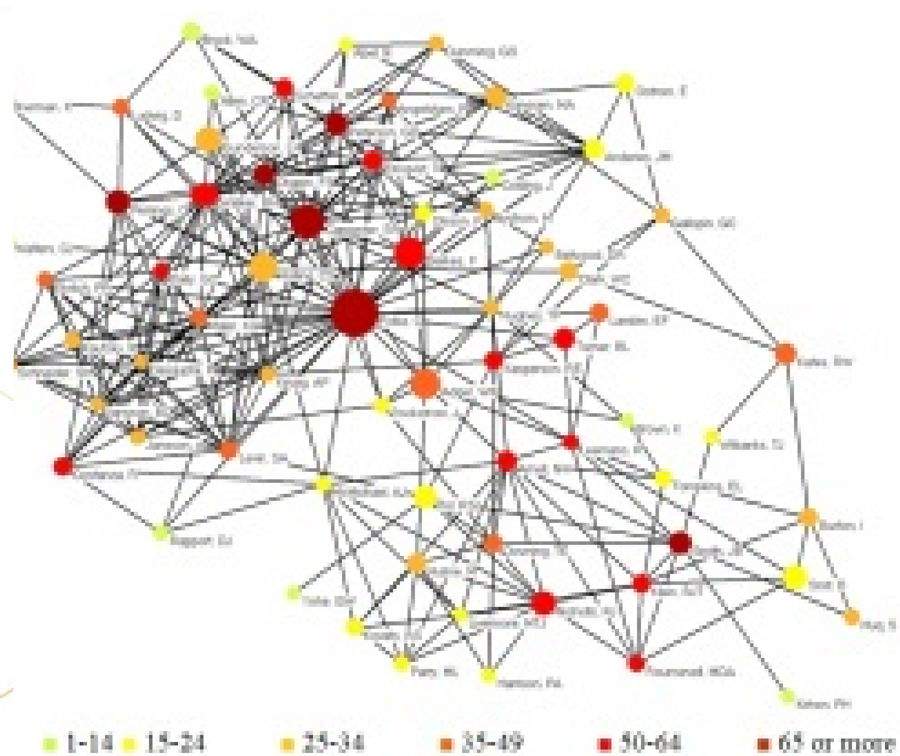
http://www.digitaltrainingacademy.com/socialmedia/2009/06/social_networking_map.php

Social networks



My co-author network in AIP journals

From AIP UniPHY

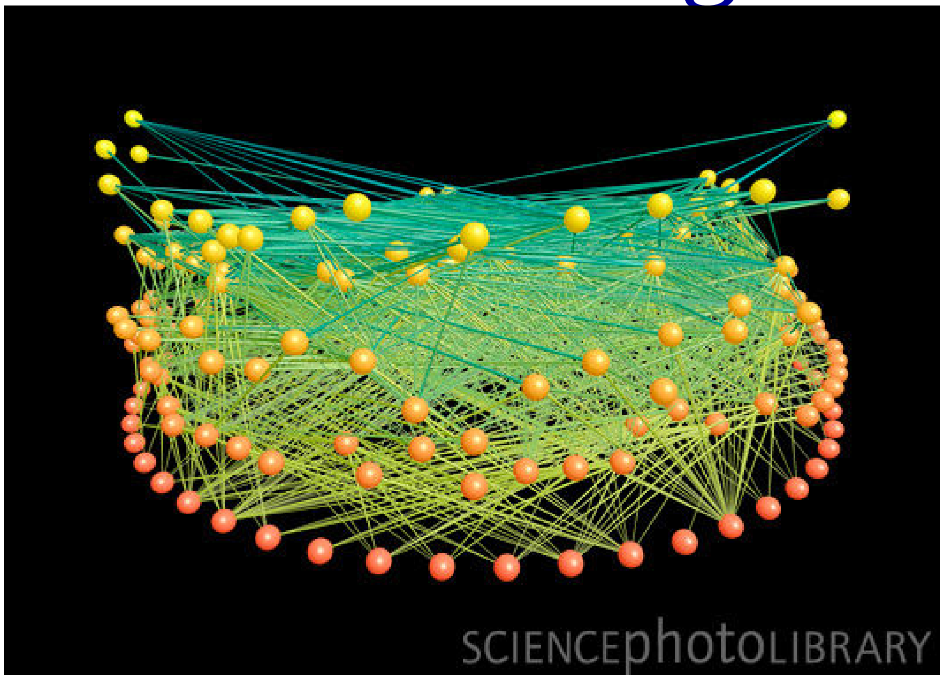


A co-author network in ecology

Janssen, M. A. 2007. *Ecology and Society* **12**(2): 9.

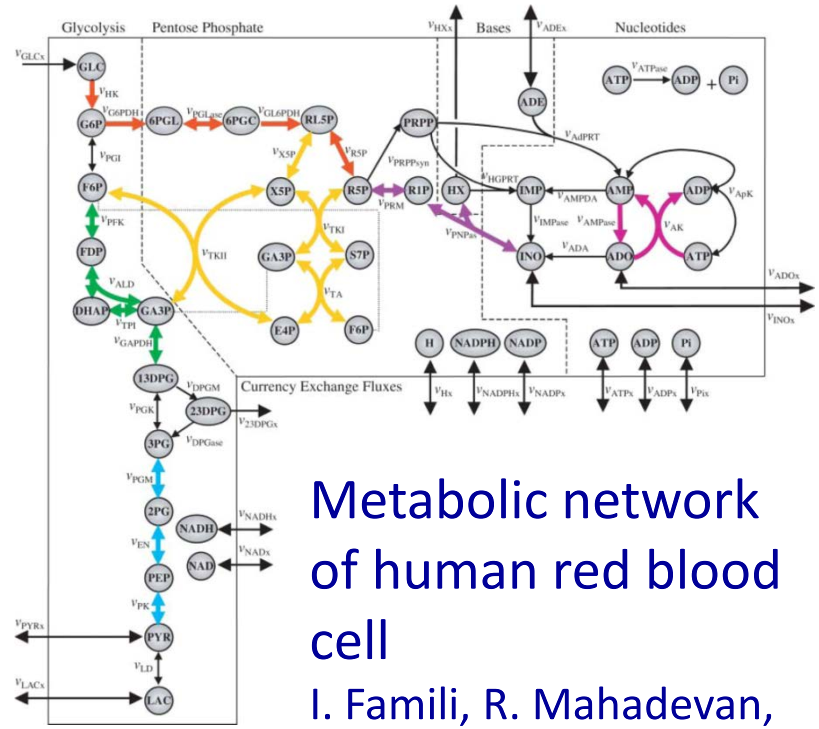
http://www.ecologyandsociety.org/vol12/iss2/art9/

Biological networks



Food web of the El Verde rainforest, Puerto Rico.

Neo Martinez. Image produced with FoodWeb3D, written by R.J. Williams and provided by the Pacific Ecoinformatics and Computational Ecology Lab (www.foodwebs.org, Yoon et al. 2004). Yoon, I., R.J. Williams, E. Levine, S. Yoon, J.A. Dunne, and N.D. Martinez. 2004. Webs on the Web (WoW): 3D visualization of ecological networks on the WWW for collaborative research and education. Proceedings of the IS&T/SPIE Symposium on Electronic Imaging, Visualization and Data Analysis 5295:124-132.



Metabolic network of human red blood cell

I. Famili, R. Mahadevan, B. O. Palsson, *Biophysical J*. **88**, 1616 (2005).

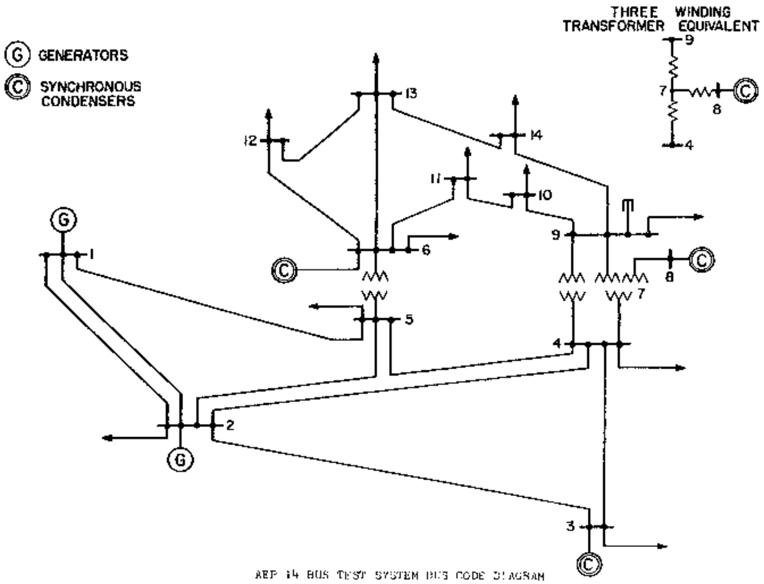
Applications of network theory to power grids

Collaborator: Prof. Svetlana V. Poroseva,
Mechanical Engineering, Univ. of New Mexico

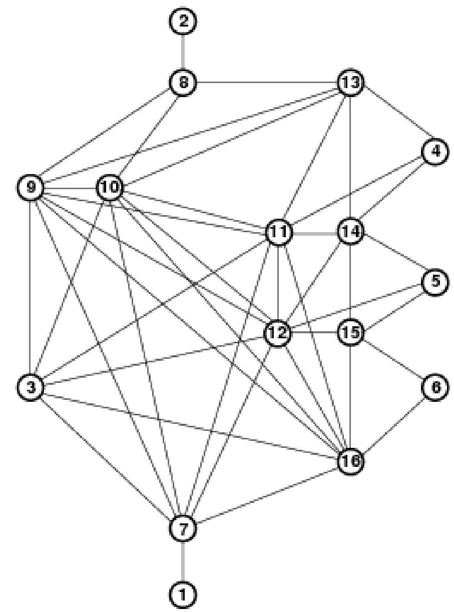
Motivation:

- Society relies heavily on power grid performance
- Modern & future power grids are large, complex, integrated
- Vulnerability to natural disasters, hostility, software failure

Approach:



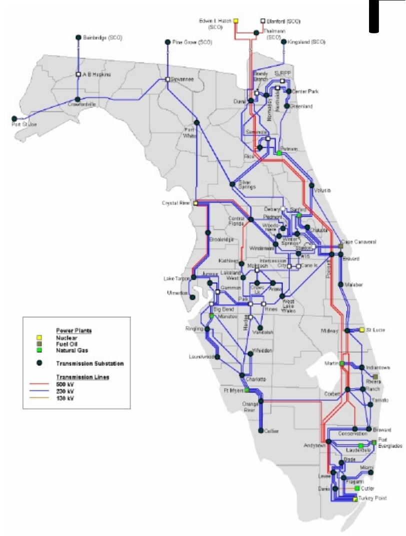
Network analysis



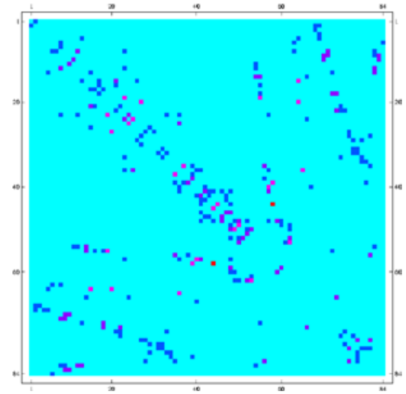
Current Focus:

- Impact of grid topology on grid performance
- Algorithm development
- Design of new grid topologies of enhanced survivability
- Bio-prototypes

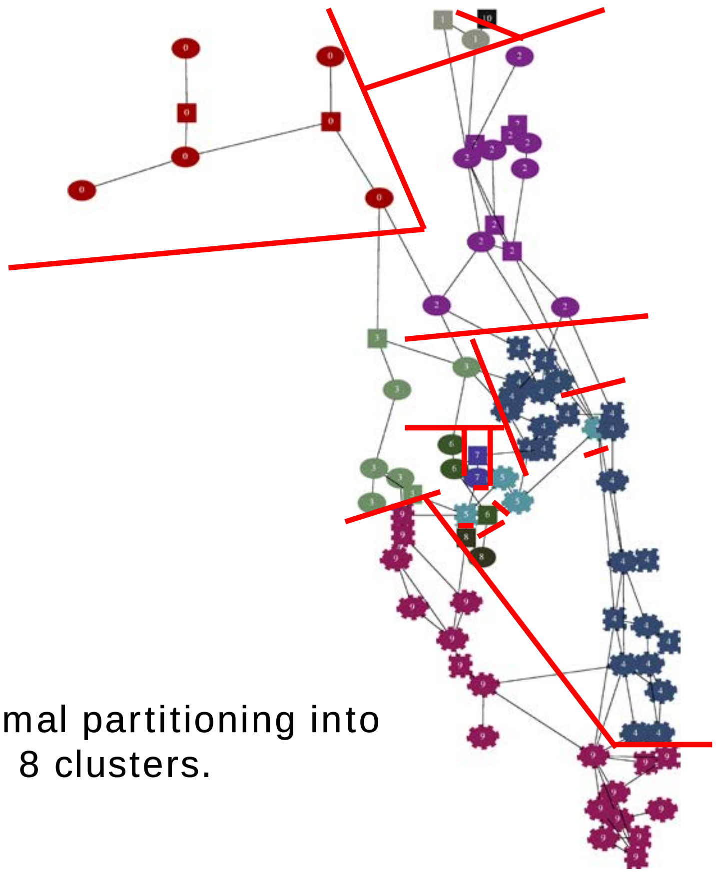
Floridian power grid



Florida electric power grid map
31 generators
53 loads



Corresponding network
84 vertices



Optimal partitioning into
8 clusters.

Conclusion

- **Statistical Physics** is about *systems that consist of* ***many*** *parts*
- Applications from
  - Nanoscience and thermodynamics
- through
  - Evolution, ecology, and sociology
- to
  - Power grids and the Internet
- **And many, many more …**