Title: Emergence and Minimal Models in Condensed Matter Physics and Biology

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Abstract: Our ability to understand the physical world has to a large extent depended on the existence of emergent properties, and the separation of scales that permits effective field theory descriptions to be useful. Exploiting this fact, we can construct minimal models that enable efficient calculation of desired quantities, as long as they are insensitive to microscopic details. This works in many instances in physics, and I give some examples drawn from the kinetics of phase transitions mediated by topological defects. In other fields, such as biology, it is not so clear that these concepts are useful, and I will discuss to what extent emergence and effective theories might be useful.

Emergence and minimal models in condensed matter physics and biology

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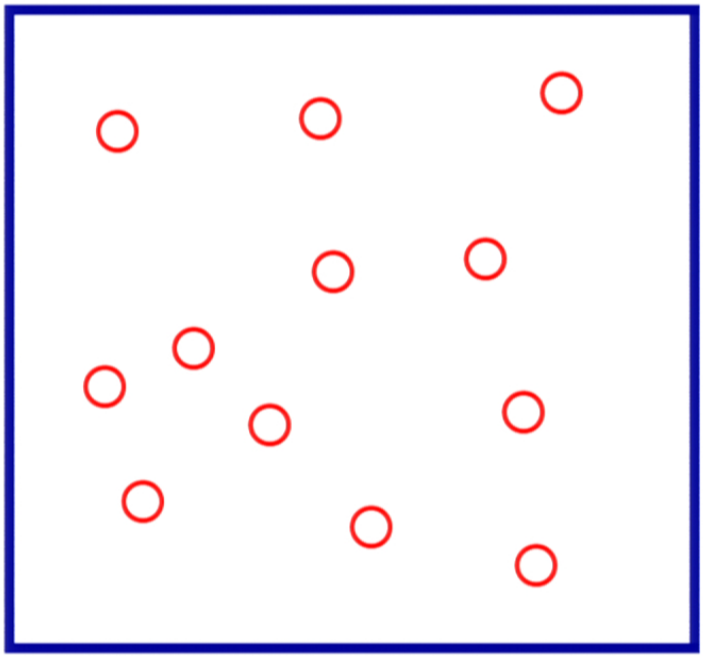
Collaborators: Yoshi Oono, M. Mondello (Cell dynamical systems); Kalin Vetsigian (evolution)

Work supported by the US National Science Foundation and NASA

Emergence of the solid state

- **Atoms in a box**
  - Fluid state
- **Low temperature**
  - Crystalline solid forms
- **Characteristics different from fluid state**
  - Periodic crystal lattice
  - Static shear rigidity



Emergence of the solid state

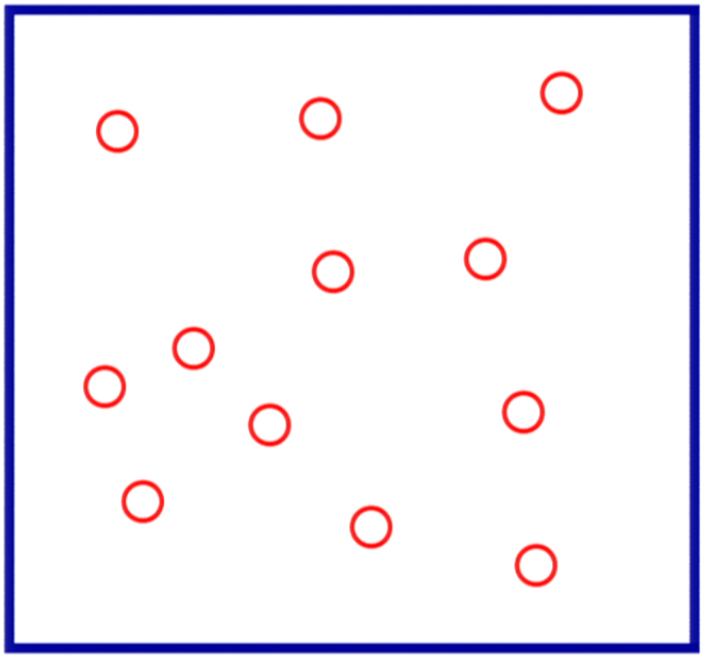
Q: *Why is this interesting?*

A: *Because the underlying physics of the crystal is* <u>exactly</u> *the same as the fluid!*

- Total Energy =

  Kinetic energy+ Potential energy

- Lowering temperature <u>has not changed</u> the interactions between the atoms



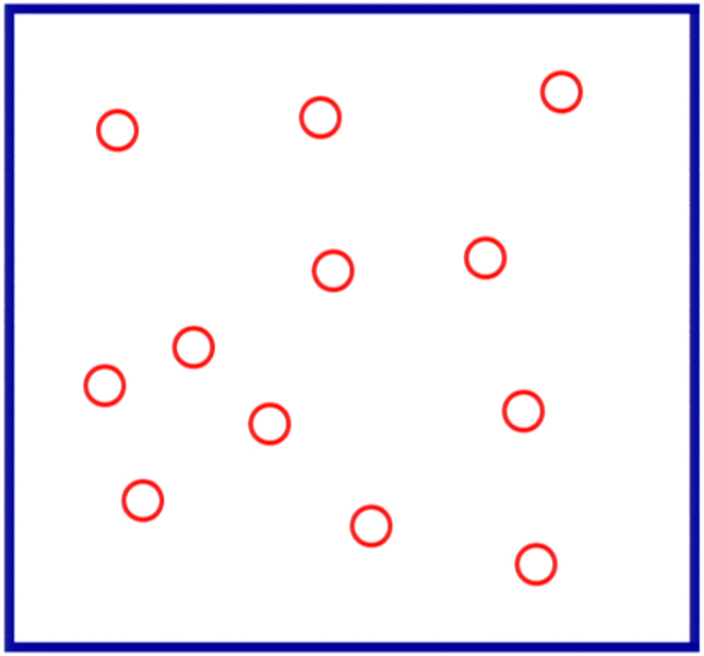
Emergence of the solid state

Conclusion:

Although the pairwise interactions between atoms did not change

the correlations between them changed when the temperature was lowered

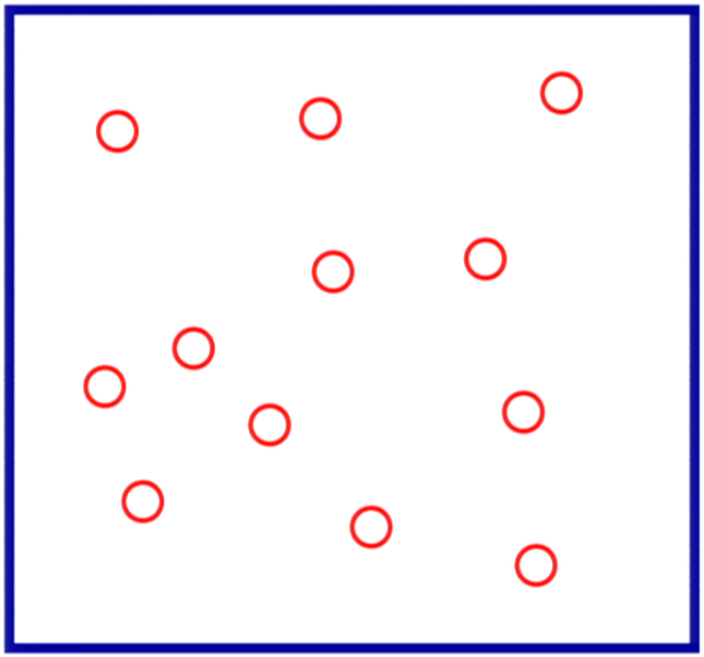
So the solid state emerged as if by magic out of the fluid state!



Emergence: the big deal

The solid state has its own new laws of physics!

- **New long-range forces that are completely distinct from the original forces between the atoms**
  - **Elasticity!**
    - **Response of solid to external disturbances completely different from that of a fluid**
- **Origin of these new laws: the collective, statistical behaviour of the atoms**



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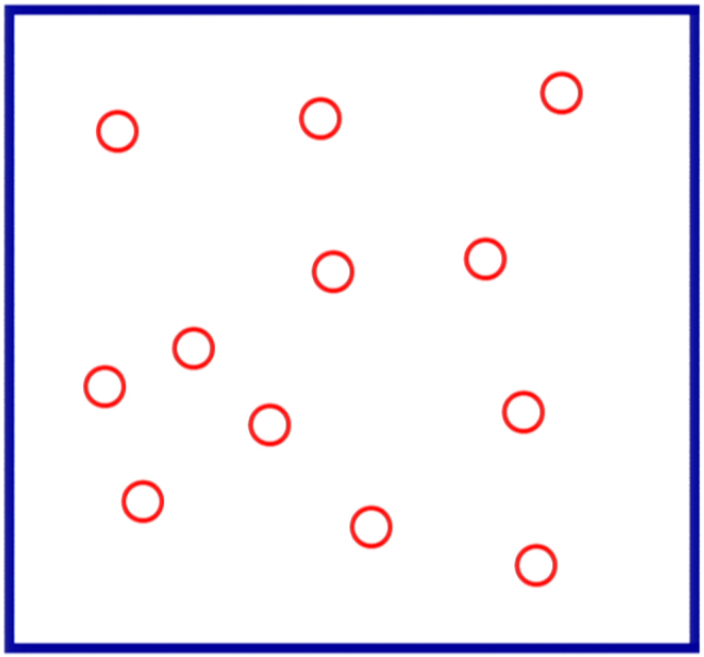
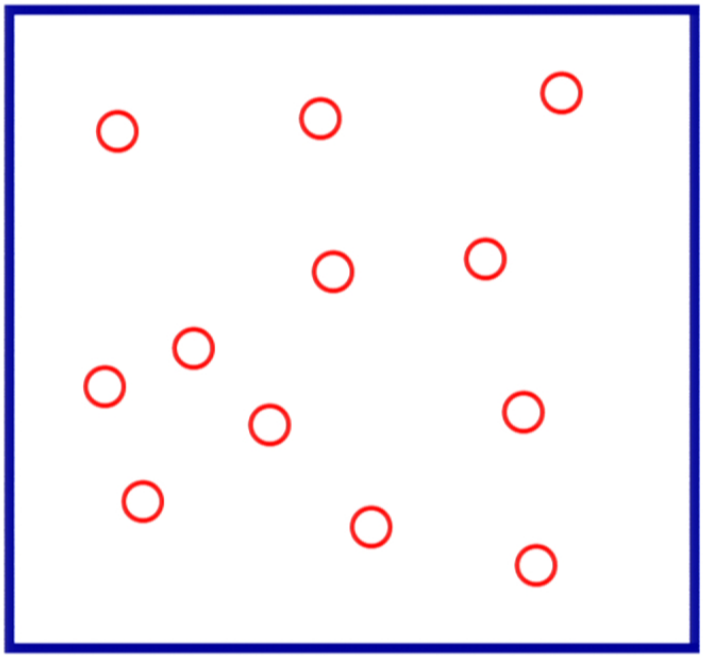


Emergence: new laws of physics?

The solid state has its own new "laws of physics"!

Really?

Well, yes! At the level of description of a solid, the actual interactions between the atoms cannot be detected --- only the continuum mechanics of the solid is observable!

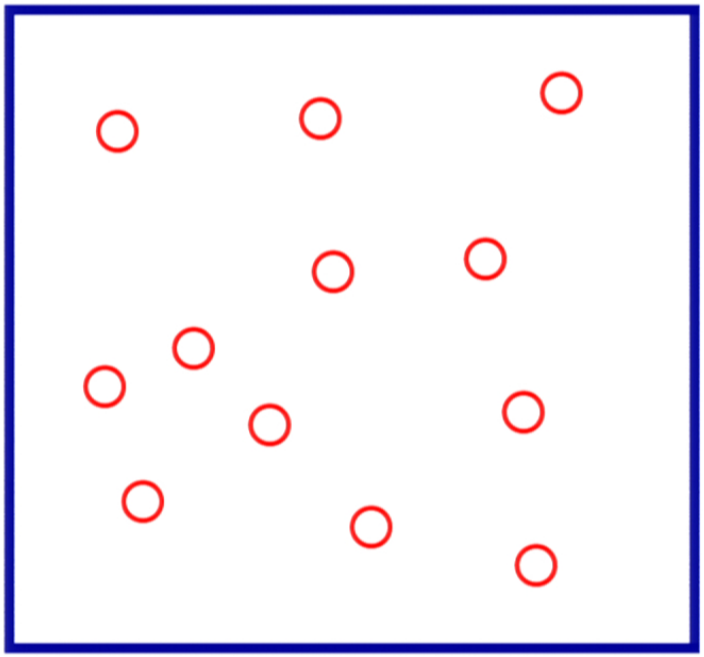


Emergence: new laws of physics?

This is why it took so long for the existence of atoms to be deduced!

Q: So where do atoms and their interactions matter?

A: The elastic forces are characterized by phenomenological parameters such as shear modulus that can only be computed from the atomic level of description.

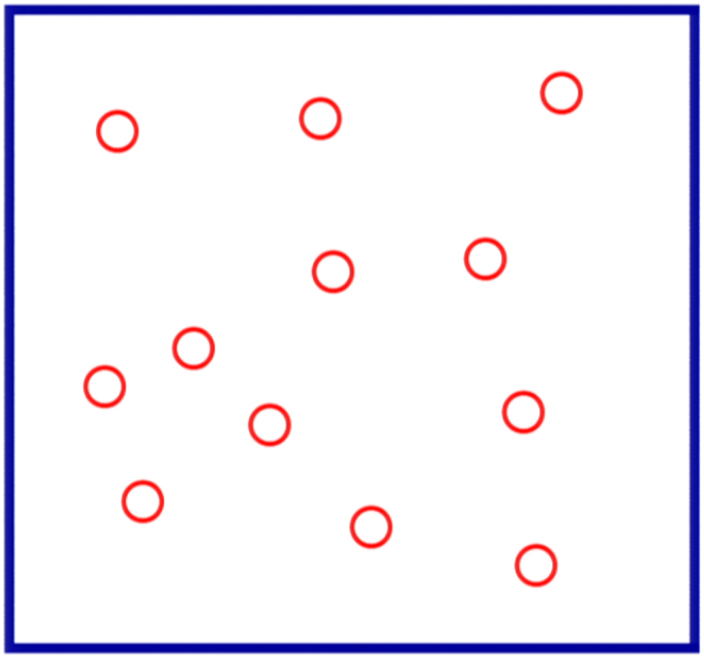


When we do atomic physics or chemistry, we do not need to take into account the mass of the top quark!

Emergence: new laws of physics?

Summary:

- **Emergent levels of description absorb the properties of lower levels of description into phenomenological parameters**
  - **Typically a small number!**



Emergence: new laws of physics?

Summary:

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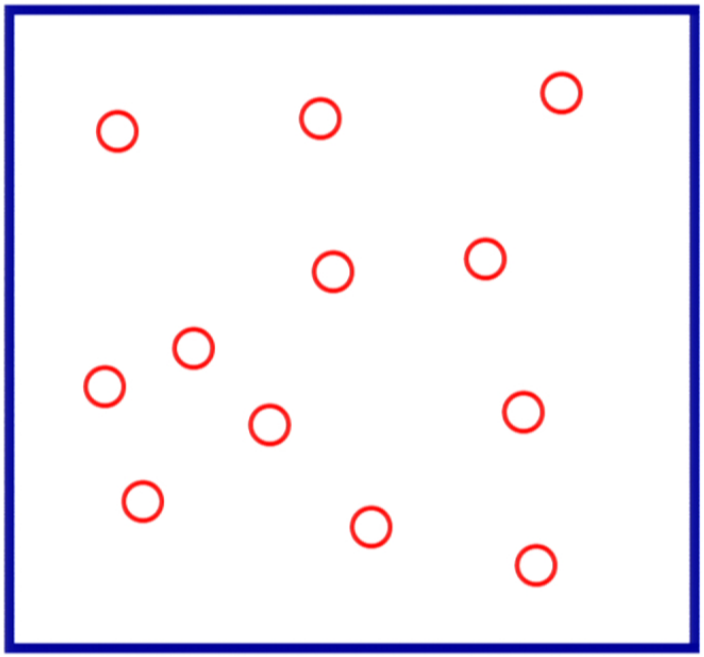
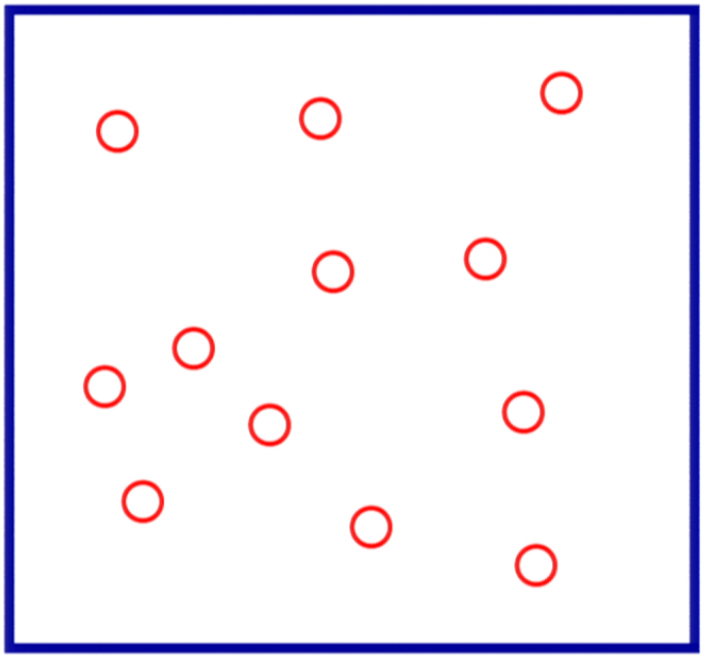
- **This makes "fundamental physics" hard, because one "goes against the flow" of emergence**



Emergence: new laws of physics?

Summary:

- **Emergent levels of description absorb the properties of lower levels of description into phenomenological parameters**
  - **Typically a small number!**
- **This makes "fundamental physics" hard, because one "goes against the flow" of emergence**
  - **Dooms reductionism!**
- **But collective properties of matter can be understood, and should be understood, without requiring knowledge "all the way down"**



Characteristics of emergence

- **Emergence is associated with loss of uniqueness**
  - Fluid state still possible at low temperature but much less likely than solid state
  - Phase transitions separate states
    - Collective, only well-defined for thermodynamically large systems
- **New, collective properties arise in emergent states**
  - Crystals, magnets, superconductors, quantum hall effects ...
  - Turbulence? Gravity? Life?
  - Do emergent phenomena bring molecules to life?

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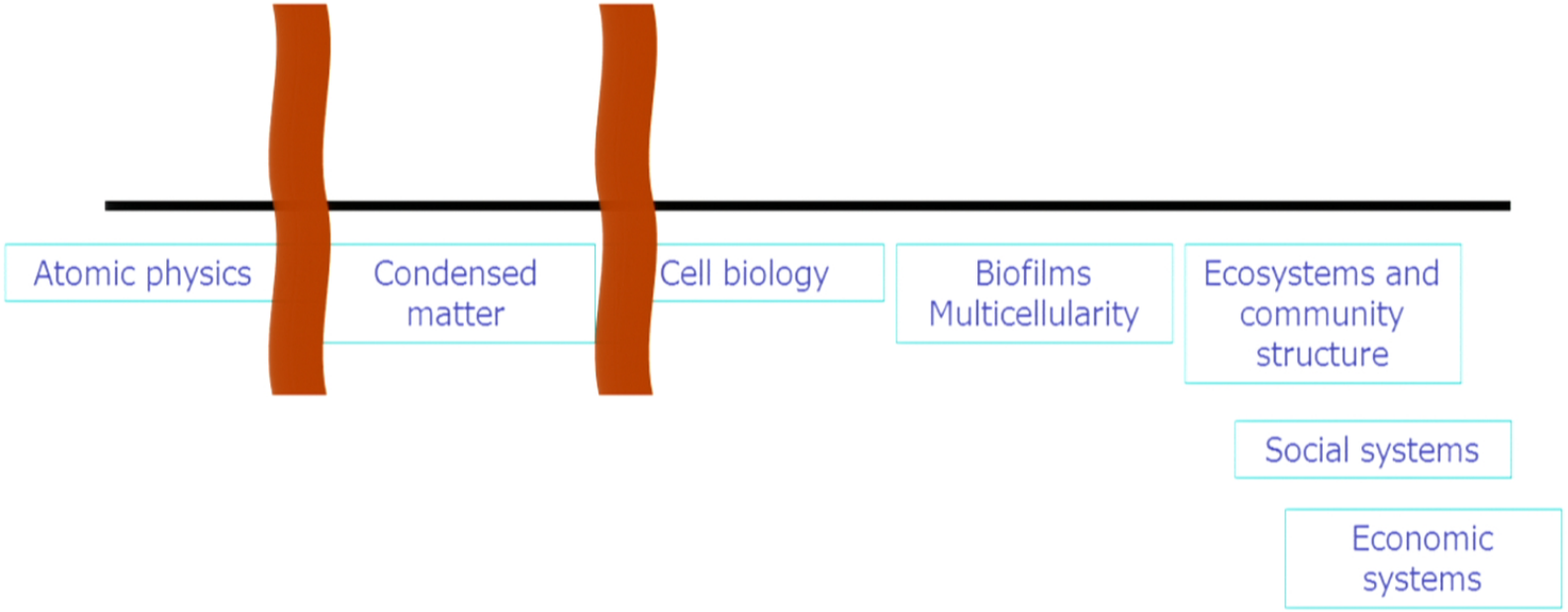
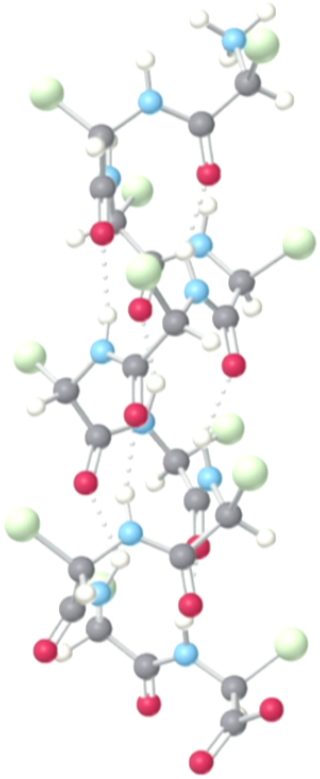
Emergence => complexity

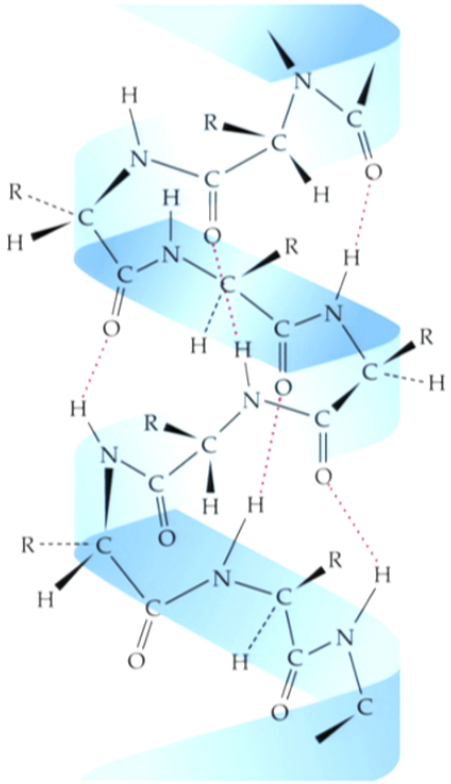


Overview

- **Minimal models and universality**
  - What aspects of physical phenomena should we try to capture?
  - What aspects of physical phenomena should we try to predict?
- **Modelling without calculus**
  - Cell dynamical systems
- **Space-time patterns during phase transitions**
  - Universal features of pattern formation
  - Comparison with experiment
- **Minimal models in biology – a waste of time?**

Perceptions of reality: polymers

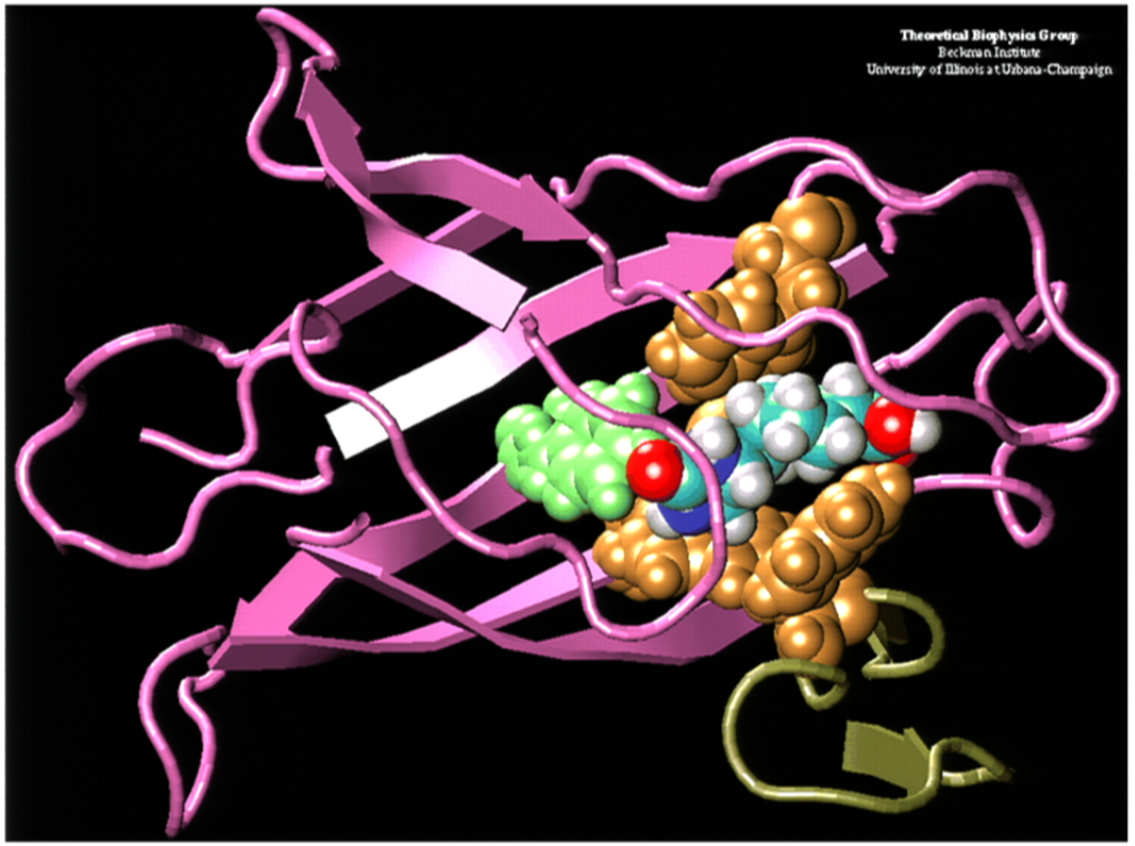




From *Chemistry* by McMurry & Fay

Chemist

Perceptions of reality: polymers



Schulten group UIUC

Computational biologist

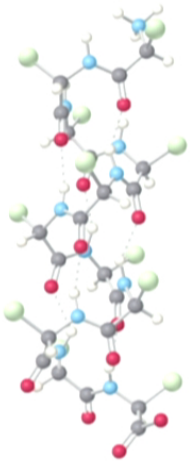
Perceptions of reality: polymers

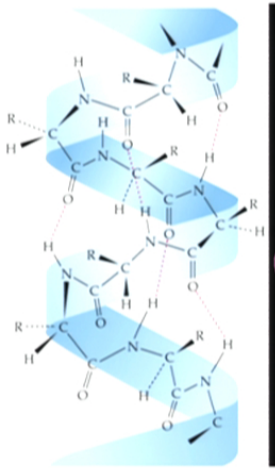
The Gutsy Gourmet

Theoretical physicist

Perceptions of reality: polymers

What questions can each of these representations answer?





Chemical bonding, reactions, …

Elasticity, large scale motions, folding

Thermodynamics, light scattering, rheology

Perceptions of reality: polymers

- **How big is a polymer?**

Total length of polymer is $L = N \ell$

Perceptions of reality: polymers

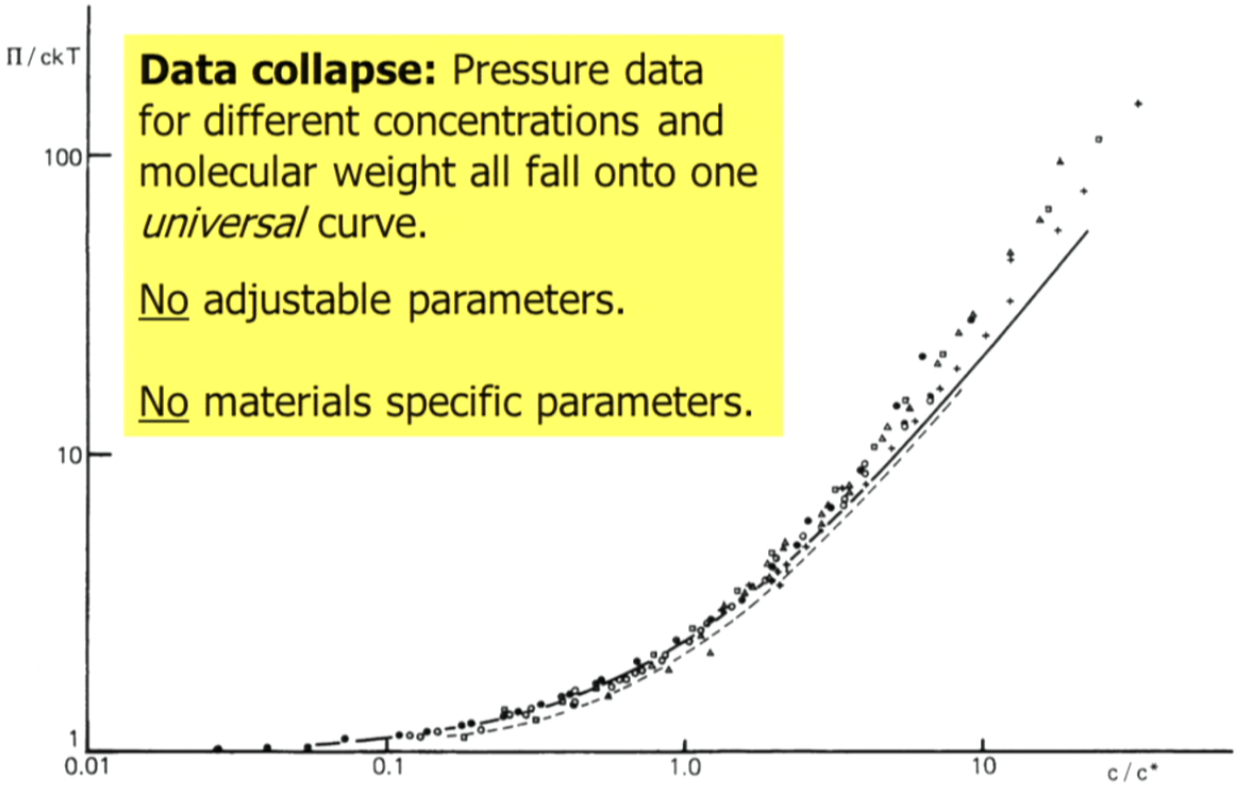
- **How big is a polymer?**
  - Chemistry
    - model bond angles and energy barriers to rotational states, solvent molecules
    - Sample over long times, or many independent conformations
    - Predict R in Angstroms
  - Physics
    - **Random walk of N steps each of length ℓ**
    - **Einstein argument: $R^2 = N\ell^2 = \ell L$**
    - **Excluded volume: polymer cannot cross itself, because two atoms cannot occupy same position. Expect chain to swell:**

$$R = A(\ell)\, L^{0.588} \quad \text{as } L \to \infty$$

    - **The scaling with L is:**
      - Universal, i.e. independent of the chemical structure
      - Asymptotic for large chains
    - **Cannot predict R in Angstroms**

Total length of polymer is $L = N\ell$

Perceptions of reality: polymers



Data collapse: Pressure data for different concentrations and molecular weight all fall onto one *universal* curve.

No adjustable parameters.

No materials specific parameters.

Osmotic pressure of polystyrene in solution as a function of concentration. Data from Wiltzius *et al* (1983) for $10^4 < M_W < 10^7$ in two different solvents. Theory by Ohta and Oono (1982).

Perceptions of reality: polymers

- **The spaghetti model of a polymer is an example of a *minimal model***
  - Flexible, random walk
  - Self-avoidance: two atoms cannot occupy same point
  - Statistical thermodynamic equilibrium
- **Good for answering certain questions**
  - Universal quantities: pressure, scaling of size with number of monomers, …
- **Lousy at answering other questions**
  - E.g. what is the size of the polymer coil (in Angstroms)?

Universality in physics

- **Successful scientific predictions are always the result of minimal models!**
  - Cannot include every detail in a model.
    - **Physics: usually only a few details important: some separation of energy scales. "Easy".**
      - Standard model of high energy physics is a minimal model (23 adjustable parameters!) Do you really think this is a "fundamental" theory?
    - **Chemistry: usually need a lot of details, but at the atomic level. Separation of energy scales. Don't worry about quarks. "Hard".**
    - **Economics: every detail matters, it seems. No obvious separation of scales. "Impossible".**

Part 1: Condensed matter

Universality in complex patterns

- **Complex patterns can arise from simple models, algorithms, or equations**
  - E.g. diffusion-limited interface dynamics
- **Can we model microstructure realistically using minimal models?**
- **Shape, scaling: yes Dimensions: no**
  - Useful for predicting morphology phase diagram

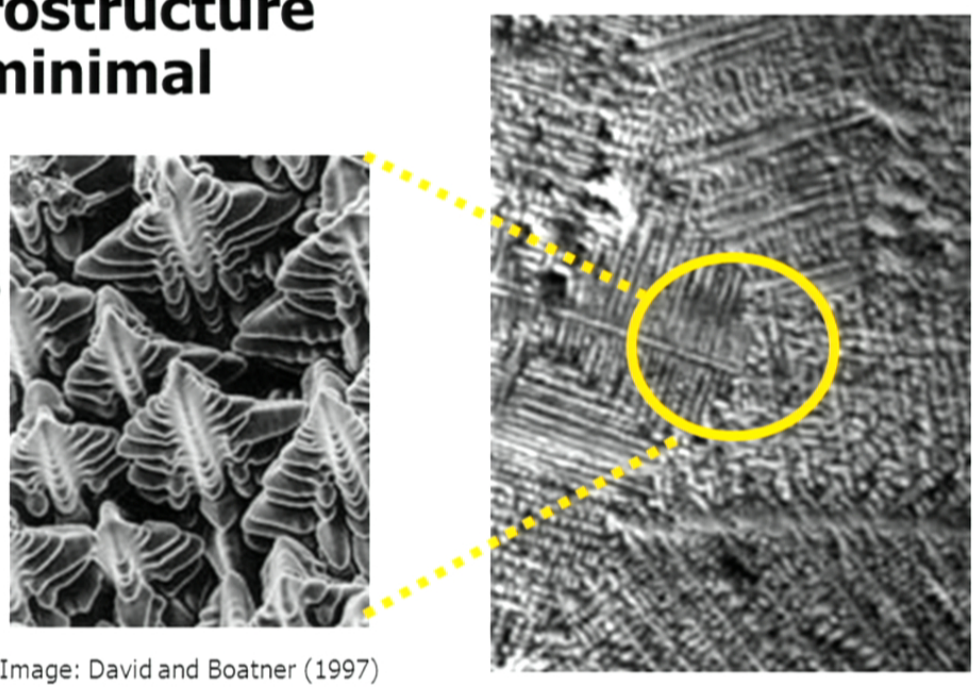
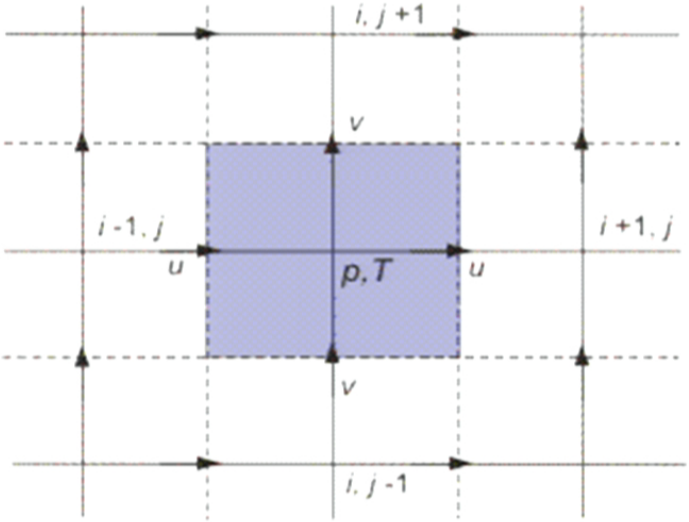


Image: David and Boatner (1997)

Numerical analysis: lattice vs. continuum

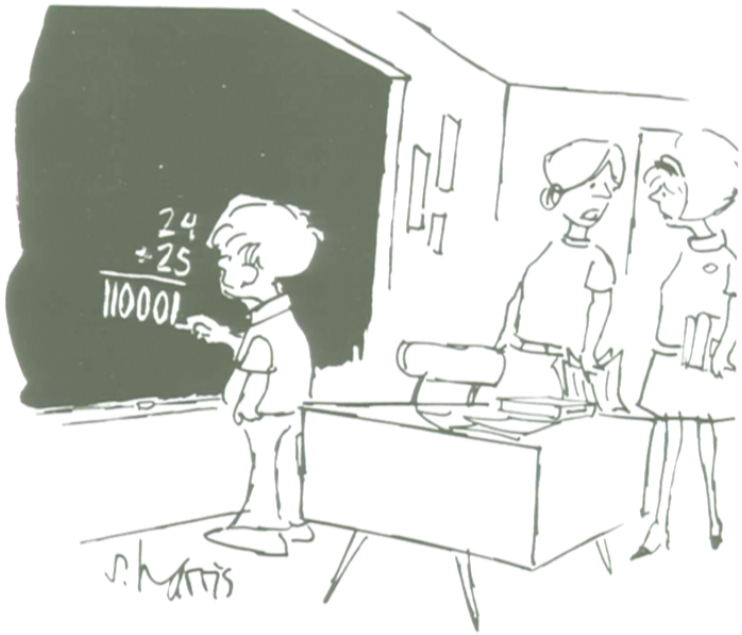


Can we study properties of materials without taking the continuum limit? Are the lattice model and the continuum model in the same universality class?

Conventional approach is to require grid convergence

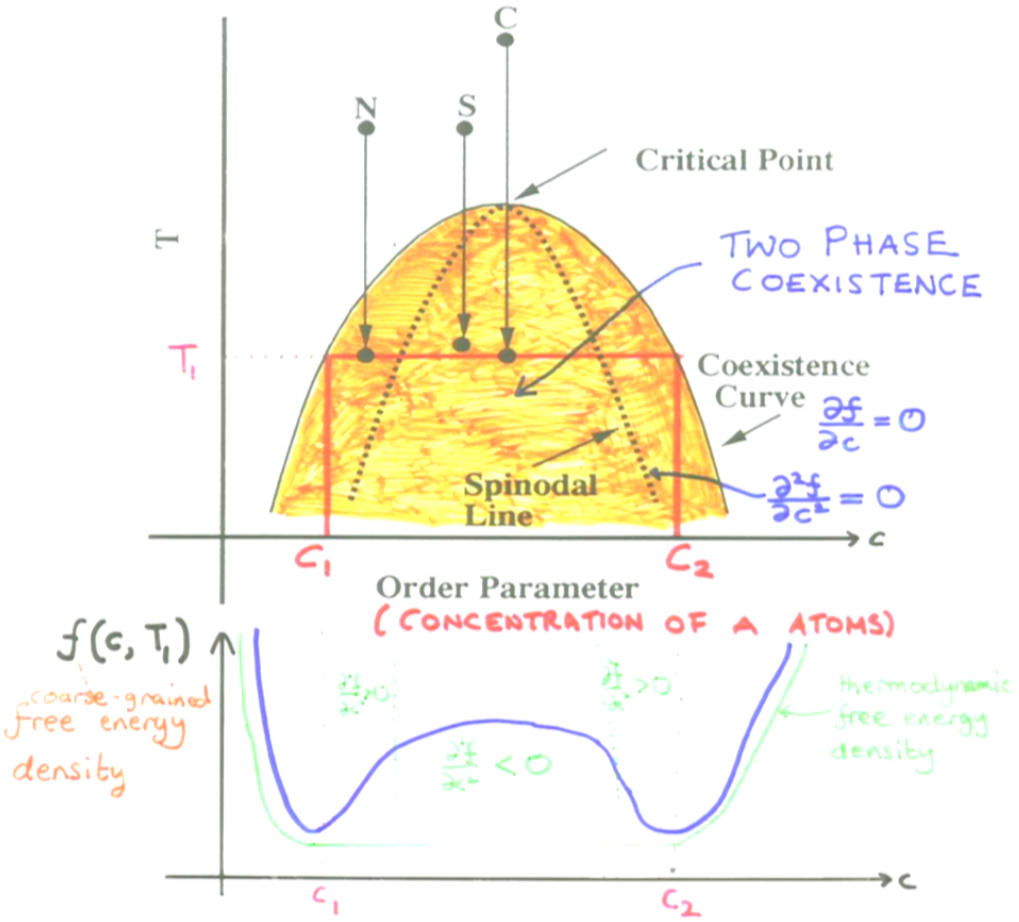
http://www.thermopedia.com/content/5413/787NHTFig3.gif

CONVENTIONAL	CDS
MODEL AS P.D.E.	MODEL AS COUPLED MAPS
DISCRETIZE P.D.E.	COMPUTE
COUPLED MAPS	
COMPUTE	



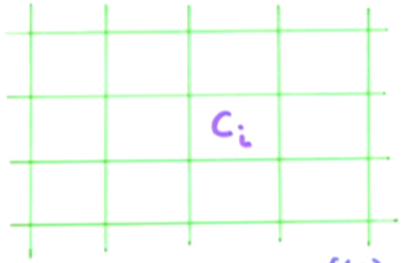
"It was bound to happen — they're beginning to think like binary computers."

PHASE DIAGRAM OF A-B ALLOY

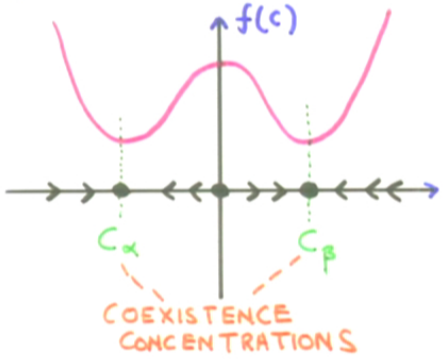


PROTOTYPE CDS: SPINODAL DECOMPOSITION

Y. OONO + S. PURI, Phys. Rev. Lett. 58, 836(87)
Phys. Rev. A 38, 434(88); ibid. 38, 1542(88).



COARSE-GRAIN SYSTEM ON SCALE OF CORRELATION LENGTH



IN EACH CELL, CONCENTRATION RELAXES IN "POTENTIAL" FROM FREE ENERGY

DYNAMICS HAS THREE FIXED POINTS

- MODEL CELL DYNAMICS BY ANY MAP WHICH HAS FIXED POINT STRUCTURE OF EVOLUTION EXPECTED ON PHYSICAL GROUNDS. NOT DISCRETISATION OF PDE!
- COUPLE CELLS: CELL CONCENTRATION ALSO EVOLVES ACCORDING TO THE AVERAGE CONCENTRATION OF NEIGHBOURING CELLS.
- IMPLEMENT CONSERVATION LAW

Minimal model for approach to equilibrium

- **Discrete coupled map lattice**
  - No continuum limit taken:
    - **dt, dx =O(1)**
  - But patterns and correlations correctly reproduced
- **Not naïve discretisation of Cahn-Hilliard**
  - Instead use onsite map that is injective
  - Algorithm is topologically stable
    - **No numerical instabilities as artifacts**
- **Use isotropic discretisation of Laplacian**
- **Impose conservation law after each time step**

CDS FOR SPINODAL DECOMPOSITION

$C_t(\underline{n})$ ≡ CONCENTRATION (i.e. OF SPECIES A) IN CELL AT $\underline{n}$ AT TIME STEP t.

EQUATION OF MOTION :

$$C_{t+1}(\underline{n}) = C_t(\underline{n}) + I_t(\underline{n}) - \langle I_t(\underline{n}) \rangle$$

EVOLUTION — IMPLEMENT CONSERVATION

EVOLUTION : $F(x) = A \tanh\left[\left(\tanh^{-1}\frac{1}{A}\right)x\right]$, $A = 1.15$

$$I_t(\underline{n}) = F(C_t(\underline{n})) - C_t(\underline{n}) + D\left(\langle C_t(\underline{n}) \rangle - C_t(\underline{n})\right)$$

SINGLE CELL DYNAMICS — COUPLING BETWEEN CELLS = DIFFUSION, $D = 0.7$

AVERAGING :

$$\langle U \rangle \equiv \frac{1}{6} \sum_{j \text{ n.n.}} U_j + \frac{1}{12} \sum_{j \text{ n.n.n.}} U_j \quad (+\cdots)$$

NEAREST NEIGHBOURS — NEXT NEARGST NEIGHBOURS

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Algorithm models same thing as the PDE: both in same universality class as physical process.

Does it work?

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EQUATION OF MOTION :

$(\underline{n}) - \langle I_t(\underline{n}) \rangle$

IMPLEMENT CONSERVATION

$\tanh\left[\left(\tanh^{-1}\frac{1}{A}\right)x\right]$, A=1.15

$+ D\left(\langle C_t(\underline{n})\rangle - C_t(\underline{n})\right)$

SINGLE CELL DYNAMICS

COUPLING BETWEEN CELLS = DIFFUSION

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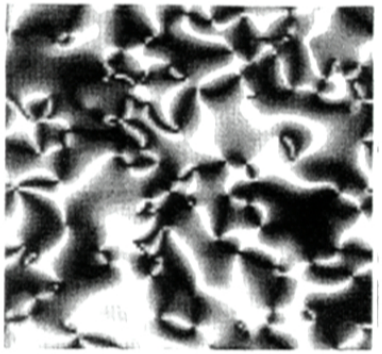
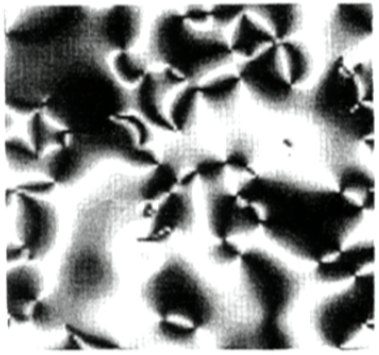
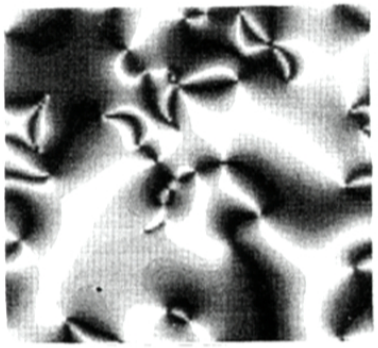


a) $t = 500$



b) $t = 1000$



c) $t = 2000$

FIG. 17. Intensity of light transmitted through a uniaxial nematic film situated between crossed polarizers (the Schlieren pattern). We show a system of size 100×100 at times $t = 500$, $t = 1000$, and $t = 2000$ after the quench. The defects appear in the pictures as the intersections of two bright and two dark lines.

Zapotowcky et al. (1995).

Experimental data: dynamics of disclination coarsening in liquid crystals film.

Cross-polarisers shows the dynamics of disclination lines and other topological defects

Coarsening reflected in growth of mean separation of defects

Nagaya *et al.* J. Phys. Soc. Jpn. **64**, 78 (1995).

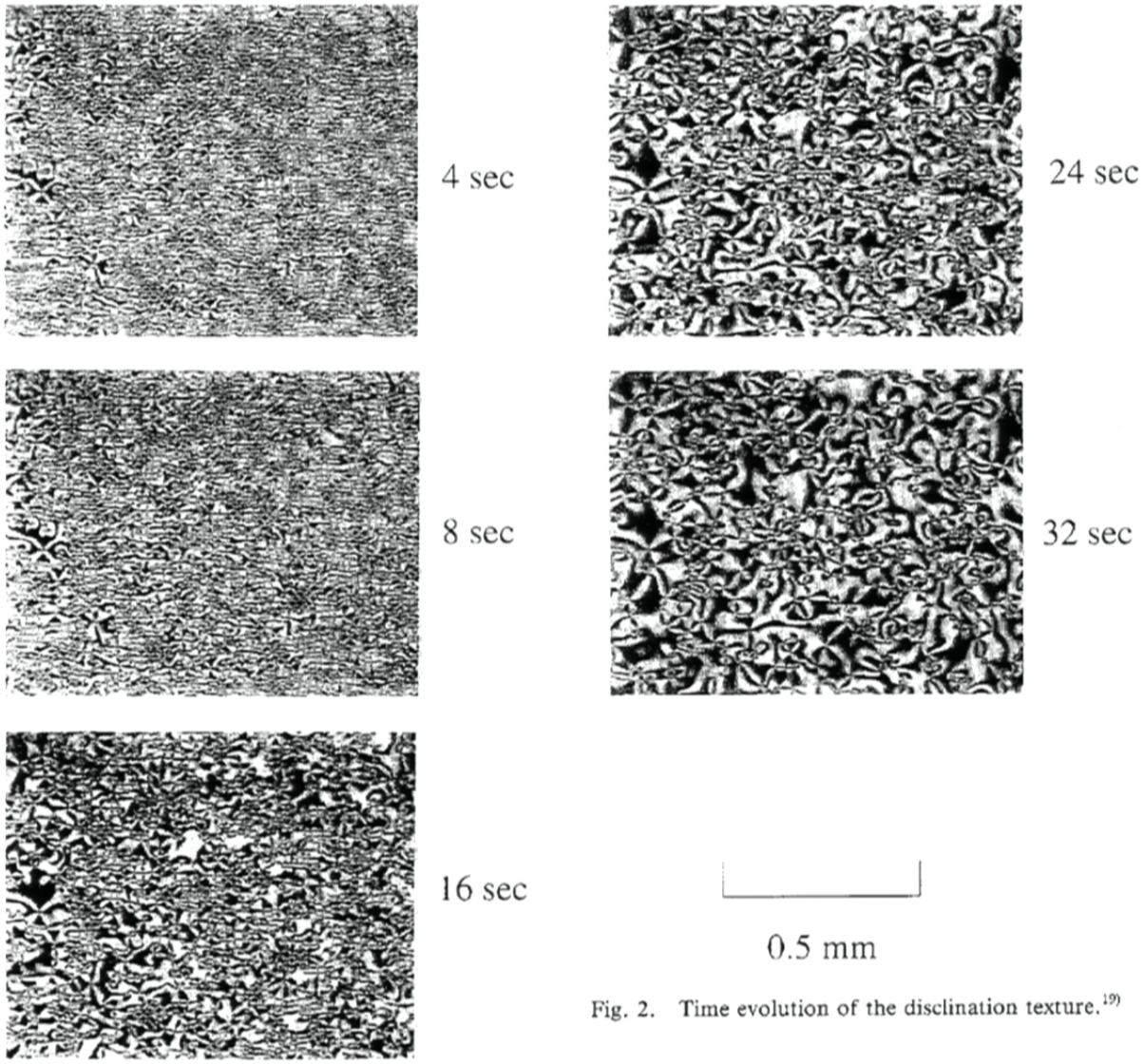


Fig. 2. Time evolution of the disclination texture.[19]

Scaled defect correlation function as a function of scaled distance.

Raw data are correlation function at different positions at different time.

Data collapse predicted by theory.

Experiment agrees with simulation with no adjustable parameters.

Mean field theory by Liu and Mazenko gives good description except near defect core.

Mondello and NG, *Phys. Rev. A* **45**, 657 (1992).

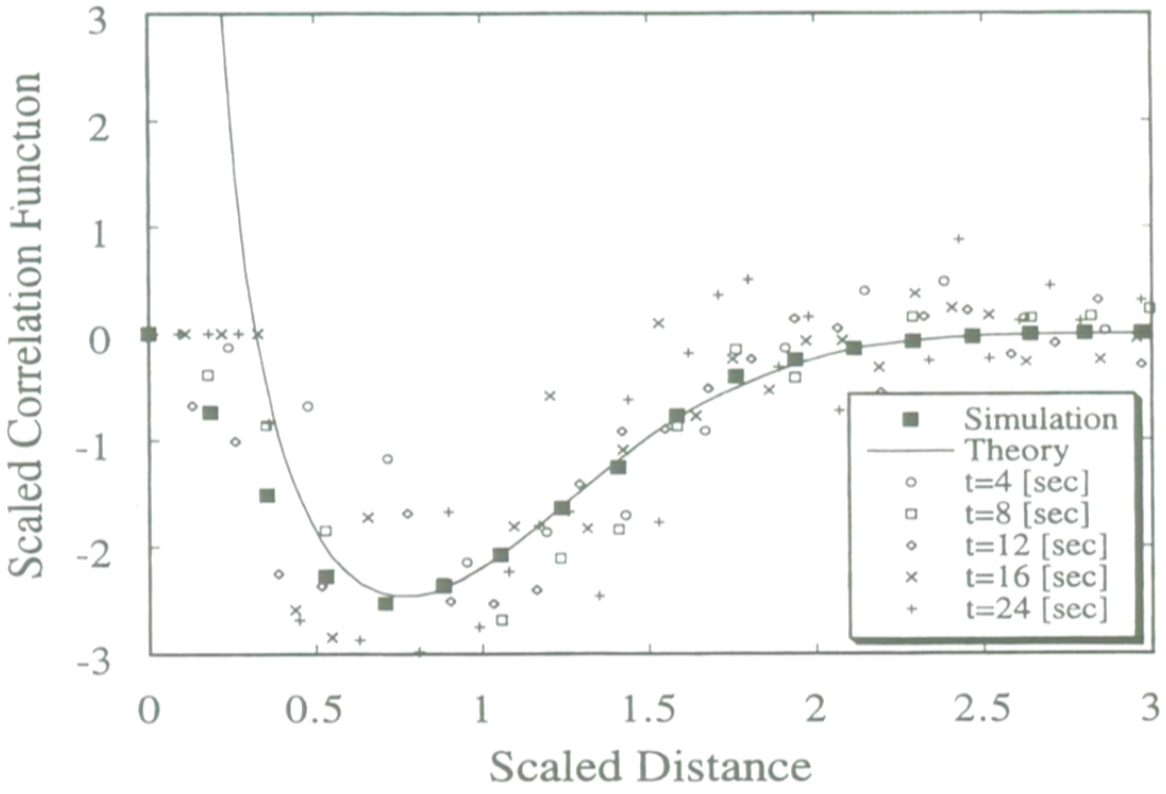


Fig. 6. The scaled correlation function of defect densities. The solid line and the large closed squares indicate the theoretical curve by Lue *et al.*[11] and the data of simulation by Mondello *et al.*,[8] respectively.

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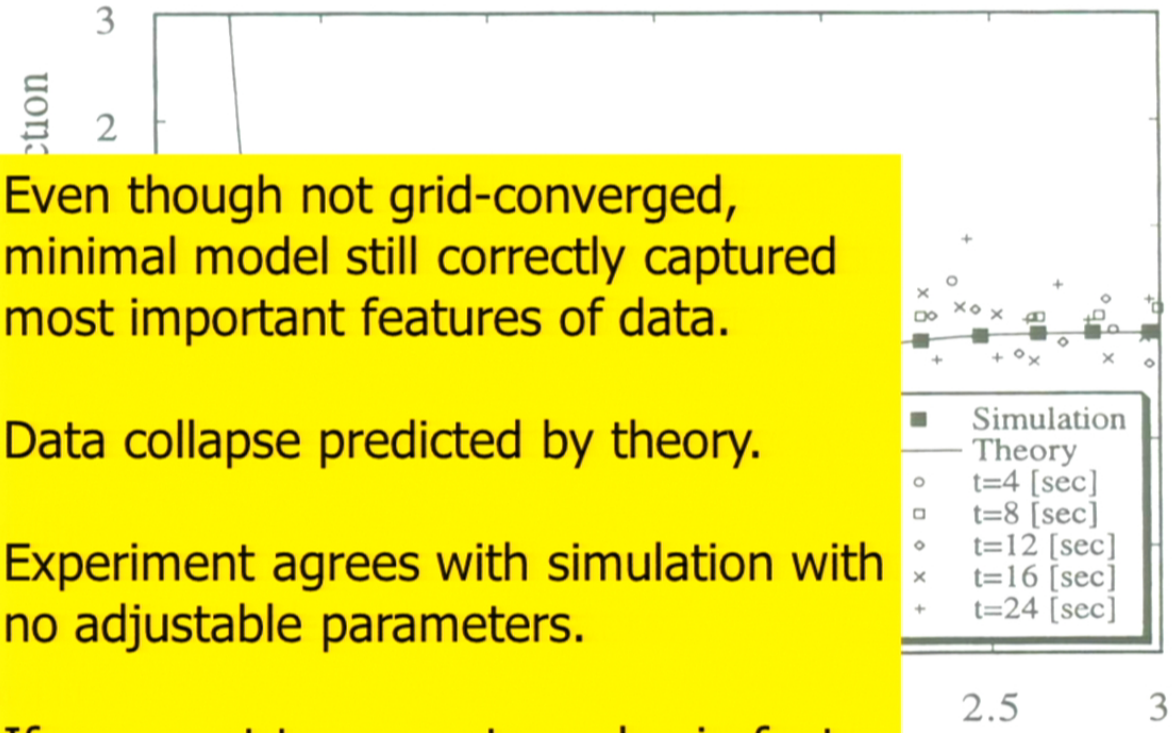

Even though not grid-converged, minimal model still correctly captured most important features of data.

Data collapse predicted by theory.

Experiment agrees with simulation with no adjustable parameters.

If you want to compute scales in feet, you're out of luck: solution – measure one length.

defect densi-
squares indi-
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of simulation by Mondello *et al.*,[8] respectively.

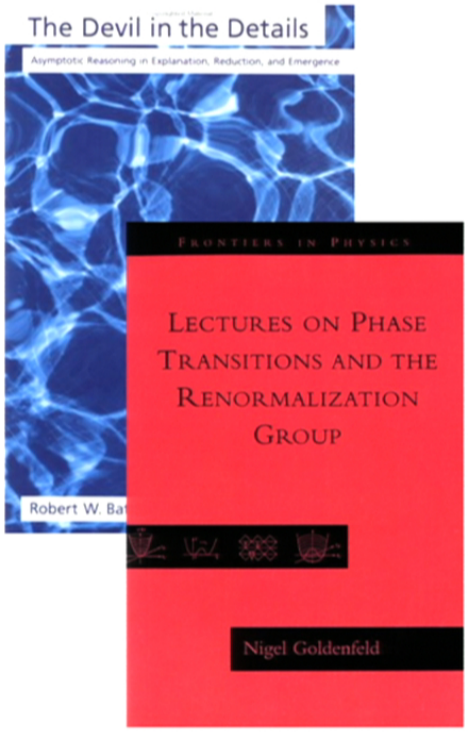
Summary

- **Predictions rely on existence of minimal models**
  - Parameter independent, universal quantities
- **Computational algorithms can model very simple processes that generate complicated space-time structures**
- **Quantitative prediction of universal quantities in excellent agreement with experiment**

Further reading

Tutorial on emergence and complexity

http://media.nakfi.org/2008/complexity/goldenfeld/goldenfeld.htm

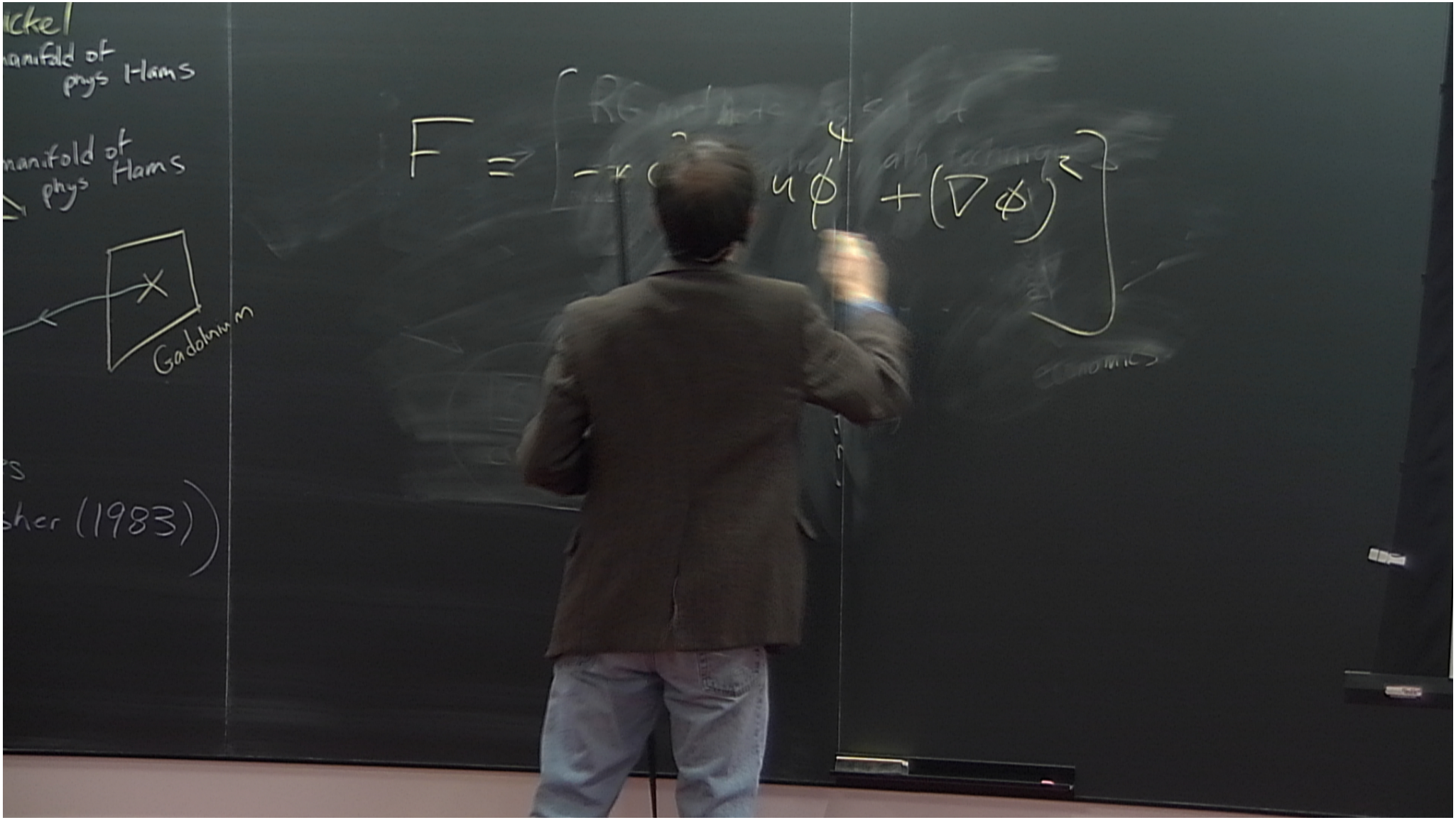


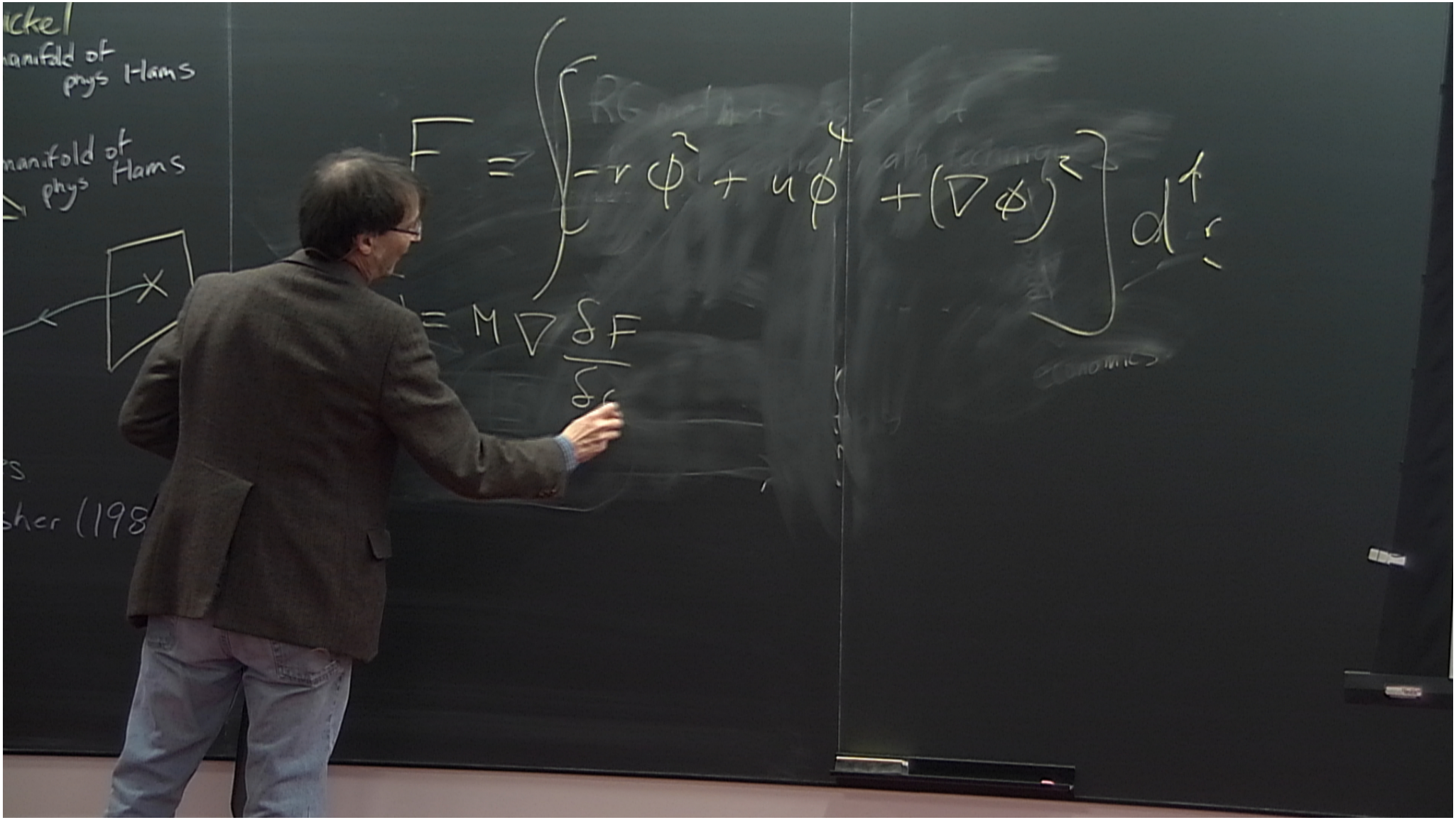
Philosophy of science: R. Batterman has written about the use of asymptotic reasoning and RG as a scientific methodology:

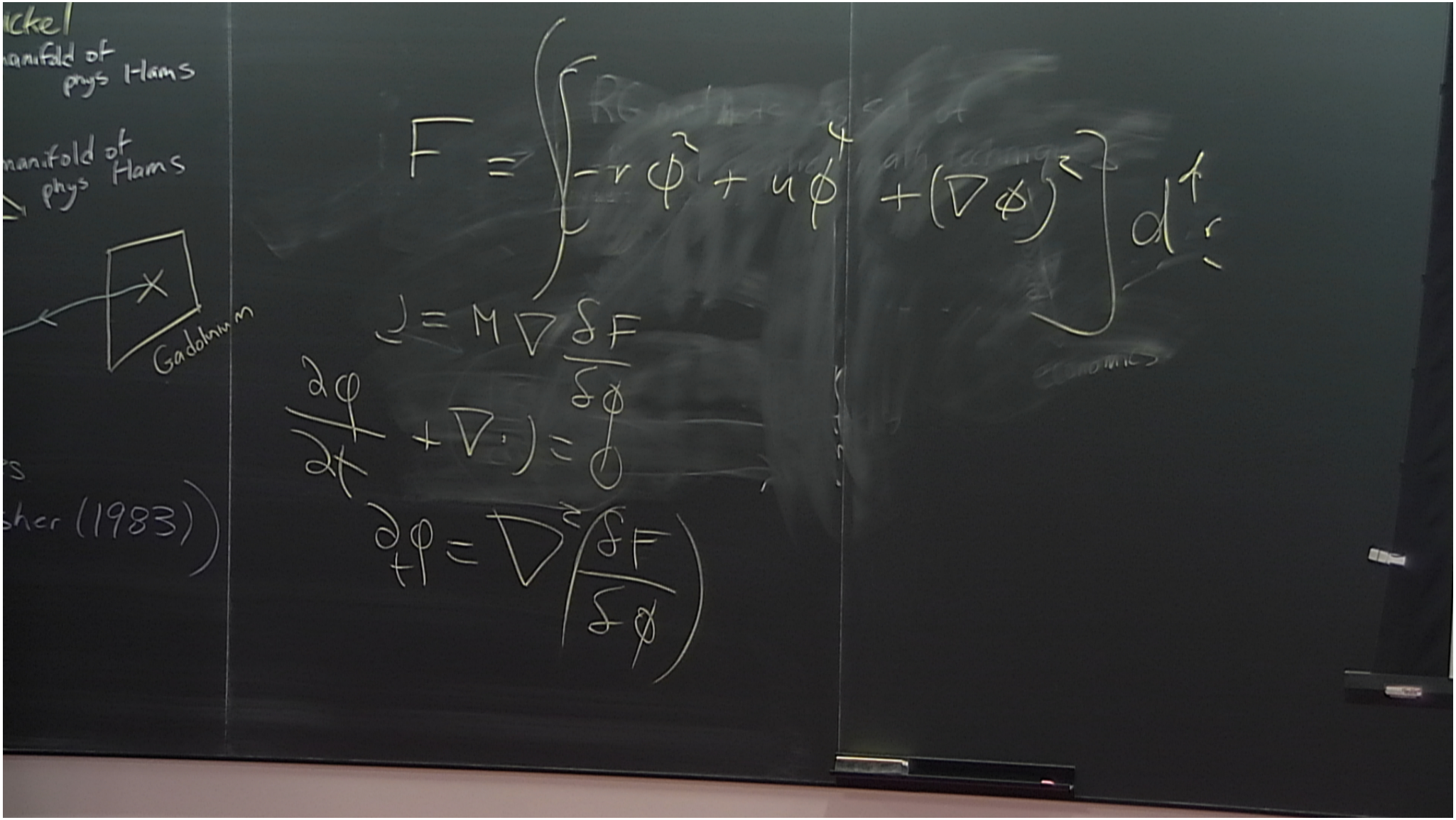
The Devil in the Details: asymptotic reasoning in explanation, reduction and emergence by Robert Batterman.

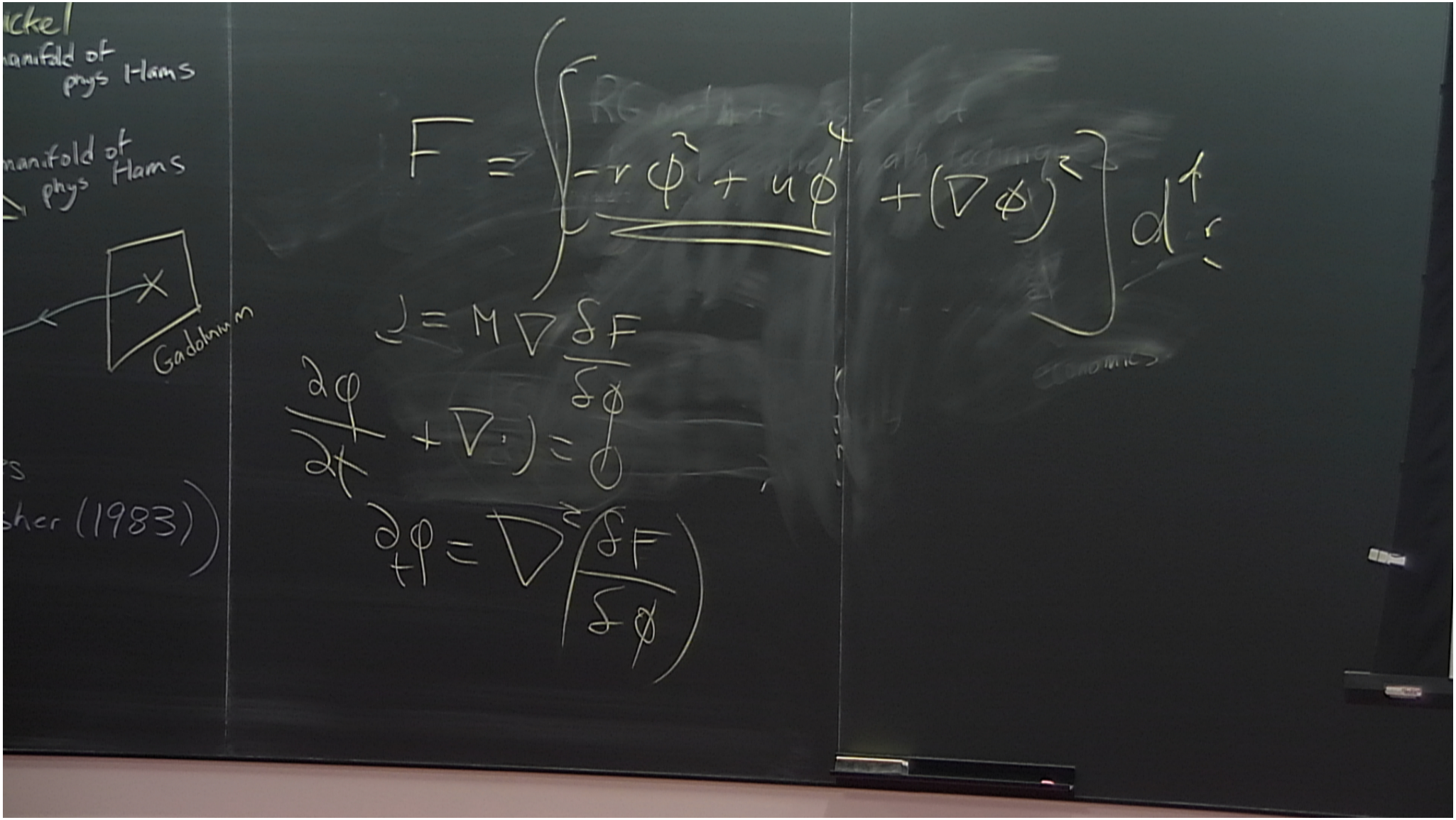
Renormalization group applied to modelling and the solution of partial differential equations:

Lectures on phase transitions and the RG by NG.


manifold of
phys Hams
manifold of
phys Hams
Gadolinium
$F = [\ -r\phi^2 + u\phi^4 + (\nabla\phi)^2\ ]$


manifold of
phys Hams
manifold of
phys Hams
X
$F = \int \left[-r\phi^2 + u\phi^4 + (\nabla\phi)^2 \right] d^d r$
$= M \nabla \frac{\delta F}{\delta}$


ckel
manifold of
phys Hams
manifold of
phys Hams
Gadolinium
sher (1983))
$F = \int \left[-r\phi^2 + u\phi^4 + (\nabla\phi)^2 \right] d^d r$
$J = M \nabla \frac{\delta F}{\delta \phi}$
$\frac{\partial \phi}{\partial t} + \nabla \cdot J = 0$
$\frac{\partial \phi}{\partial t} = \nabla^2 \left(\frac{\delta F}{\delta \phi} \right)$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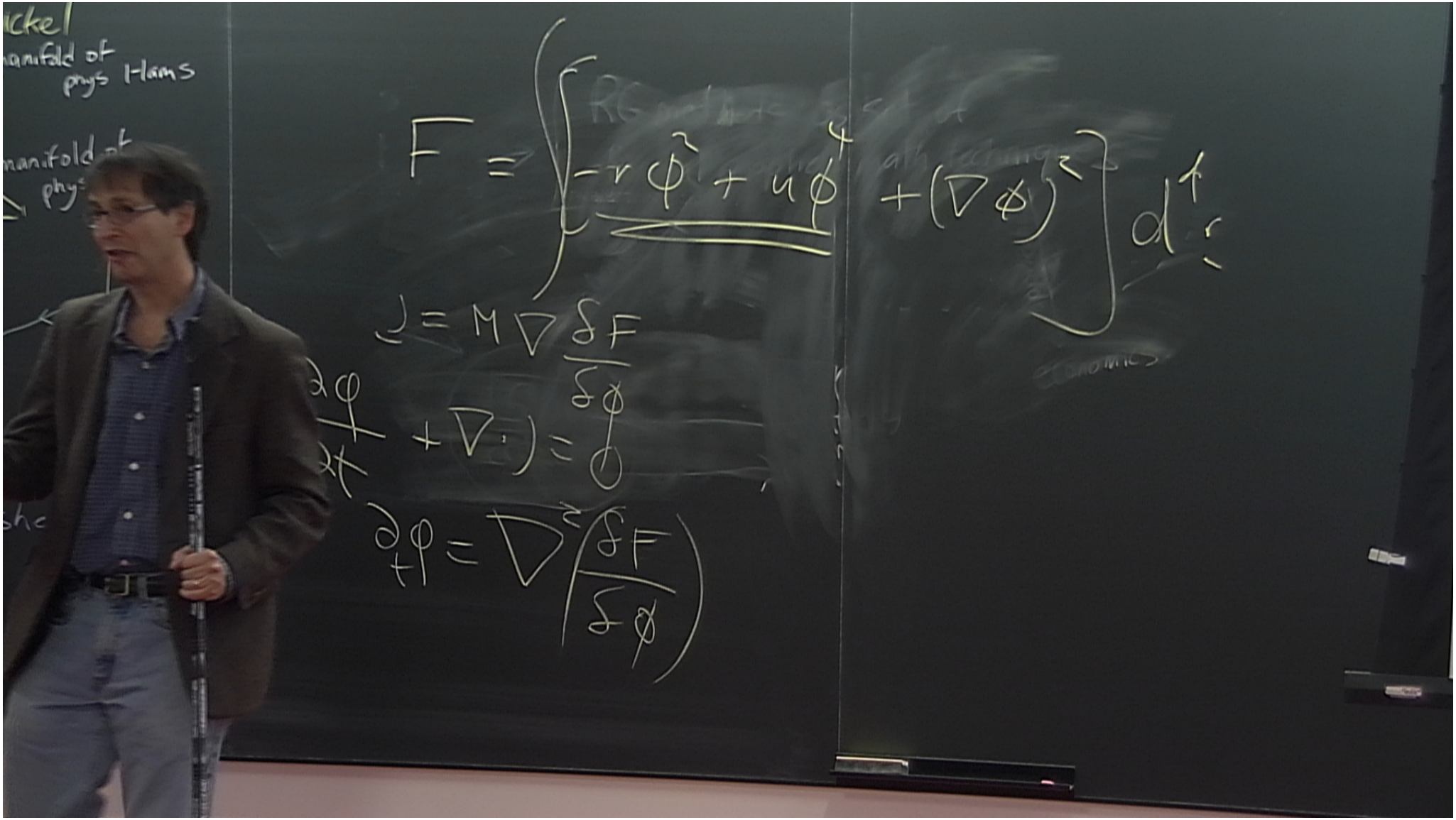
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