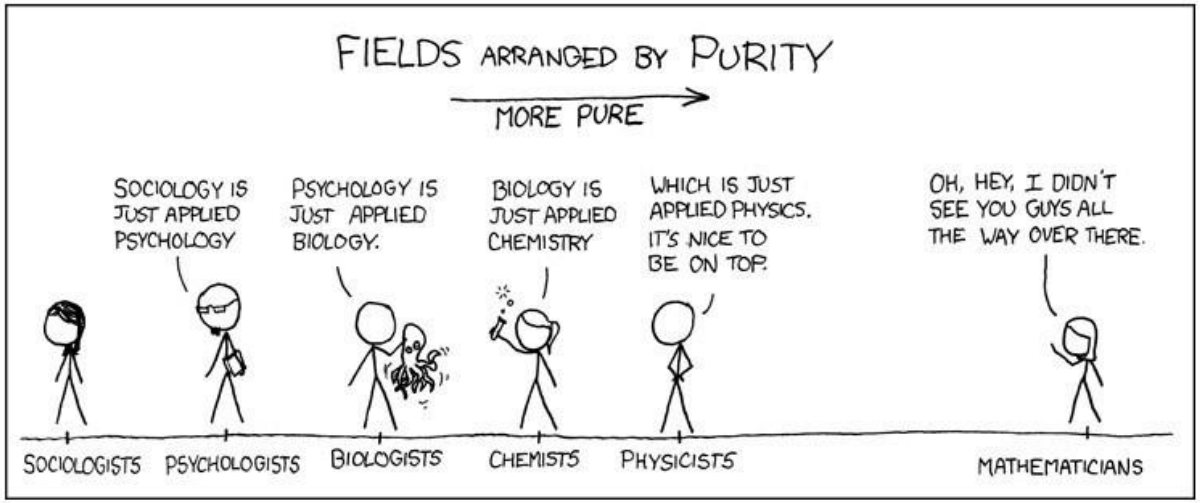
Statistical Field Theory in Biological Systems

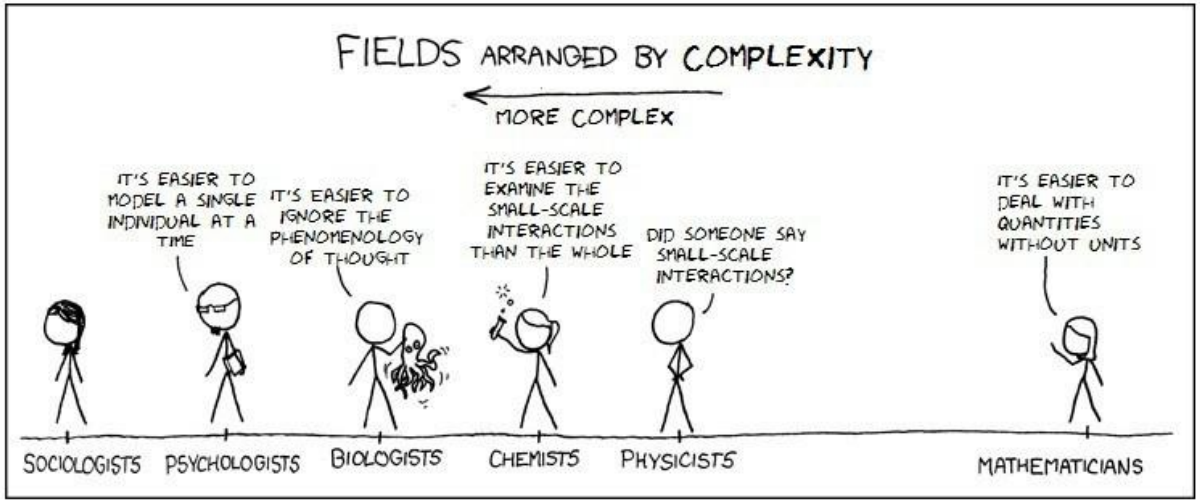
Maria A. Gutierrez

Part III Seminar Series

4/12/2020

Introduction


FIELDS ARRANGED BY PURITY
MORE PURE
SOCIOLOGY IS JUST APPLIED PSYCHOLOGY
PSYCHOLOGY IS JUST APPLIED BIOLOGY.
BIOLOGY IS JUST APPLIED CHEMISTRY
WHICH IS JUST APPLIED PHYSICS. IT'S NICE TO BE ON TOP.
OH, HEY, I DIDN'T SEE YOU GUYS ALL THE WAY OVER THERE.
SOCIOLOGISTS
PSYCHOLOGISTS
BIOLOGISTS
CHEMISTS
PHYSICISTS
MATHEMATICIANS


FIELDS ARRANGED BY COMPLEXITY
MORE COMPLEX
IT'S EASIER TO MODEL A SINGLE INDIVIDUAL AT A TIME
IT'S EASIER TO IGNORE THE PHENOMENOLOGY OF THOUGHT
IT'S EASIER TO EXAMINE THE SMALL-SCALE INTERACTIONS THAN THE WHOLE
DID SOMEONE SAY SMALL-SCALE INTERACTIONS?
IT'S EASIER TO DEAL WITH QUANTITIES WITHOUT UNITS
SOCIOLOGISTS
PSYCHOLOGISTS
BIOLOGISTS
CHEMISTS
PHYSICISTS
MATHEMATICIANS

Motivation

- **Complexity** and **diversity**
- Unified quantitative theory of biology?
- **“Life”** not about the properties of fundamental constituents but **interactions**
- **Emergent collective phenomena** of life...use **statistical mechanics**?
- This talk: big picture > details
    - *Not* about biological details
    - Statistical Field Theory / Statistical Physics

Today’s plan:

- **Maximum Entropy Models**
- Ising, Potts and XY models
- **Ising models** for networks of **neurons**.
- **Potts models** for sequences of **amino acids**.
- Dynamical **XY model** + **RG** for flocks of **birds**.
- Concluding remarks

Maximum Entropy Models

Real unknown probability distribution $P_r(\sigma)$ approximated by **model distribution** $P_m(\sigma)$ that **maximizes entropy**

$$S[P_m] = -\sum_\sigma P_m(\sigma) \log P_m(\sigma)$$

subject to measured **observables**

$$\langle \mathcal{O}_a(\sigma) \rangle_m = \langle \mathcal{O}_a(\sigma) \rangle_r$$

Lagrange multipliers → Boltzmann distribution

$$P_m(\sigma) = \frac{1}{Z} e^{\sum_a \beta_a \mathcal{O}_a(\sigma)} \equiv \frac{1}{Z} e^{-\beta E(\sigma)}$$

Ising Model

Spin +1 or -1

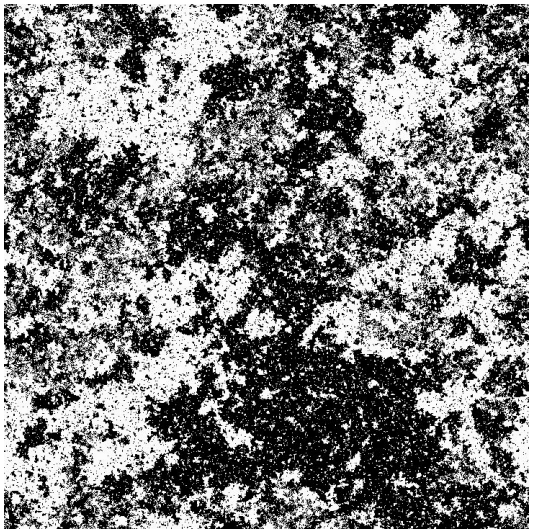
$$E(\sigma) = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i$$

External magnetic field h at each site

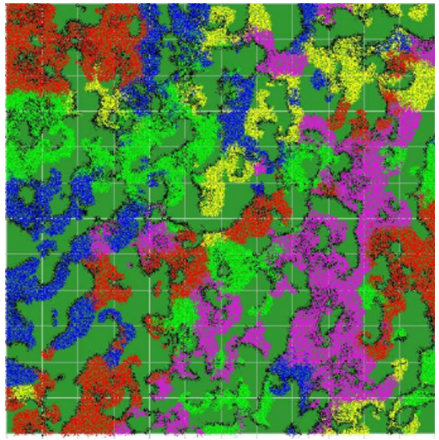
Interaction term between **adjacent spins**.

Long Range Ising

$$\sum_{\langle ij \rangle} \rightarrow \sum_{i,j}$$



Potts Model



-Generalizes Ising model

-Spins can take **one of q values**
uniformly distributed about a circle, at angles

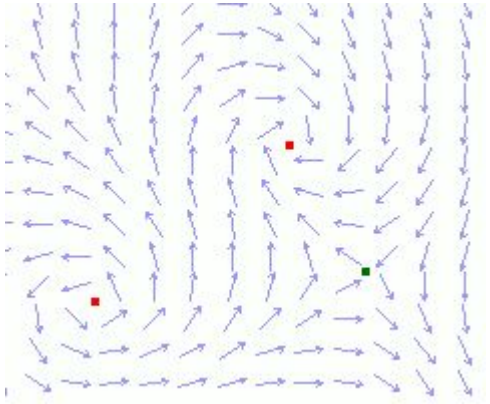
$$\theta_n = \frac{2\pi n}{q}$$

$$n = 0, \ldots, q-1$$

Commonly,

$$E = -J \sum_{\langle ij \rangle} \cos\left(\theta_{\sigma_i} - \theta_{\sigma_j}\right) - \sum_i h_i \sigma_i$$

XY model



Potts with $q \to \infty$

Spin can take **continuous values** in a circle $|\sigma_i| = 1$

Interaction term J translational invariant

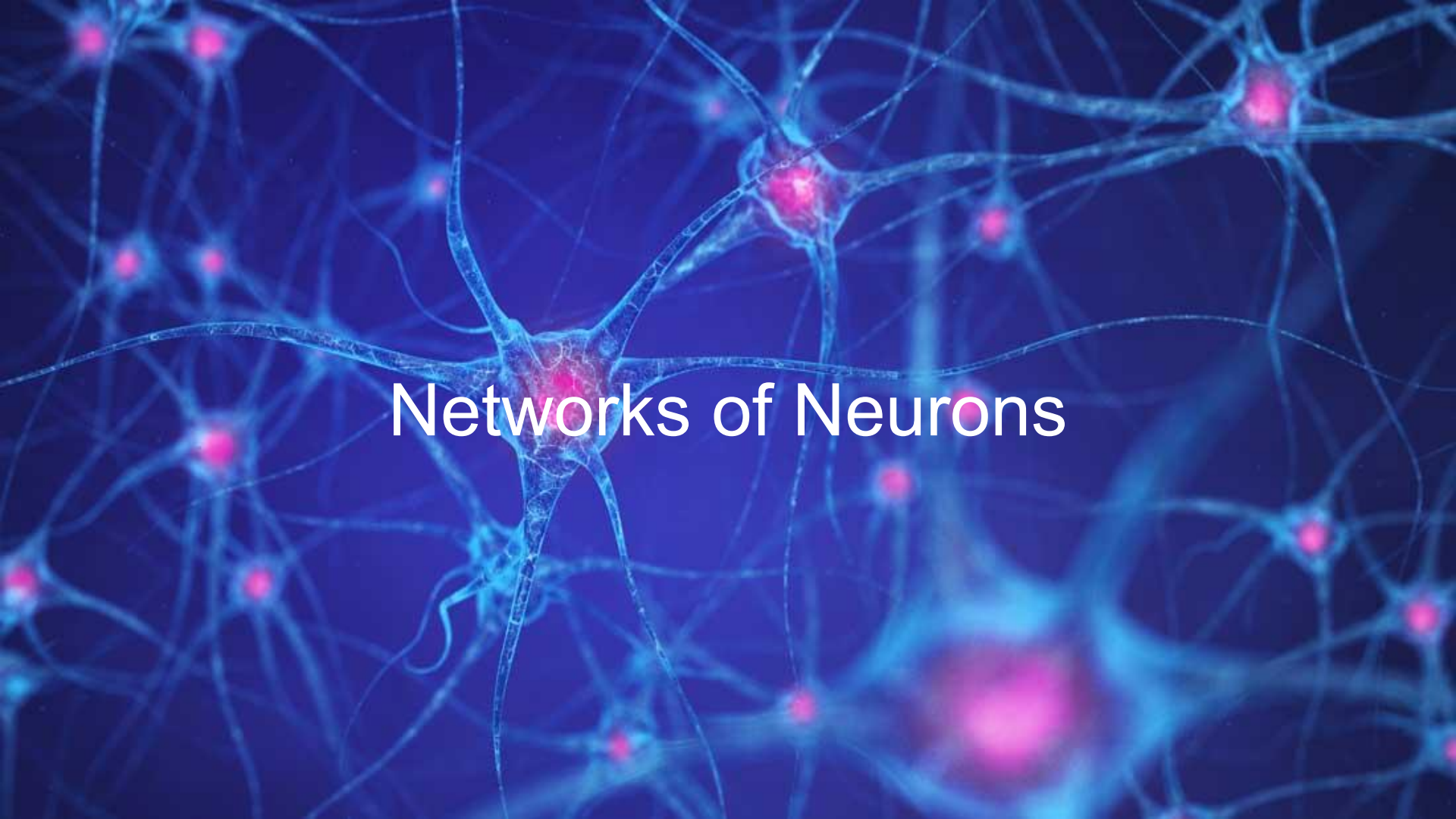
$$E = -\sum_{i \neq j} J_{ij} \sigma_i \cdot \sigma_j = -\sum_{i \neq j} J_{ij} \cos\left(\theta_{\sigma_i} - \theta_{\sigma_j}\right)$$

Coarse-graining:

$$F[\psi(\mathbf{x})] = \int d^d x \left[\frac{\gamma}{2}|\nabla\psi|^2 + \frac{\mu^2}{2}|\psi|^2 + g|\psi|^4 + \ldots\right]$$

Equation of motion

$$\gamma\nabla^2\psi = \mu^2\psi + 4g\psi|\psi|^2 + \ldots$$

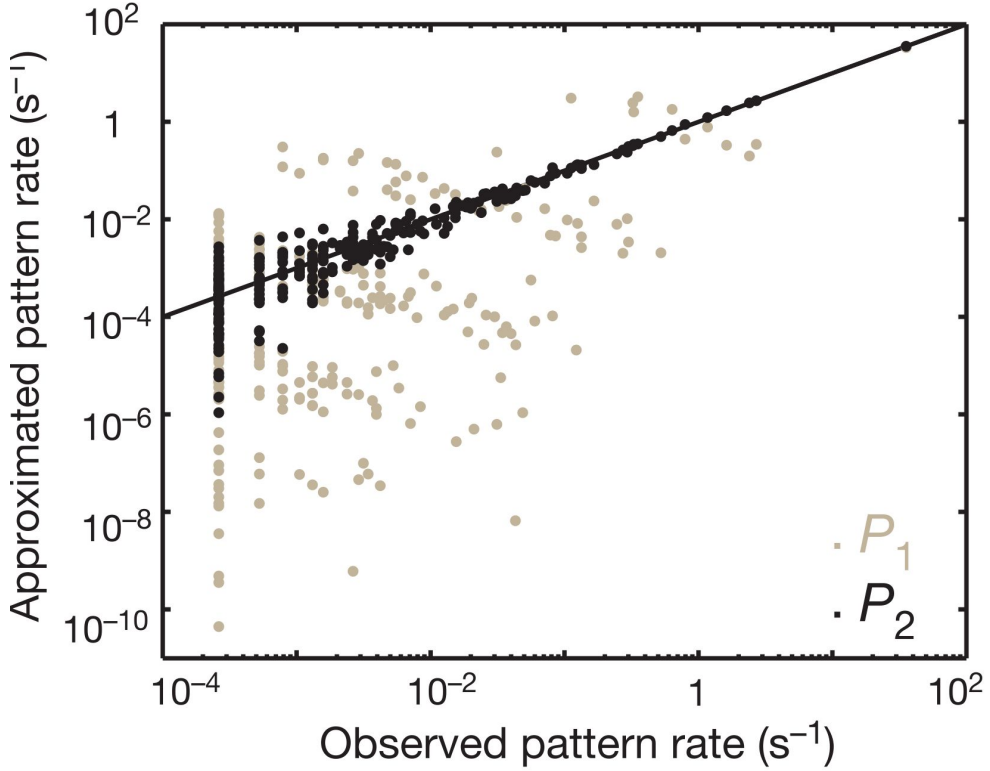

Networks of Neurons

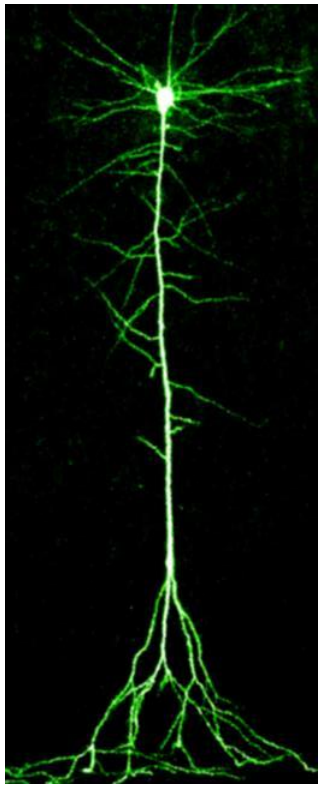
Disordered (long range) Ising model

$$E(\sigma) = -\sum_i h_i \sigma_i - \sum_{i<j} J_{ij} \sigma_i \sigma_j$$

$$\bar{r}_i = \left\langle \frac{1+\sigma_i}{2} \right\rangle \frac{1}{\Delta\tau}$$

$$\sigma_i = \pm 1$$





Heat Capacity

Introduce fictitious temperature

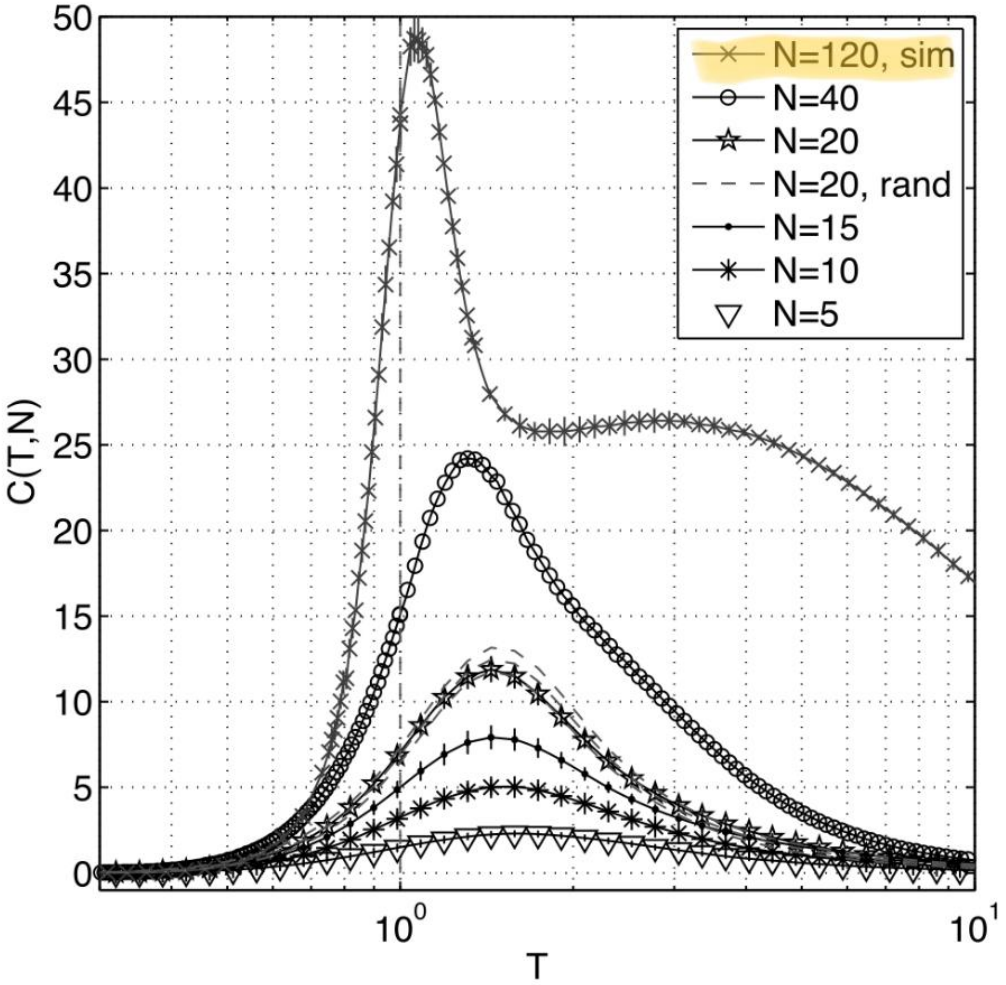
$$h_i \rightarrow h_i/T$$

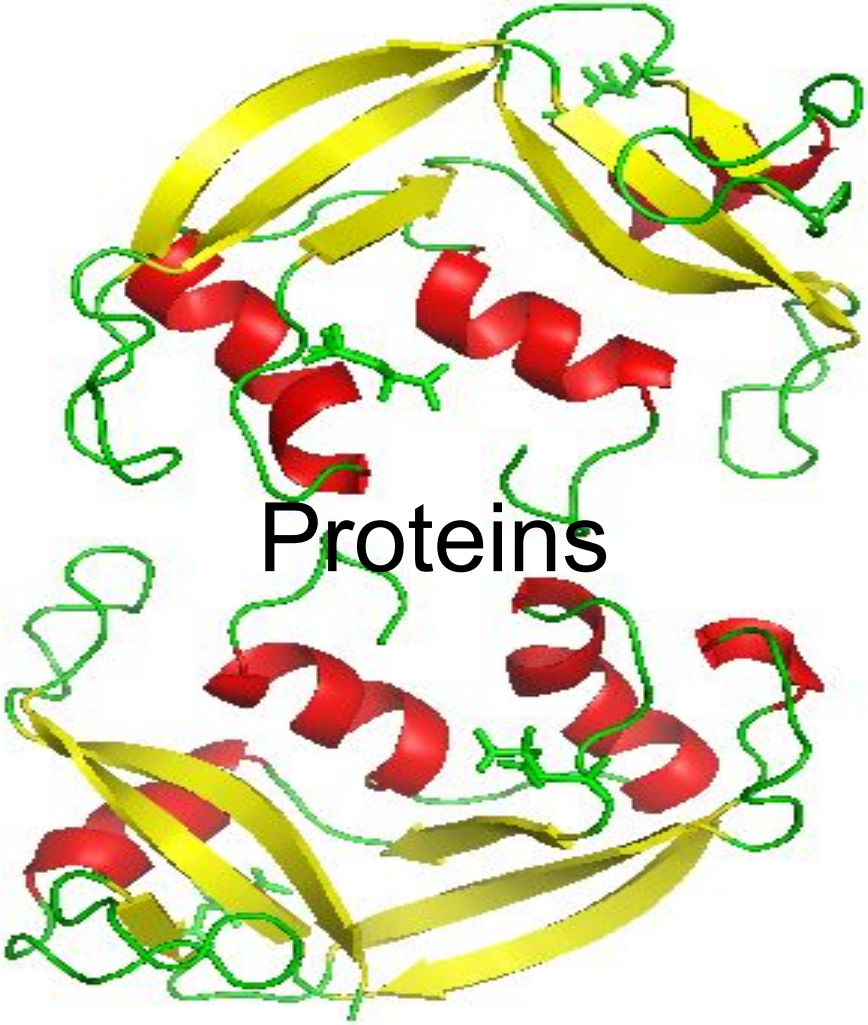
$$J_{ij} \rightarrow J_{ij}/T$$

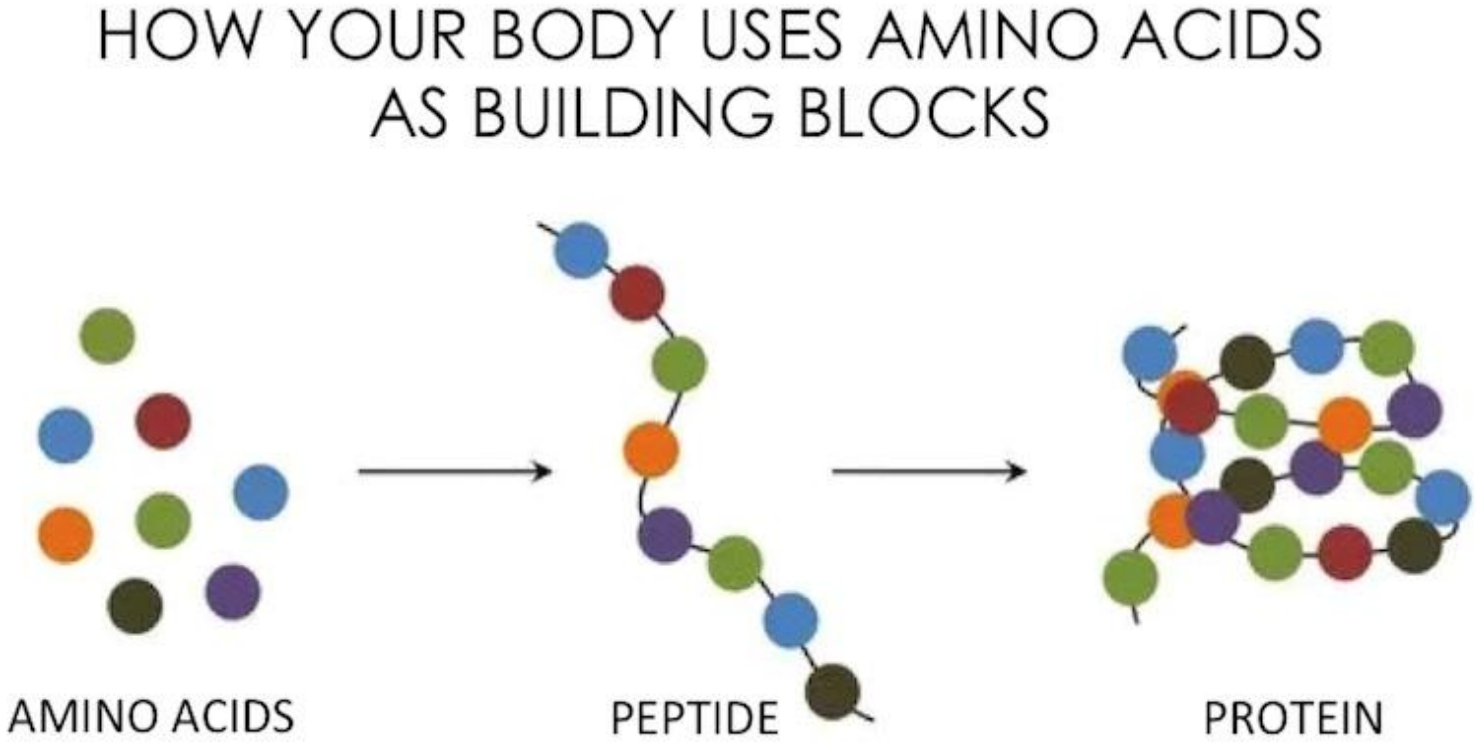
$$C(T) = \frac{N}{T^2}\left[-\frac{d^2 S(E)}{dE^2}\right]^{-1}$$

Divergent near T=1? Critical point?

$$C \sim C_{\pm}|T - T_c|^{-\alpha}$$

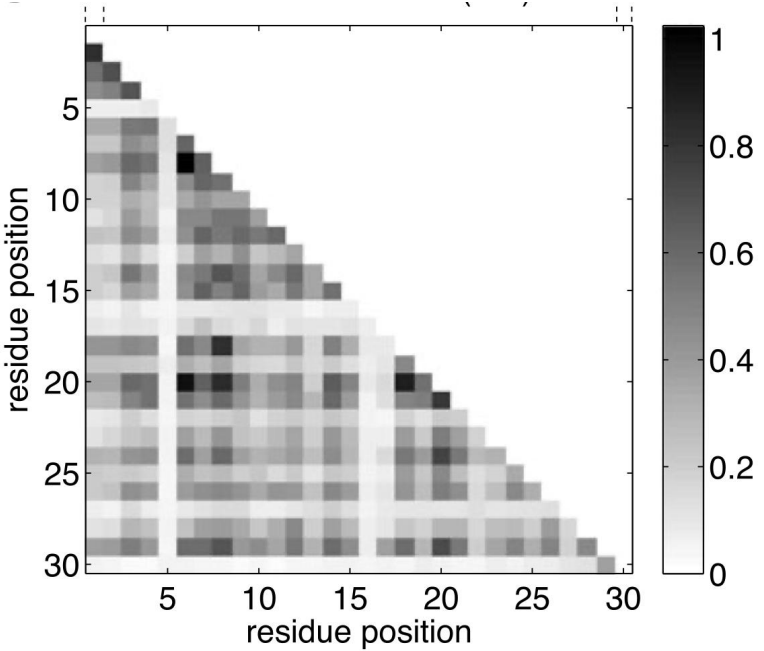



Proteins



Understanding amino acid mapping is equivalent to solving the **protein folding problem**

Pairwise correlations in WW domains



σ_i 1 of 20 amino acids or gap

Independent probabilities not enough for binding free energy

Disordered Potts model

“D segments”: good to study diversity and already sequenced experimentally. But:

- Sequences cannot be aligned
- Varying length. 0-8 amino acids

$$P(\sigma) = \frac{1}{Z} e^{\sum_i h(\sigma_i) + \sum_{ij} J_{(i-j)}(\sigma_i, \sigma_j) + \mu[L(\sigma)]}$$

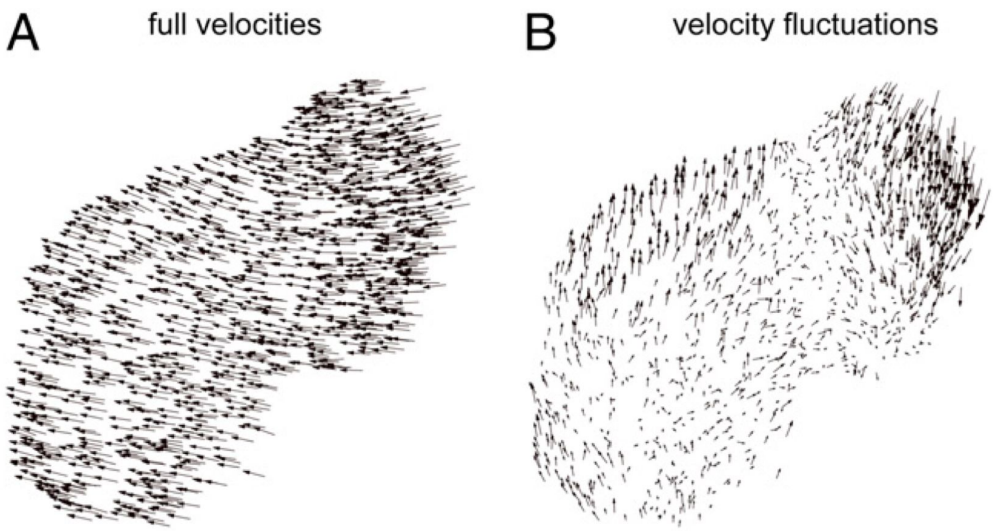
Translational invariant

Chemical potential depends on sequence length L.

Gradient descent + Monte Carlo: correlations between nearest and second to nearest neighbors agrees with 70-90% of info

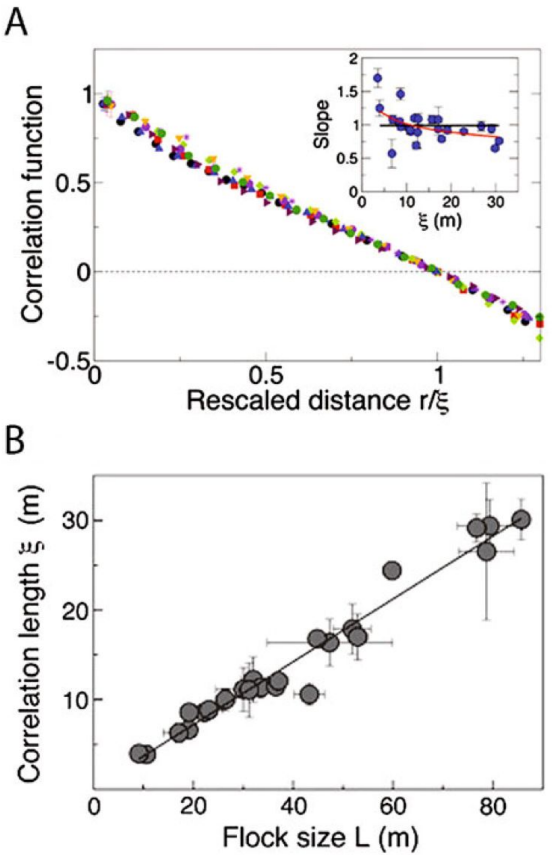
~10 metastable states, sign of criticality


Flocks of Birds



$$C(r) = \frac{1}{r^{\gamma}} f(r/\xi)$$

System near critical point?



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Long-Range Order in a Two-Dimensional Dynamical *XY* Model: How Birds Fly Together

John Toner[1,2] and Yuhai Tu[1]

[1]*IBM T. J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598*

[2]*Department of Physics, University of Oregon, Eugene, Oregon 97403-1274**

(Received 9 June 1995)

We propose a nonequilibrium continuum dynamical model for the collective motion of large groups of biological organisms (e.g., flocks of birds, slime molds, etc.) Our model becomes highly nontrivial, and different from the equilibrium model, for $d < d_c = 4$; nonetheless, we are able to determine its scaling exponents *exactly* in $d = 2$ and show that, unlike equilibrium systems, our model exhibits a broken continuous symmetry even in $d = 2$. Our model describes a large universality class of microscopic rules, including those recently simulated by Vicsek *et al.*

"Violates" **Mermin-Wagner theorem**: a continuous symmetry cannot be spontaneously broken in d=2 dimensions.

Model

$$\partial_t \vec{v} + (\vec{v} \cdot \nabla)\vec{v} = \alpha \vec{v} - \beta |\vec{v}|^2 \vec{v} - \nabla P + D_L \nabla(\nabla \cdot \vec{v}) + D_1 \nabla^2 \vec{v} + D_2 (\vec{v} \cdot \nabla)^2 \vec{v} + \vec{f}\,, \tag{1}$$

$$\gamma \nabla^2 \psi = \mu^2 \psi + 4g\psi|\psi|^2 + \ldots$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{v}\rho) = 0\,, \tag{2}$$

$$\alpha < 0 \Rightarrow \text{disordered phase } \langle |\vec{v}| \rangle = 0$$

$$\alpha > 0 \Rightarrow \text{ordered phase } \langle |\vec{v}| \rangle = \sqrt{\alpha/\beta}$$

Renormalization Group

Scaling dimensions

$$\vec{x}_\perp \longrightarrow b\vec{x}_\perp, \quad x_\parallel \longrightarrow b^\zeta x_\parallel, \quad t \longrightarrow b^z t, \quad \vec{v}_\perp \longrightarrow b^\chi \vec{v}_\perp$$

$$z = \frac{2(d+1)}{5}, \quad \zeta = \frac{d+1}{5}, \quad \chi = \frac{3-2d}{5}$$

Define non-linear effective coupling constants g_n

RG flow (beta functions) to find:

g_1, g_2 **relevant** for d<4 $g_{n>2}$ **irrelevant** near d=4

Findings and follow up paper

1. Model differs from equilibrium system for d<4
2. Can calculate exactly the scaling exponents for d=2
3. Model has a *stable* spontaneous symmetry broken state even in d=2
    - d=4-epsilon expansion

Flocks, herds, and schools: A quantitative theory of flocking

John Toner, Yuhai Tu. arXiv:cond-mat/9804180 **[cond-mat.stat-mech]**

- Goldstone modes, Landau-Ginzburg theory…
- Anisotropic model in d=3: preference for flying horizontally

Concluding remarks

We have seen:

- **Ising models** for networks of **neurons**.
  - Divergent heat capacity
- **Potts models** for sequences of **amino acids**.
  - Metastable states
- Dynamical **XY model** for flocks of **birds**.
  - Scale invariant correlations
  - RG flow

Criticality

- Evidence towards critical behaviour in different systems
- **But** criticality in biological networks is still to be tested

Why would biological systems be near critical?

How criticality (a tiny region in parameter space) can be achieved in so many different systems?

Mora, T., Bialek, W. **Are Biological Systems Poised at Criticality?**.
J Stat Phys 144, 268–302 (2011). https://doi.org/10.1007/s10955-011-0229-4

Final ideas

- Universality
- Criticality
- Coarse-graining: renormalization group
- Quantitative approaches to theoretical biology

Perspectives on theory at the interface of physics and biology

W Bialek - Reports on Progress in Physics, 2017

Questions' Time

Please fill up the **feedback form :)**

https://forms.gle/hB1VHzCfUsnq65Qx7

Contact: mag84 or pm on Fb

THANK YOU!