Patterns, universality and computational algorithms

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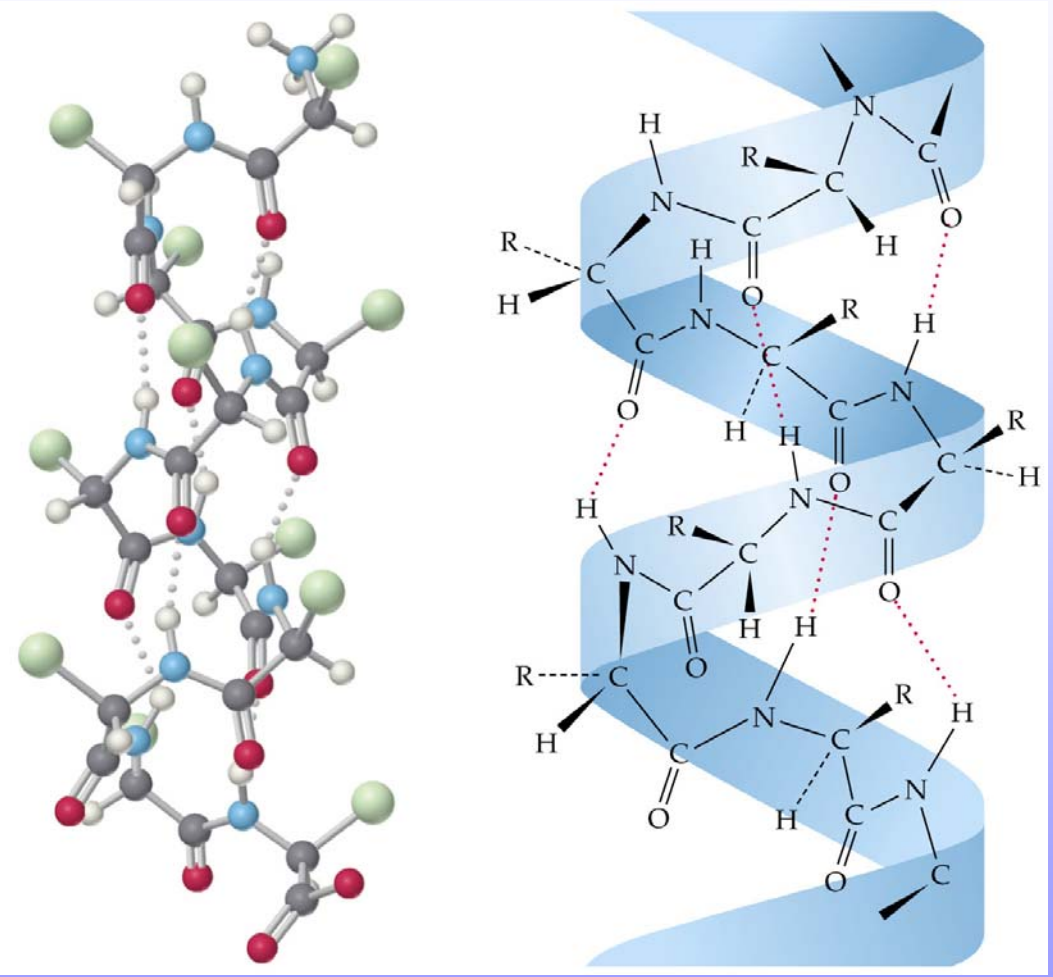
Navot Israeli (Cellular automata)
Badrinaryan Athri and Jon Dantzig (Multiscale modeling)

Work supported by the US National Science Foundation and NASA

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
- **Can we make simple theories of complex phenomena?**
  - Computational irreducibility
- **Multiscale modeling of patterns**
  - Renormalization group approach to large-scale simulation of materials processes

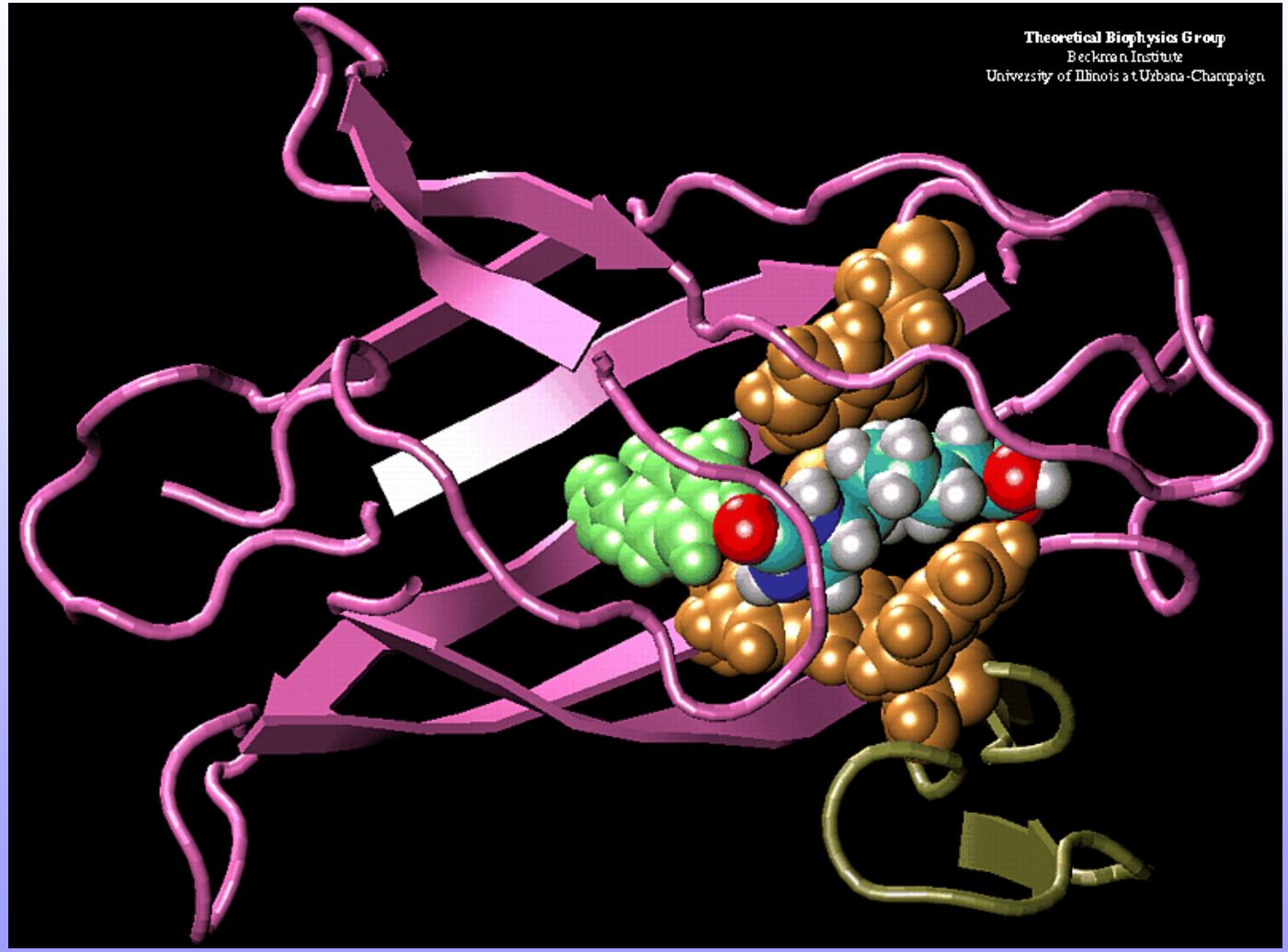
Perceptions of reality: polymers



From *Chemistry* by McMurry & Fay

Chemist

Perceptions of reality: polymers



Schulten group UIUC

Computational biologist

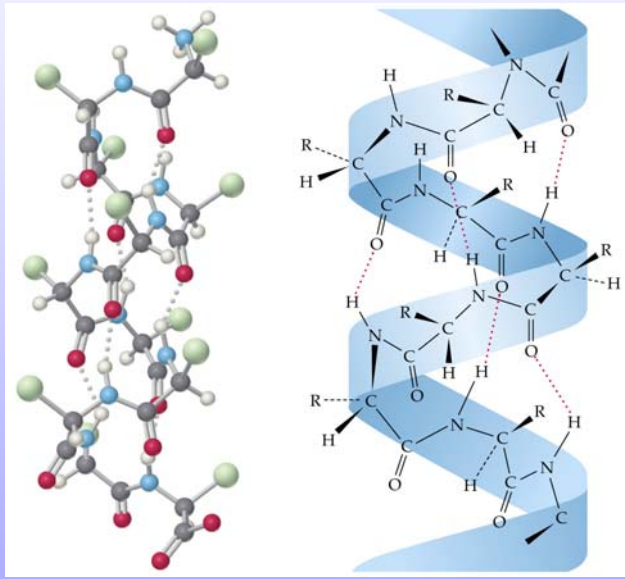
Perceptions of reality: polymers

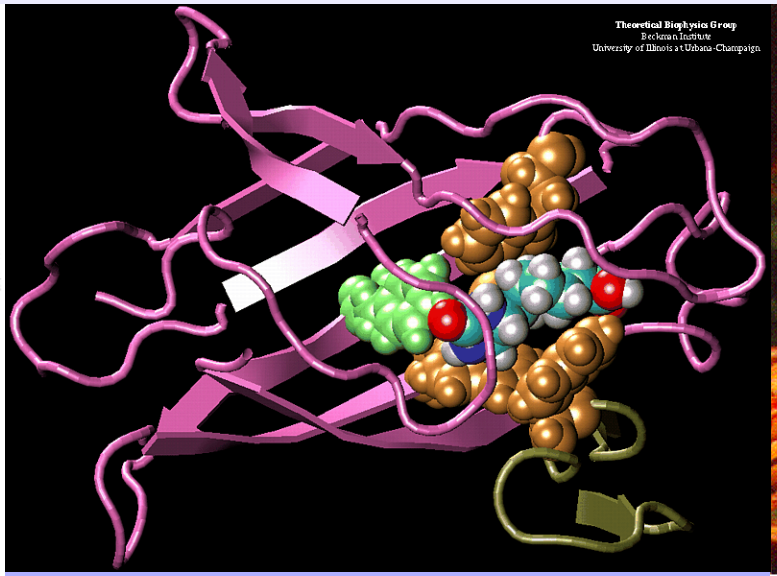
The Gutsy Gourmet

Theoretical physicist

Perceptions of reality: polymers

What questions can each of these representations answer?





Chemical bonding, reactions, ...

Elasticity, large scale motions, folding

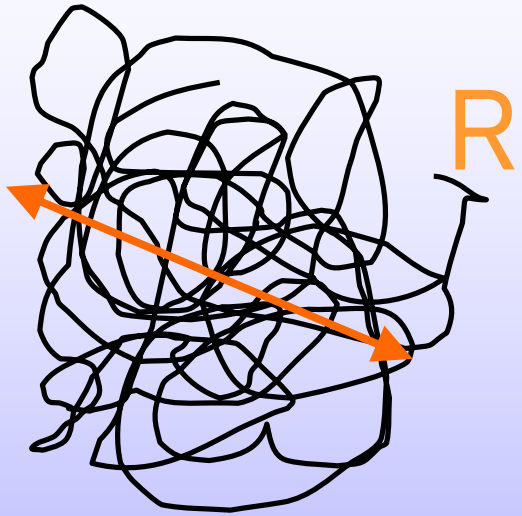
Thermodynamics, light scattering, rheology

Perceptions of reality: polymers

- **How big is a polymer?**
  - 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:**

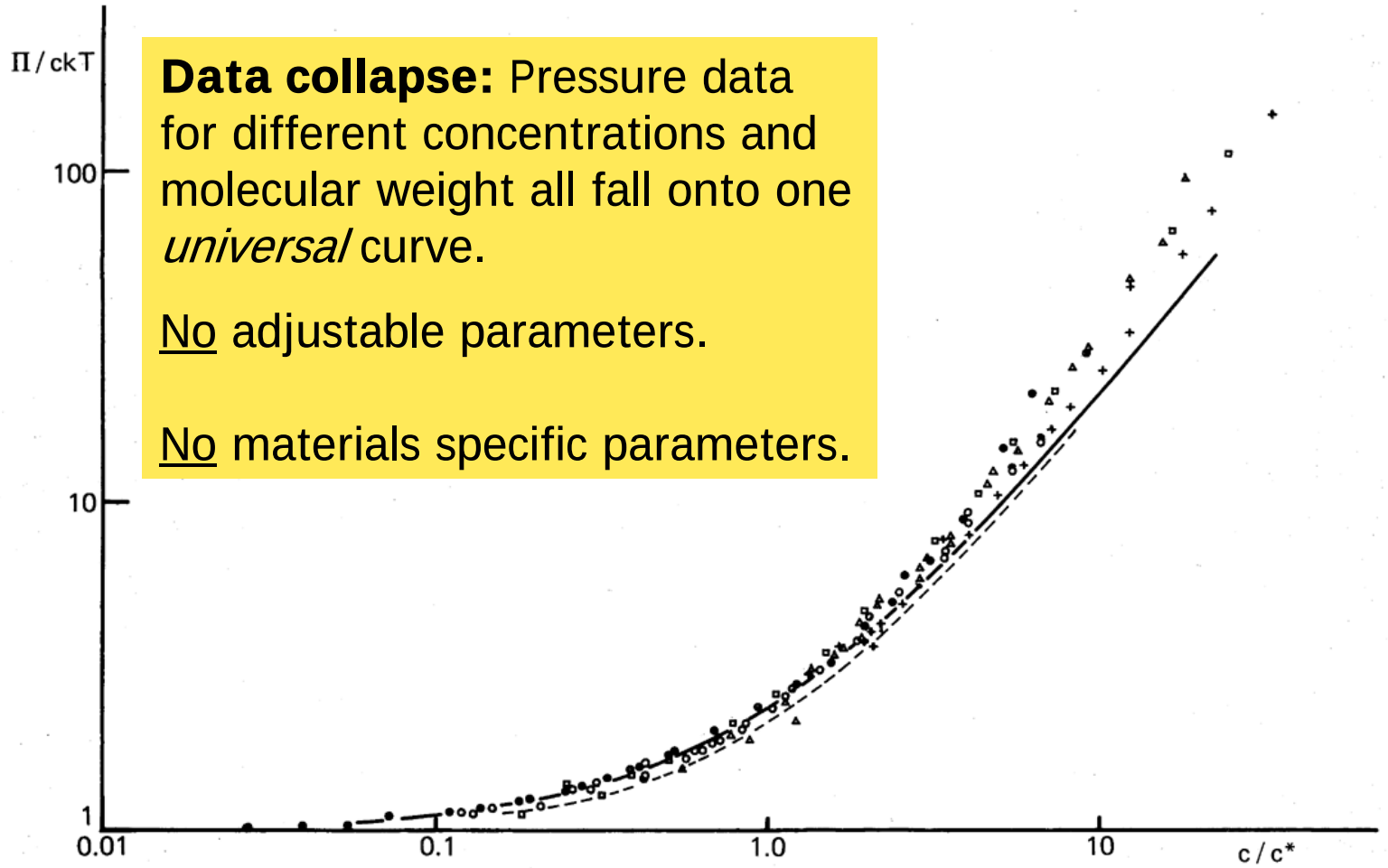
$$R = A(\ell)\, L^{0.588} \quad \text{as } L \rightarrow \infty$$

    - **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.

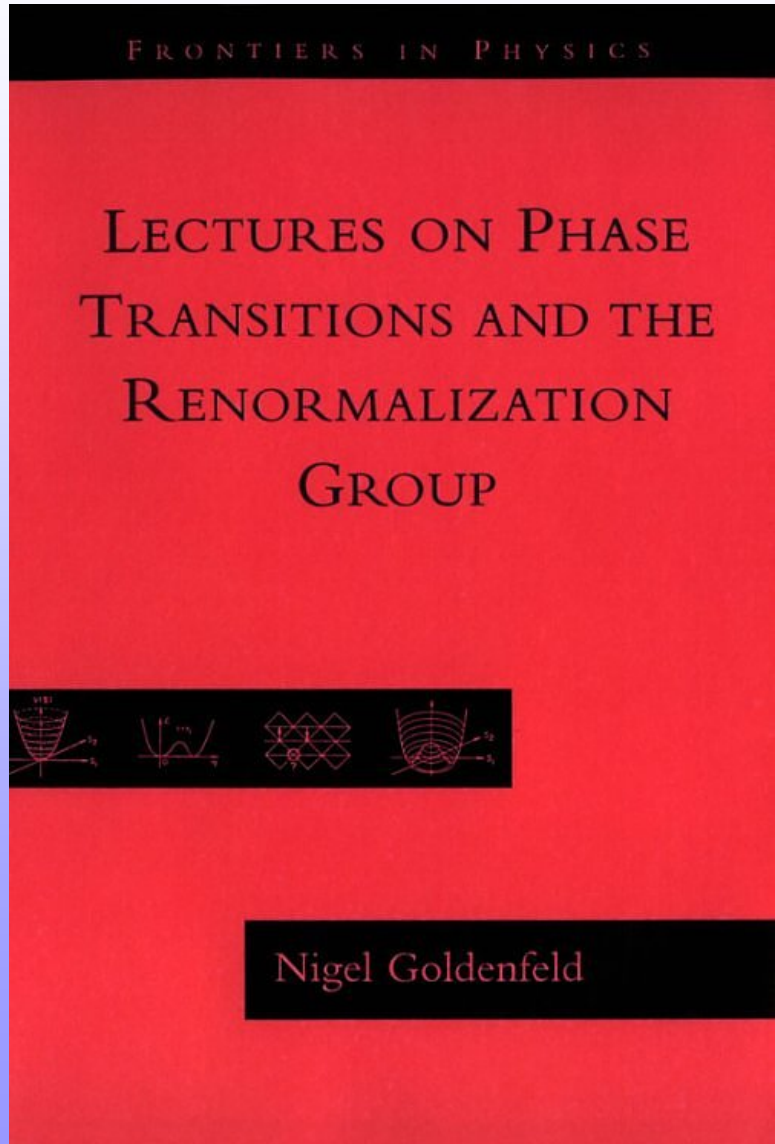
Osmotic pressure of polystyrene in solution as a function of concentration. Data from Wiltzius *et al* (1983) for $10^4 < M_w < 10^7$ in two different solvents. Theory by Ohta and Oono (1982).

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)?

Calculating universal quantities

- **Renormalization group theory**
  - First used in quantum field theory and second order phase transitions
  - Explained why thermodynamics near critical points showed universality
    - **Liquid-gas critical point = ferromagnet-paramagnet critical point: exponents**
  - Later applied to differential equations, dynamical phenomena
- **Explains how to identify universal phenomena, see what is important in model building**

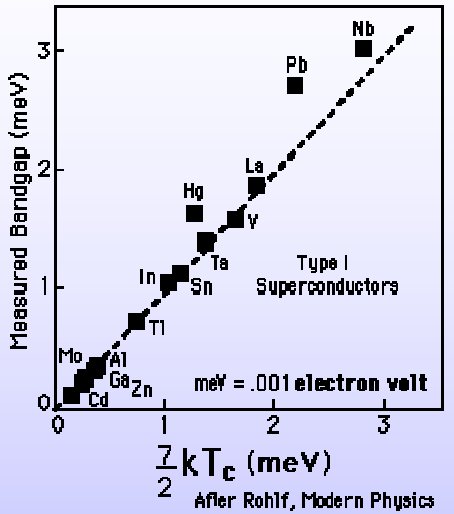


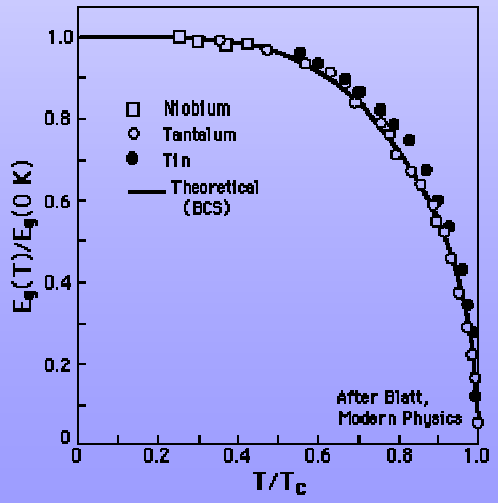
Universality in physics

- **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 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".**

Universality in physics

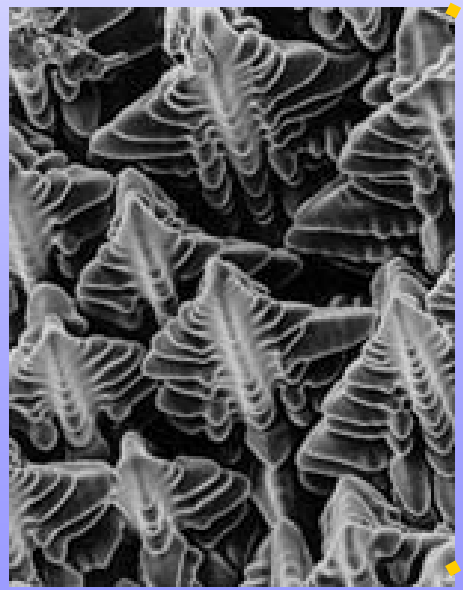
- **Example: BCS theory of superconductivity**
  - Most successful many-body theory
  - Spectacular agreement with experiment:
    - **Universal ratios: $\Delta / k_B T_c = 3.53$**
    - **Universal functions: $\Delta(T)$**
- **Poor ability to predict T_c**
- **BCS model leaves out much physics**
  - Don't even need to know what is the mechanism allowing electrons to form Cooper pairs!

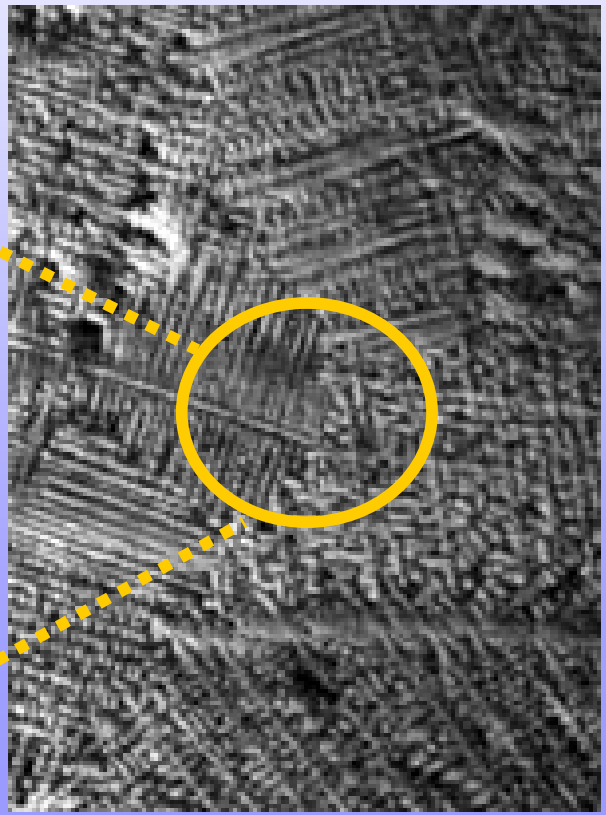




Universality in complex patterns

- **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





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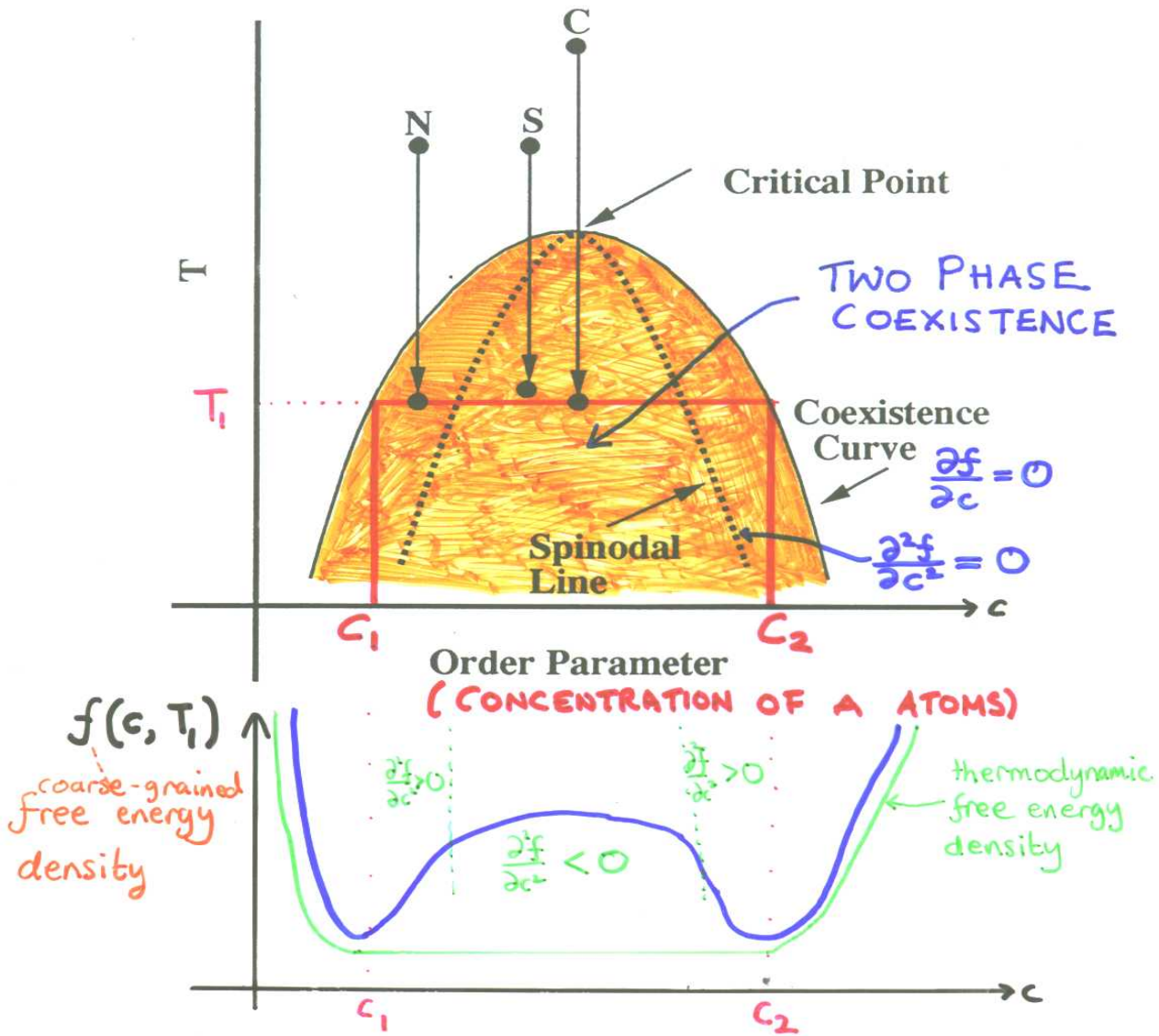
Cell dynamical systems (CDS)

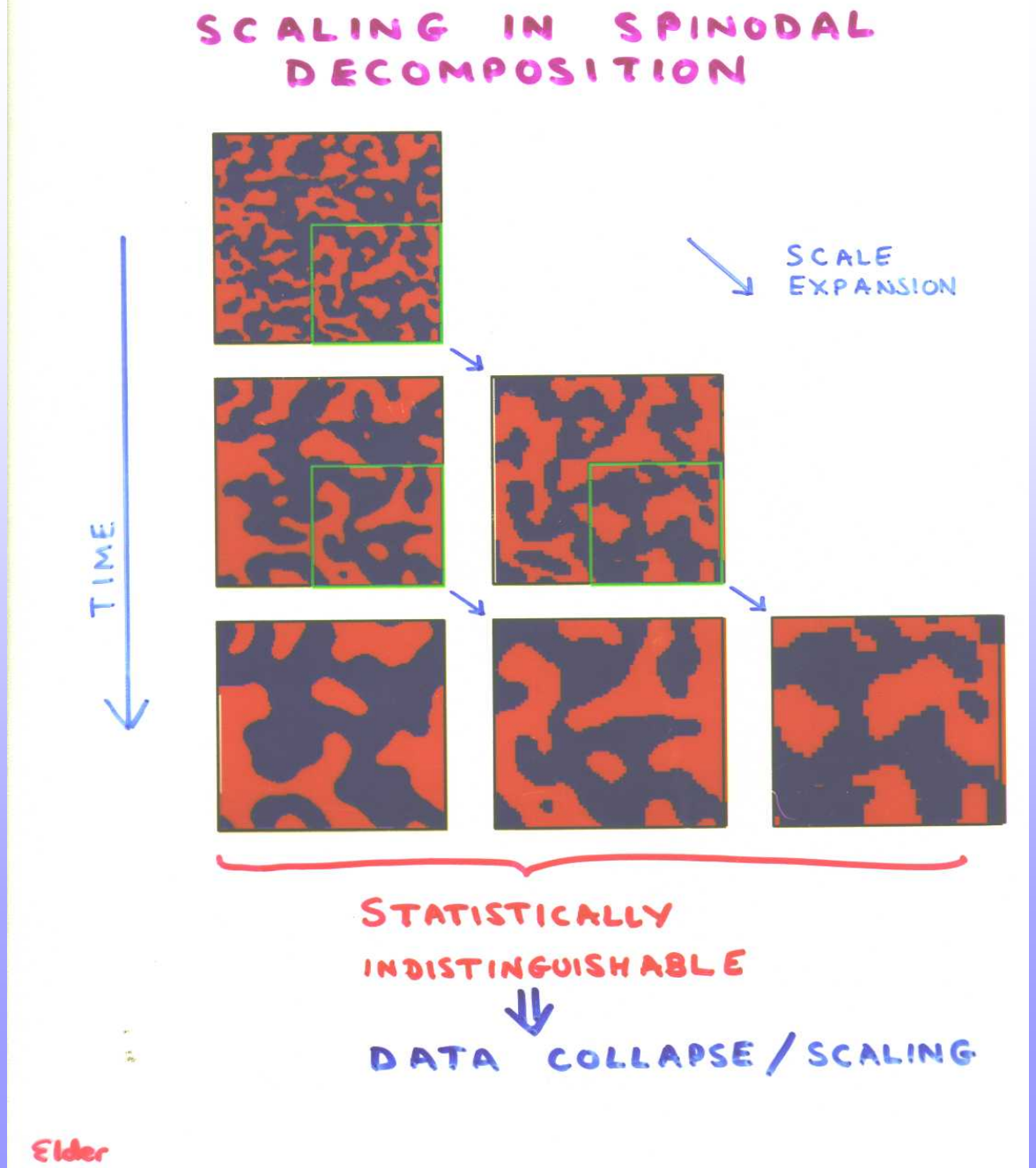
Modelling the universal aspects of phase transition dynamics

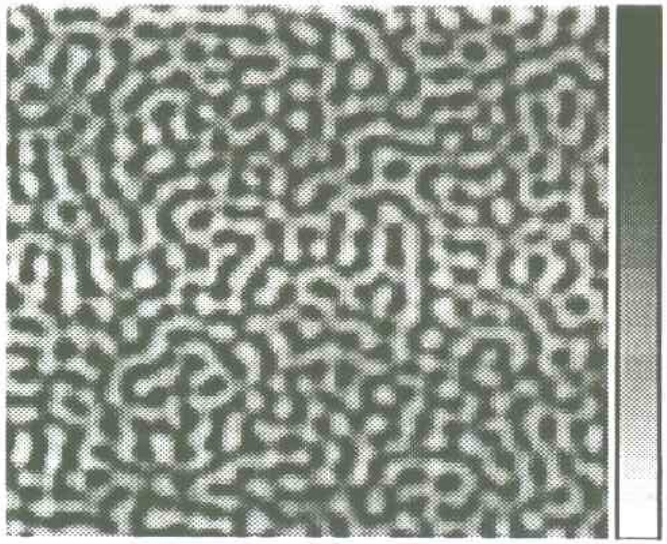
PHASE DIAGRAM OF A-B ALLOY



Scaling

- **Dynamics of spinodal decomposition**
  - Scale invariance
  - Pattern
- **Extensions to vector and tensor order parameters**
  - Topological defects
  - Correlation functions





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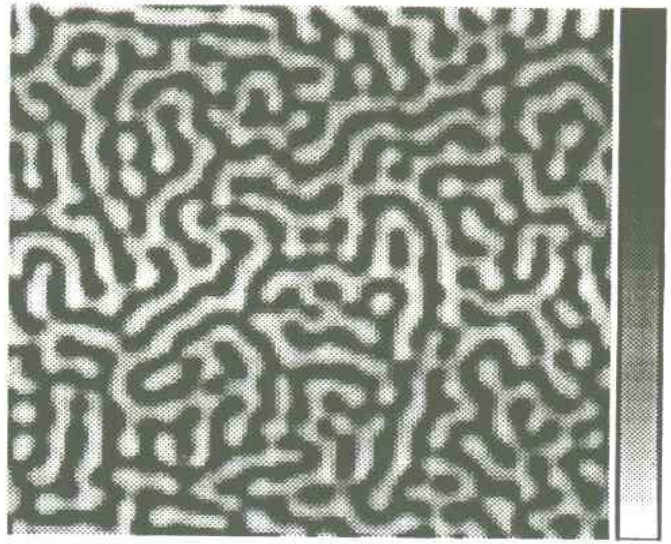

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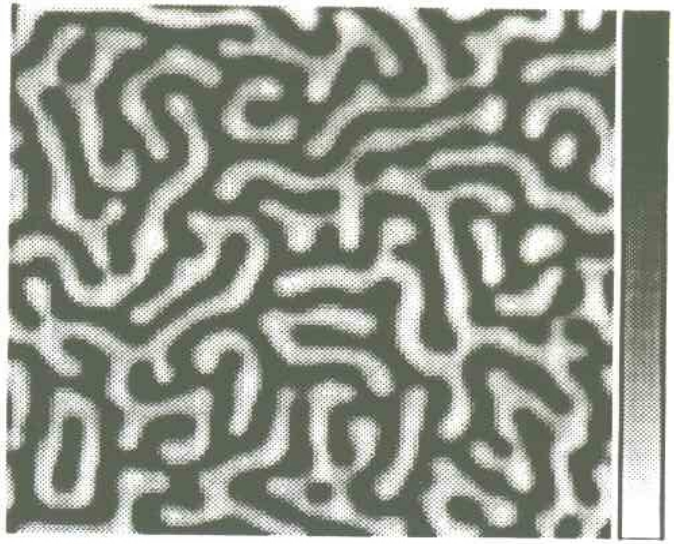

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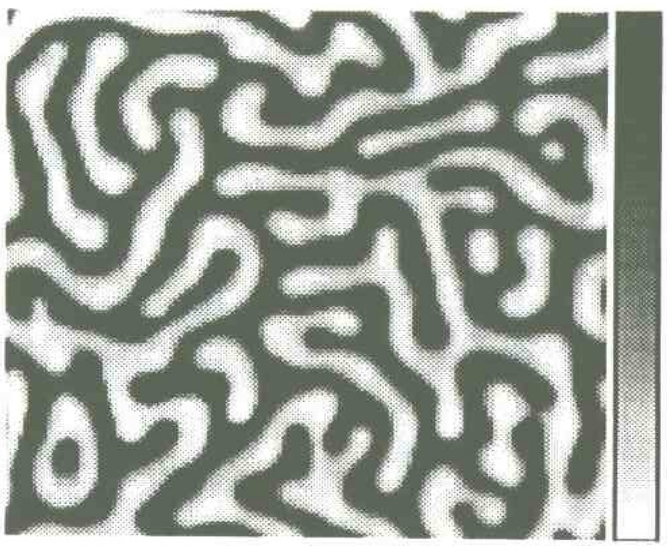

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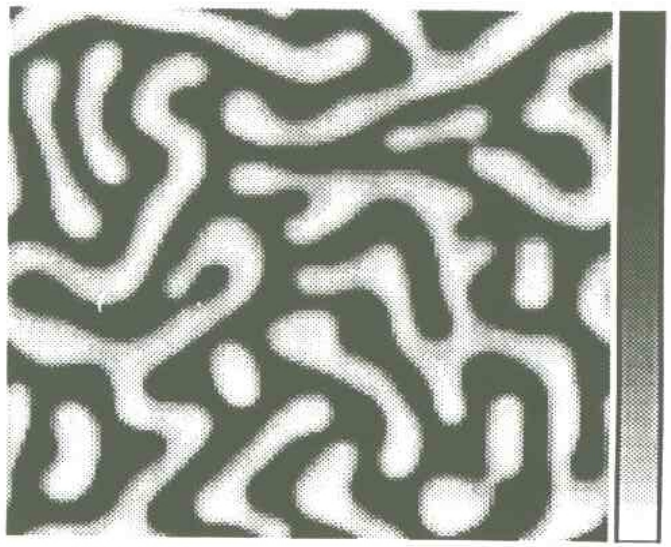

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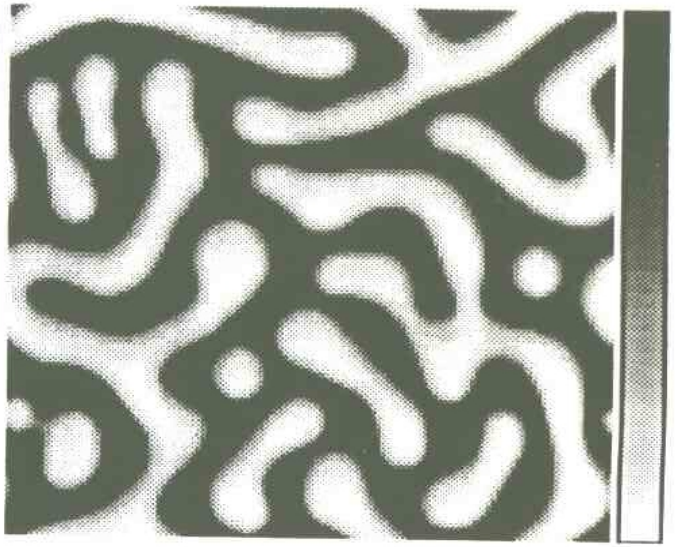

4000

CELL DYNAMIC SIMULATION OF SPINODAL DECOMPOSITION (OONO + PURI)

Dynamical scaling during the quench of a binary alloy.

Measure the concentration correlation function by neutron scattering

Observe data collapse!

Phenomenon is universal, independent of chemical composition of alloy.

In practice, lattice strain effects influence the scaling function, so direct comparison with theory not possible in this case.

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Kinetics of Phase Separation in $Mn_{0.67}Cu_{0.33}$

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and
Y. Morii
Physics Division, Japan Atomic Energy Research Institute, Tokai, Ibaraki 391-11, Japan
(Received 9 March 1987)

We have examined the kinetics of phase separation in $Mn_{0.67}Cu_{0.33}$ using time-resolved neutron-scattering techniques. In an early-time regime, the kinetics follows the Cahn-Hilliard-Cook linear theory of spinodal decomposition. There is an intermediate stage. Then, at a late time, dynamic scaling is obeyed. The time dependence of the wave vector at maximum scattering intensity (which is inversely proportional to the average linear domain size) can be well described over the entire late-time regime and much of the intermediate-time regime by arguments recently put forward for earlier-time corrections to the limitingly late-time stages of phase separation.

PACS numbers: 64.75 +g, 61.50.Ks, 81.40.Cd

EARLY TIME

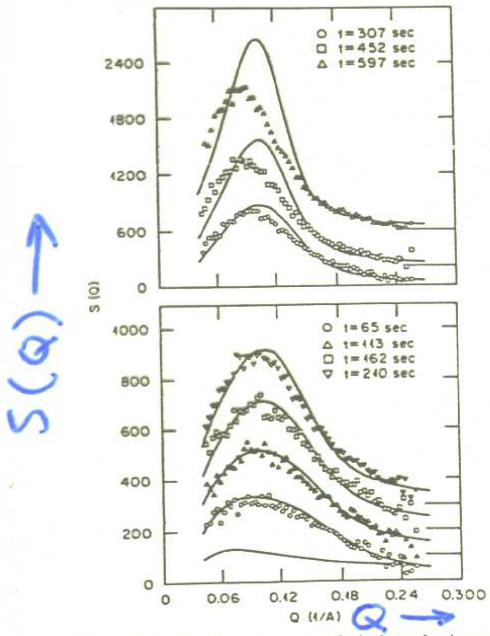


FIG. 2. The $S(Q,t)$ data sets at relatively early times. The solid lines are the results of the fit of the CHC theory [with the $\frac{1}{2}\tilde{S}(Q)$ base function shown at the bottom of the figure] to the data. Systematic discrepancies are clear for times longer than 300 sec. Data sets have zero $S(Q)$ values shown by the solid lines to the right of the panels for clarity of presentation.

LATE TIME

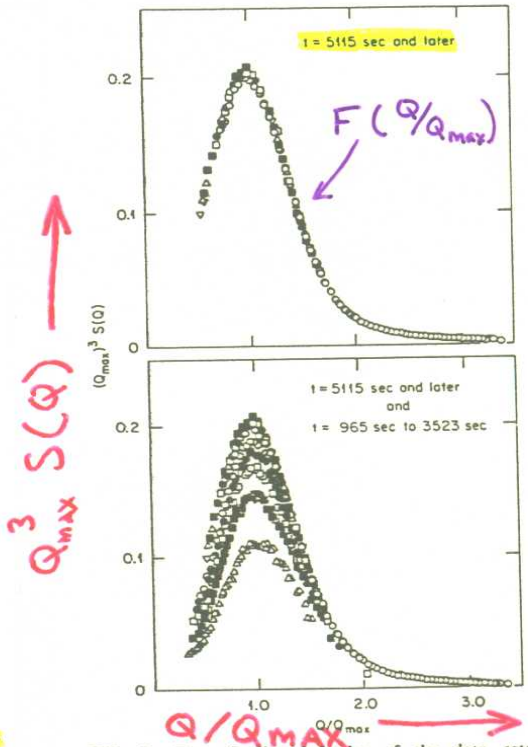


FIG. 3. Top: Scaling behavior of the data sets of $F(Q/Q_{max}) = Q_{max}^3 S(Q)$ for times exceeding 5000 sec. Bottom: Same data sets as the top panel, as well as five data sets at 965, 1602, 2239, 2886, and 3523 sec. These earlier-time data sets depart from the scaling relation to a systematically greater extent with decreasing time.

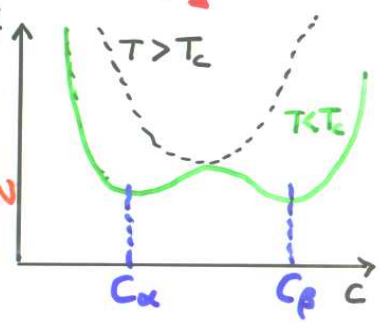
SIMPLE LINEAR THEORY

CAHN-HILLIARD "COARSE-GRAINED" FREE ENERGY

$$F\{c_\Lambda(\underline{r})\} = \int d^d\underline{r}\left[\tfrac{1}{2}(\nabla c)^2 + f(c_\Lambda(\underline{r}))\right]$$

c_Λ: COARSE-GRAINED ON SCALE Λ i.e. NO $\underline{k}$-MODES WITH $k > \Lambda$

$\tfrac{1}{2}(\nabla c)^2$: FREE ENERGY COST TO MAINTAIN CONCENTRATION GRADIENT



MASS CONSERVATION

$$\partial_t c + \underline{\nabla}\cdot\underline{J} = 0$$

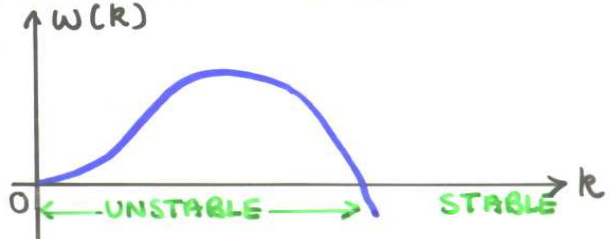
PHENOMENOLOGY (LINEAR RESPONSE)

$$\underline{J} = -M\,\underline{\nabla}\frac{\delta F}{\delta c}$$

M: MOBILITY

GROWTH OF SMALL PERTURBATIONS

$$c(\underline{r}) - c_0 \sim e^{ikx + \omega(k)t}$$



DYNAMIC SCALING

$$S(\underline{k},t) = \int d^d r \; e^{i\underline{k}\cdot\underline{r}} \langle \psi(r,t)\,\psi(0,t)\rangle$$

SCATTERING FUNCTION

ENSEMBLE OR VOLUME AVERAGE

IN GENERAL ψ IS ORDER PARAMETER

EXPERIMENT & NUMERICS GIVE

$$S(\underline{k},t) \underset{t\to\infty}{\sim} L(t)^d \, F(kL(t))$$

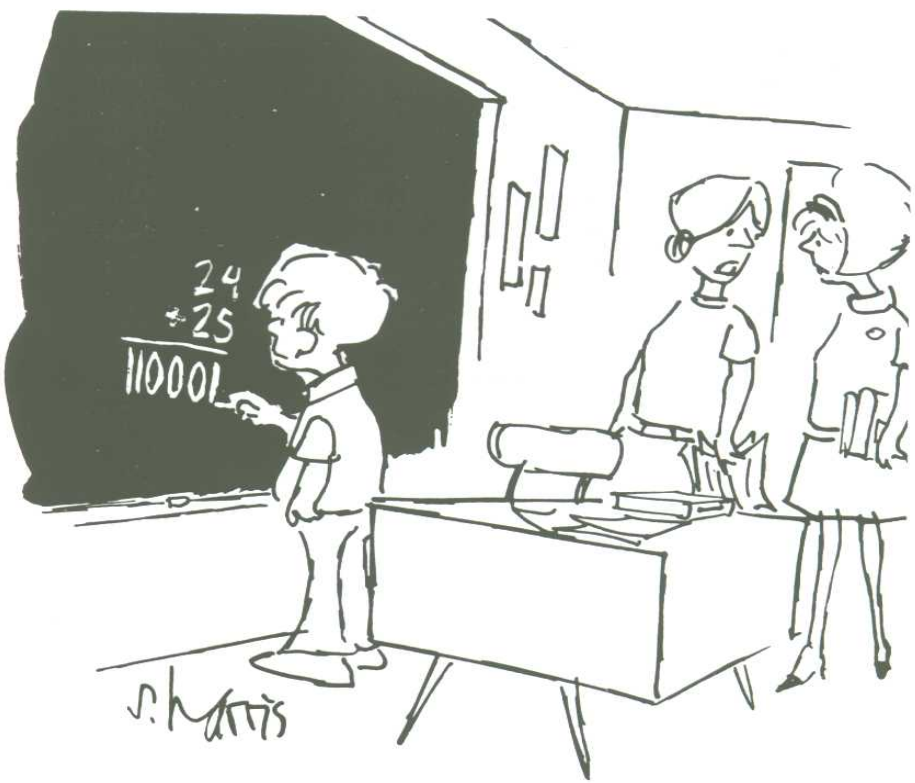
$$L(t) \sim t^{\phi}$$

IN SPINODAL DECOMPOSITION $\phi = 1/3$

$L(t)$ IS CHARACTERISTIC SCALE OF PATTERN i.e. $\exists$ ONLY ONE SUCH SCALE

COMPUTATIONAL TECHNIQUE

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."

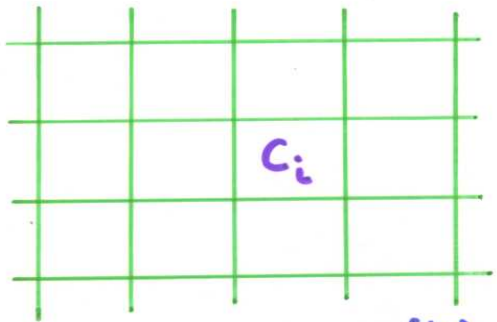
- CDS PHILOSOPHY :
  - IDENTIFY KEY PHYSICS
  - MODEL THIS FAITHFULLY
  - REMAINING INGREDIENTS ADDED AFTER

EXAMPLES:

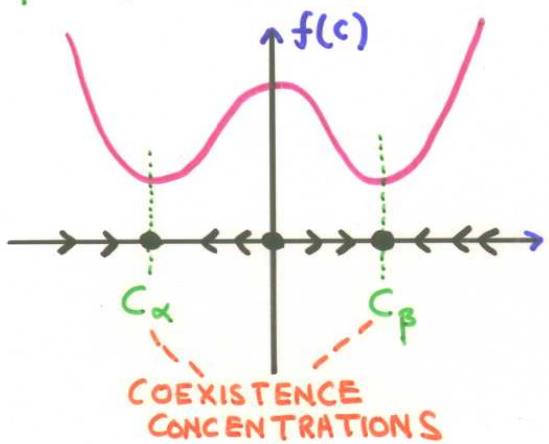
ALLOY PHASE SEPARATION	HYDRODYNAMICS AND FLOW
ON-SITE "DOUBLE WELL" POTENTIAL + DIFFUSION + CONSERVATION	ADVECTION + VISCOSITY + DRIVING FORCE

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

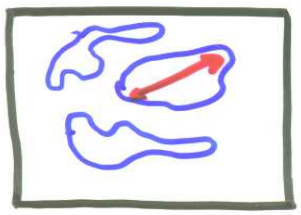


IN EACH CELL, CONCENTRATION RELAXES IN "POTENTIAL" FROM FREE ENERGY

DYNAMICS HAS THREE FIXED POINTS

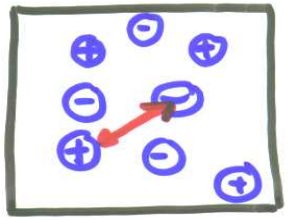
- MODEL CELL DYNAMICS BY ANY MAP WHICH HAS FIXED POINT STRUCTURE OF EVOLUTION EXPECTED ON PHYSICAL GROUNDS. NOT DISCRETISATION OF PDE!
- COUPLE CELLS: CELL CONCENTRATION ALSO EVOLVES ACCORDING TO THE AVERAGE CONCENTRATION OF NEIGHBOURING CELLS.
- IMPLEMENT CONSERVATION LAW

LEVEL OF DESCRIPTION



SCALAR

DEFECTS ARE DOMAIN WALLS

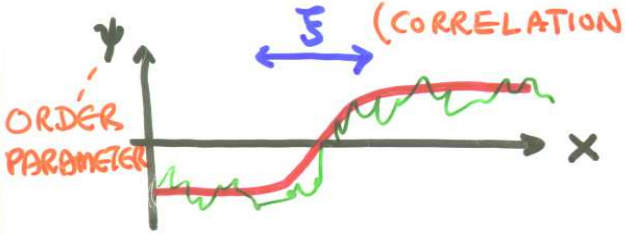


VECTOR

DEFECTS ARE VORTICES

$L(t)$

CHARACTERISTIC SCALE OF PATTERN



MICROSCOPIC DEGREES OF FREEDOM

COARSE-GRAINED DEGREES OF FREEDOM (ψ)

INTERESTED IN PHENOMENA ON SCALE OF $L(t)$. IDEALLY COULD IGNORE SCALES $< \xi$.

THERMAL FLUCTS. $\rightarrow$ SCALES $< \xi$.

$\frac{\xi}{L(t)} \rightarrow 0$ as $t \rightarrow \infty$, SO IGNORE THERMAL FLUCTUATIONS ("$T=0$")

CDS

KEY POINTS:

(1) SPACE + TIME DISCRETE.

$\Delta x \sim \Delta t \sim O(1)$

NO CONTINUUM LIMIT

(2) POTENTIAL: ONLY FIXED POINT STRUCTURE IMPORTANT

(1) MORE IMPORTANT THAN (2).

ASSUMPTION:

THIS ALGORITHM IS IN UNIVERSALITY CLASS OF P.D.E. NOT OBVIOUS!

NOTE: IN LITERATURE, CDS APPROACH USED WITH P.D.E., FOLLOWING (1) BUT NOT (2) i.e. DOING EULER BUT NOT CONTINUUM LIMIT.

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

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

SINGLE CELL DYNAMICS

COUPLING BETWEEN CELLS = DIFFUSION
$D = 0.7$

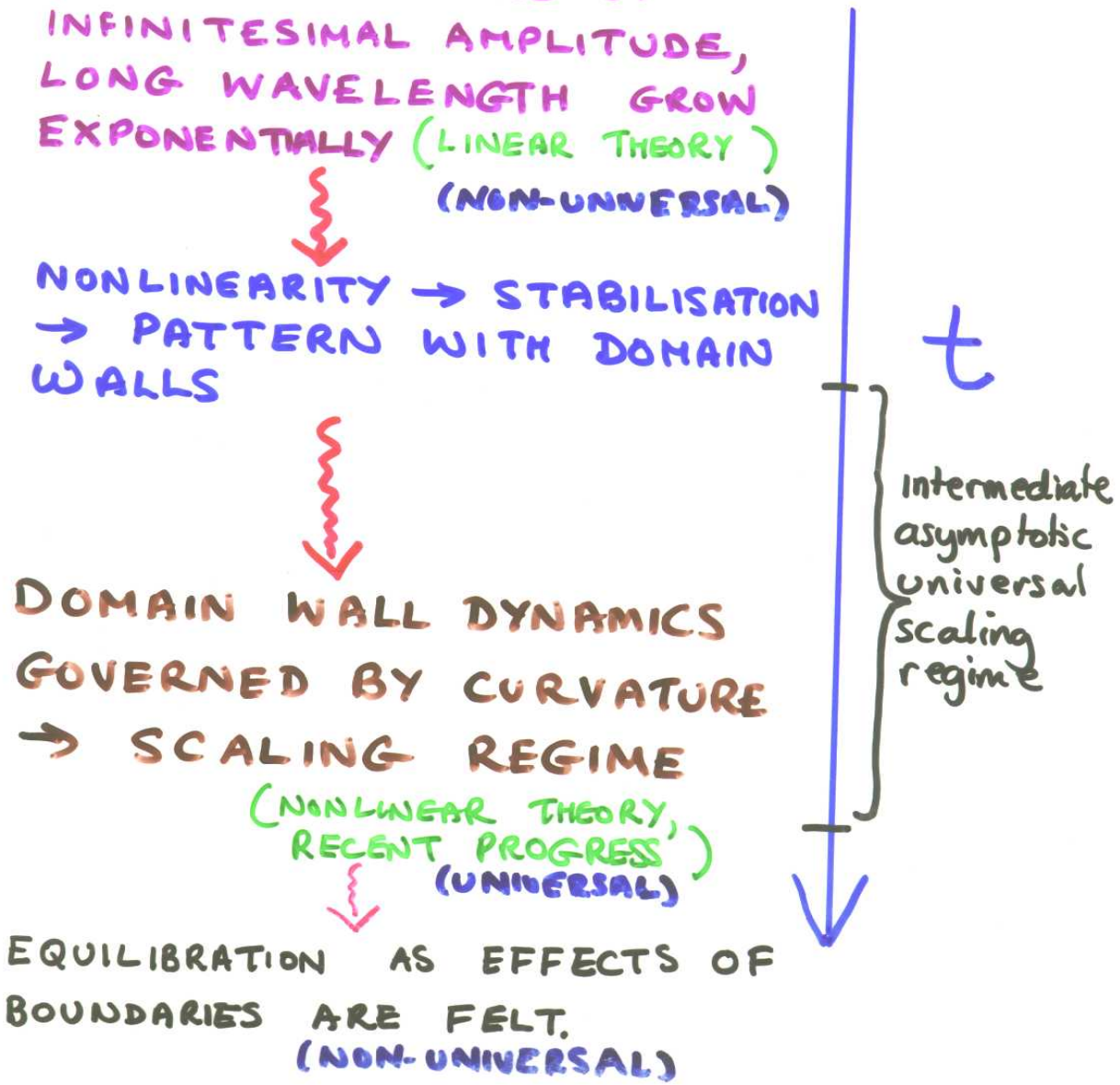
AVERAGING:

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

NEAREST NEIGHBOURS

NEXT NEAREST NEIGHBOURS

SUMMARY OF TIME REGIMES



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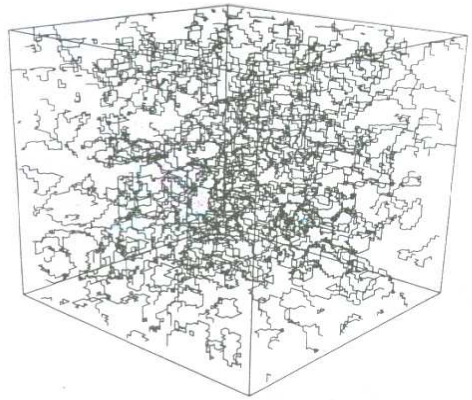
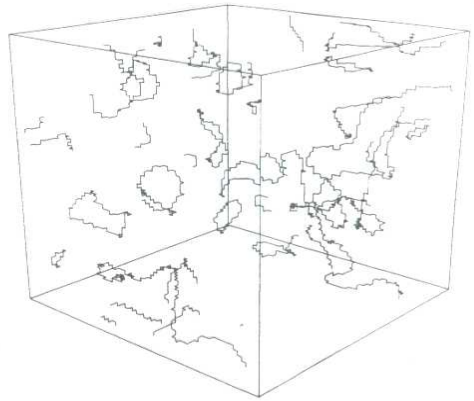
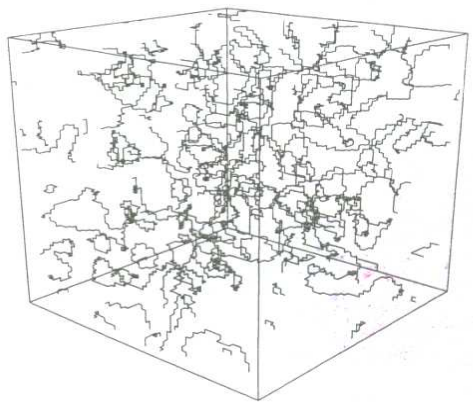
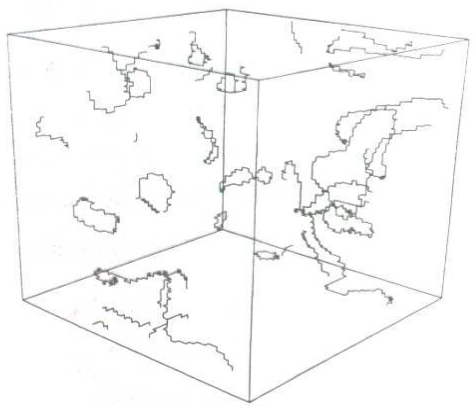
  - Renormalization group approach to large-scale simulation of materials processes

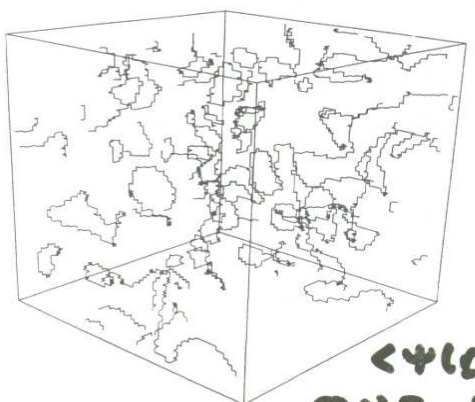


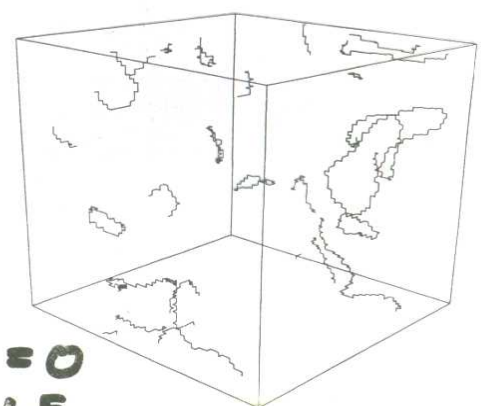


VORTEX ANNIHILATION IN O(2) MODEL



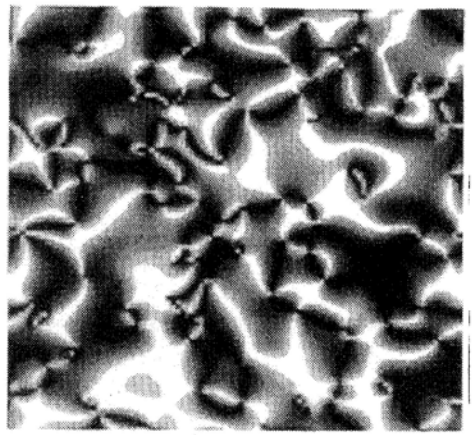




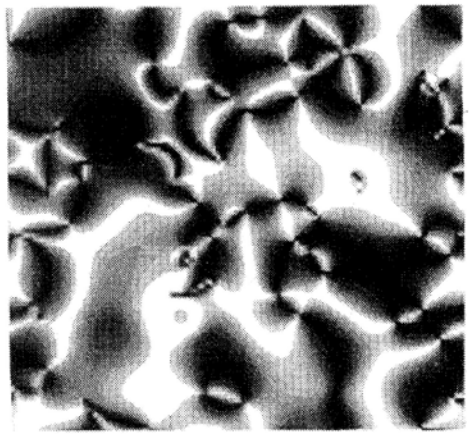


$\langle \psi(r,0) \rangle = 0$

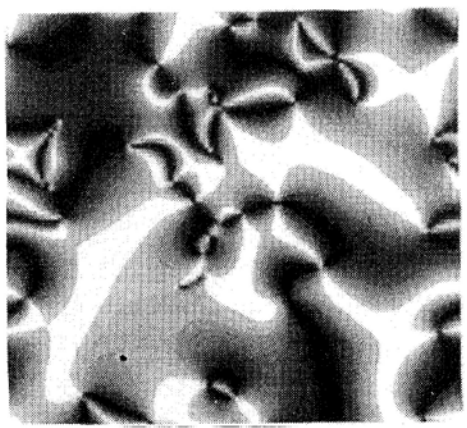
→ ONE SCALE



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).

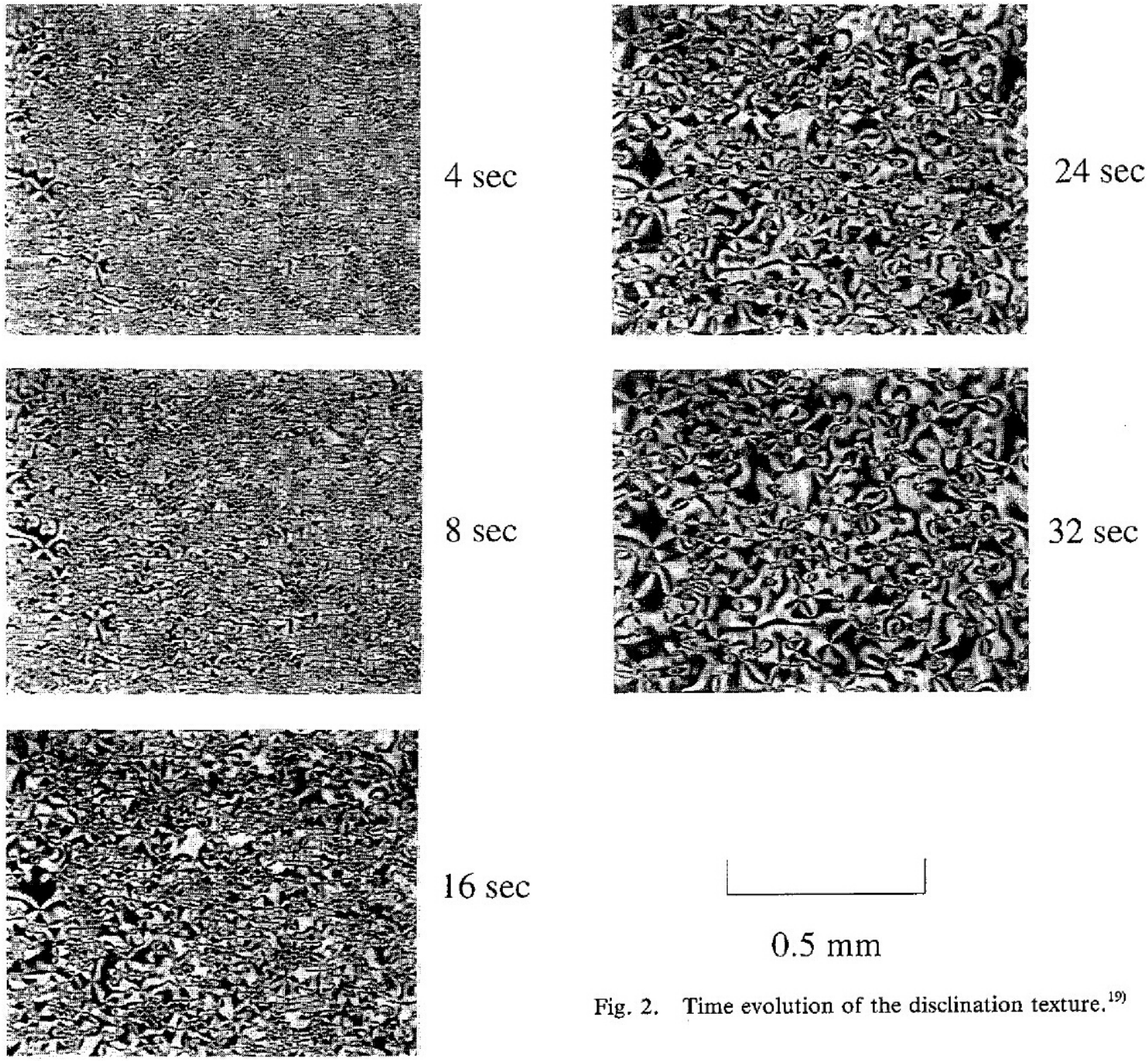


Fig. 2. Time evolution of the disclination texture.[19]

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.

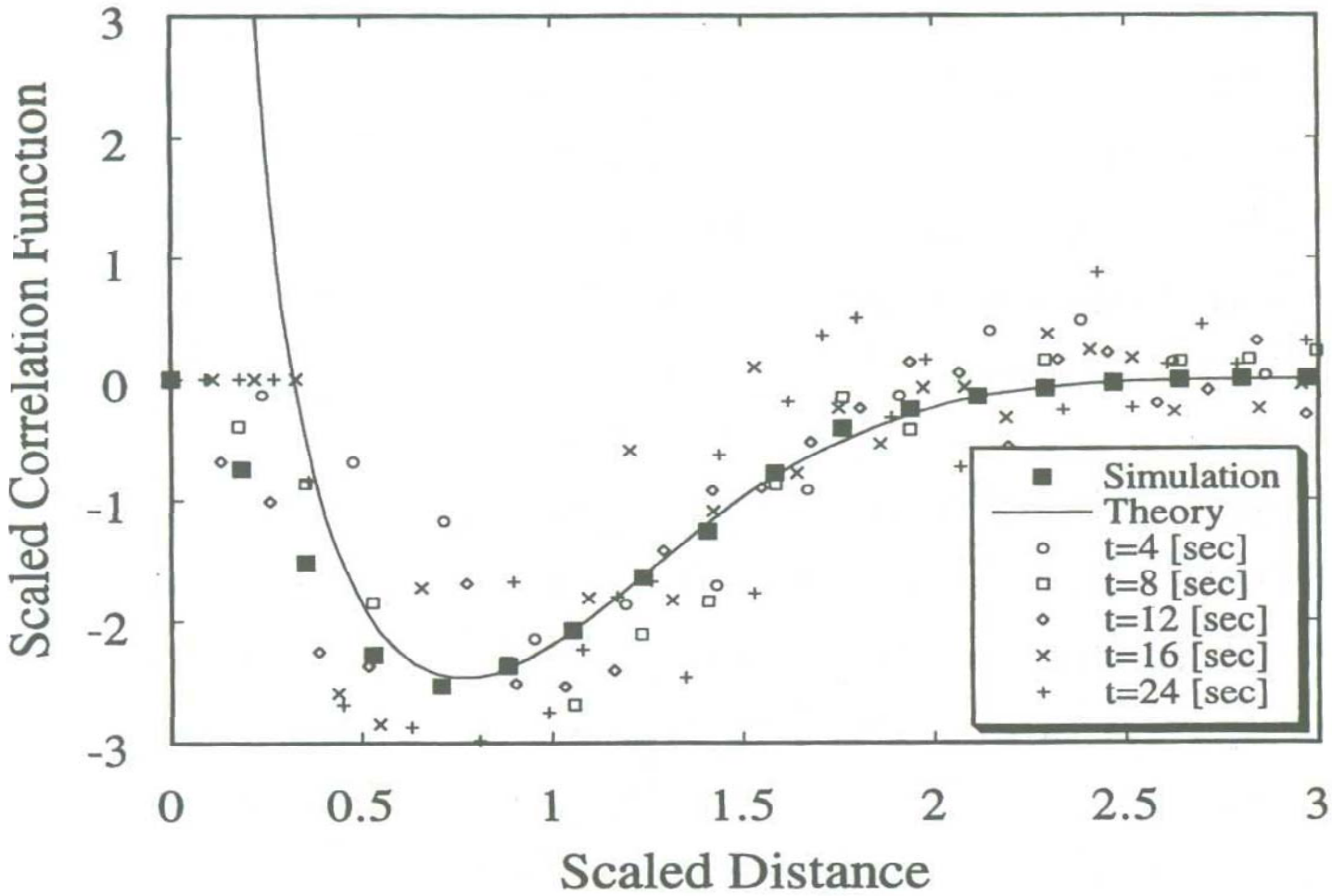


Fig. 6. The scaled correlation function of defect densities. The solid line and the large closed squares indicate the theoretical curve by Lue *et al.*[11] and the data of simulation by Mondello *et al.*,[8] respectively.

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

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**

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
- **Can we make simple theories of complex phenomena?**
  - Computational irreducibility
- **Multiscale modeling of patterns**
  - Renormalization group approach to large-scale simulation of materials processes

Computational irreducibility and the predictability of physical systems

Navot Israeli & Nigel Goldenfeld

Department of Physics

University of Illinois at Urbana-Champaign

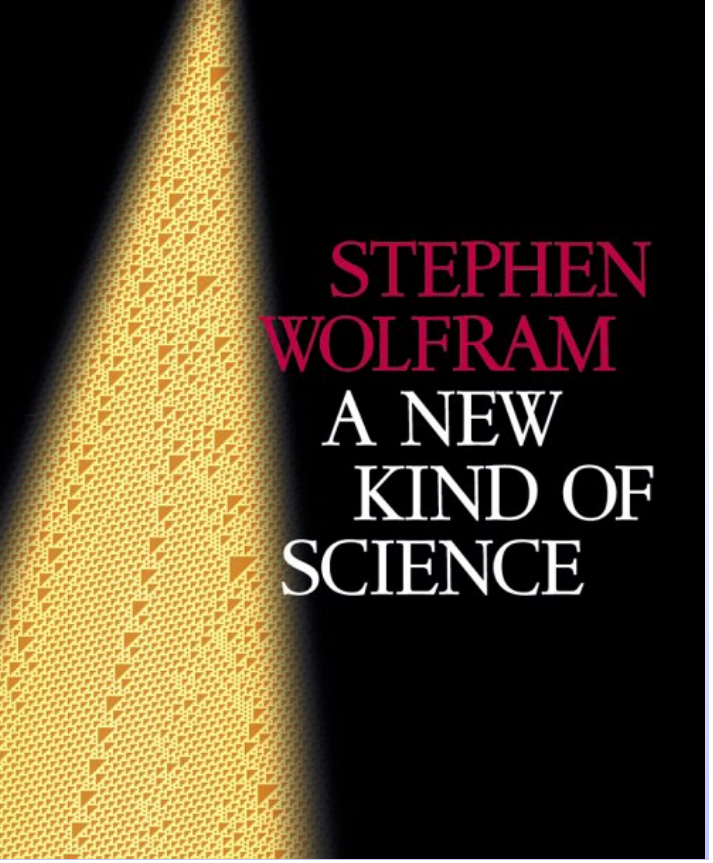
Phys. Rev. Lett. **92**, 074105 (2004)

Overview: Part II

- The story so far ...
  - **Universal features of pattern formation**
  - **Comparison with experiment**
- The question: Can we make simple theories of complex phenomena?
  - **Does computational irreducibility present a fundamental limitation to modelling complex phenomena?**
- The idea: Focus on universality and long-wavelength properties
  - **Coarse-graining of spatially-extended dynamical systems**
- What we did: Numerical experiments using one-dimensional nearest neighbour cellular automata (CA)
  - **Construct RG flow picture: CA's emulating other CA's in a coarse-grained way**
- What our results suggest: Computational irreducibility not necessarily an obstacle: approximation can be computationally reducible
  - **Good enough for physicists!**

Modelling Complex Systems

Can we go beyond simulation?



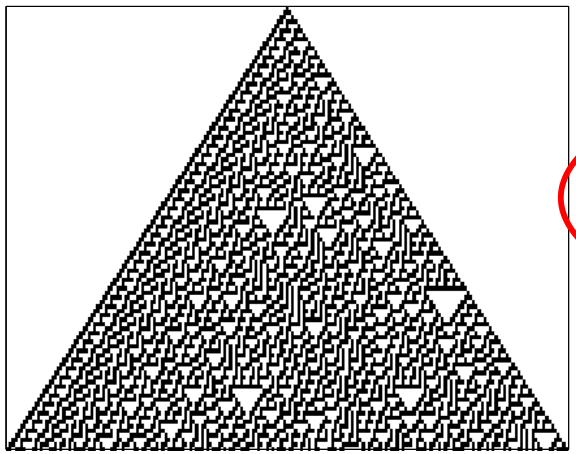
Are complex systems unpredictable?

In traditional science it has usually been assumed that if one can succeed in finding definite underlying rules for a system then this means that ultimately there will always be a fairly easy way to predict how the system will behave.

Several decades ago chaos theory pointed out that to have enough information to make complete predictions one must in general know not only the rules for a system but also its complete initial conditions.

But now computational irreducibility leads to a much more fundamental problem with prediction. For it implies that even if in principle one has all the information one needs to work out how some particular system will behave, it can still take an irreducible amount of computational work actually to do this.

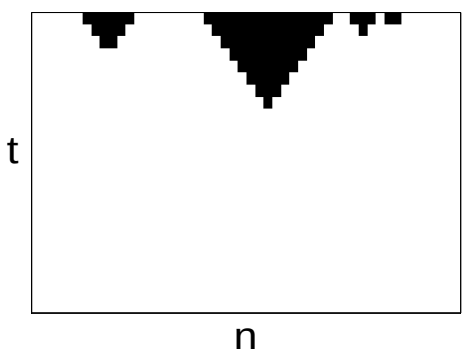
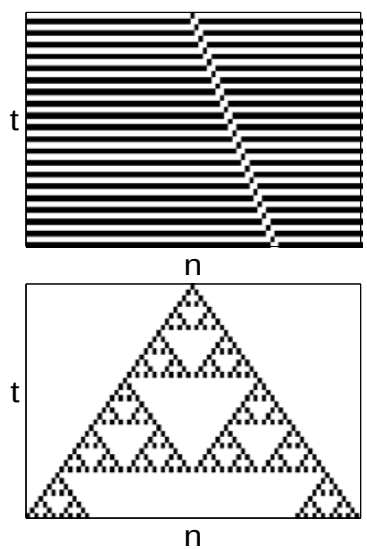
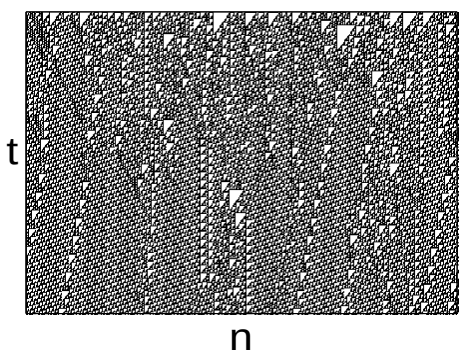
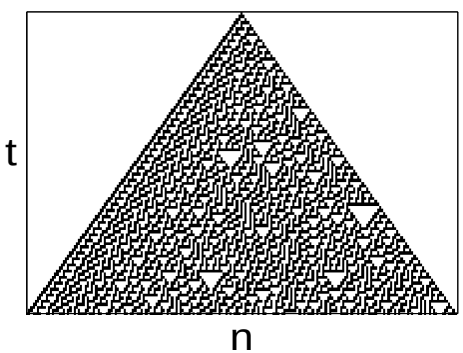
Indeed, whenever computational irreducibility exists in a system it means that in effect there can be no way to predict how the system will behave except by going through almost as many steps of computation as the evolution of the system itself.



Cellular automata as a proxy for a complex system

Wolfram's classification of CA

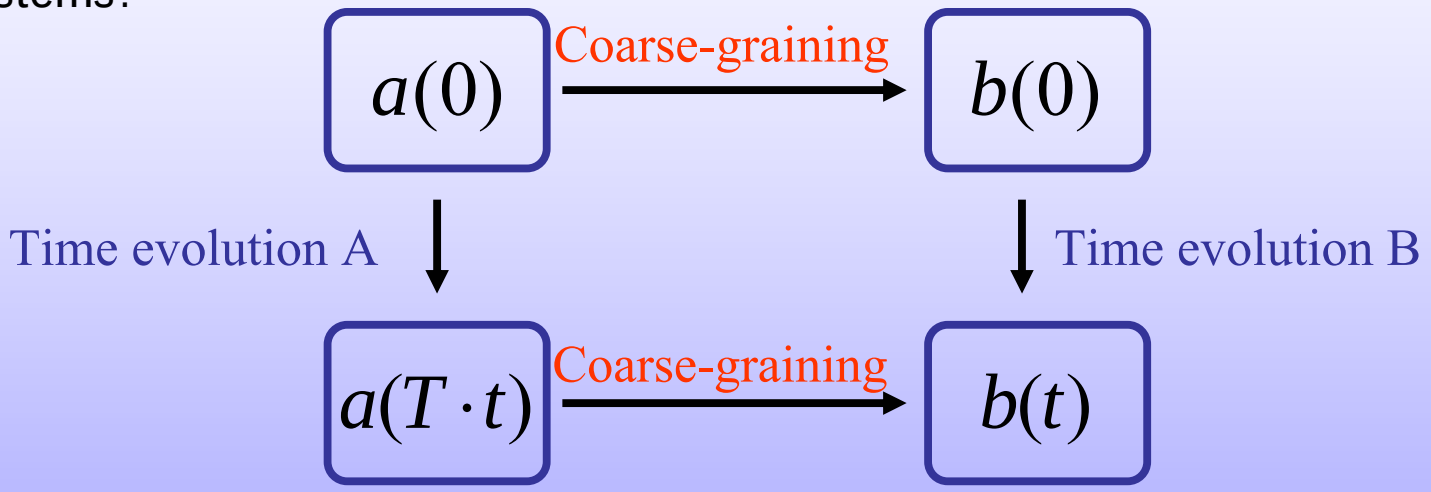
Classification according to apparent complexity:

Class 1 **Decaying structures**	**Class 2** **Periodic or nested**	**Class 4** **Interacting structures**	**Class 3** **Chaotic behavior**
			

- Classification is only qualitative, there is no classification algorithm.
- CA seem to cover the full range of complexity found in nature.
- Some CA are ***computationally irreducible*** (Wolfram hypothesized that most of class 3 and 4).
- Some CA are ***universal*** Turing Machines (Wolfram hypothesized that class 4 is the threshold).

Usually in physics, we do not seek exact predictions.

What happens if we coarse-grain computationally-irreducible dynamical systems?



Not obvious how to coarse-grain a spatially-extended dynamical system such as a cellular automata.

Construct using exhaustive search ...

Elementary Cellular Automata

$$A = \left(a(t), S_A, f_A\right)$$

lattice of cells

alphabet

update function

	$a_{n-1}(t)$	$a_n(t)$	$a_{n+1}(t)$	
		$a_n(t+1)$		

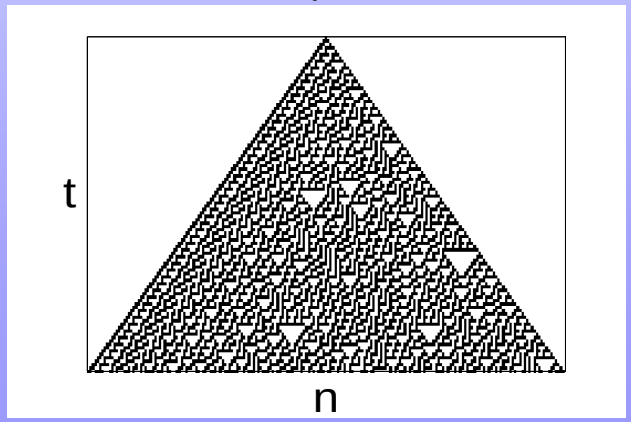
$$S_A = \{0,1\}$$

for elementary CA

$$a_n(t+1) = f_A\left[a_{n-1}(t), a_n(t), a_{n+1}(t)\right]$$

(256 possible functions)

A dynamical system capable of rich behavior.



Wolfram's rule notation:
read 
as a binary number.

Computational Irreducibility and Predictability

- Some complex CA are ***computationally irreducible***. Wolfram hypothesized that most of class 3 and 4 CA are irreducible.

- ***Computational irreducibility*** = the system behavior can be predicted only by running it. There is no computationally more efficient way.

- In analogy to the real world:
  - Many physical processes that seem complex are probably computationally irreducible.
  - Most physical systems have too many degrees of freedom for direct simulation.
  - Are Complex Systems inherently unpredictable?

Predictable Coarse-Grained Behavior

- Usually infinite precision is not required in Physics and coarse-grained or even statistical information is sufficient.

- Can CA be coarse-grained?

- Coarse-grain-able CA are ***compactable***. They have a coarse description with a smaller phase space.

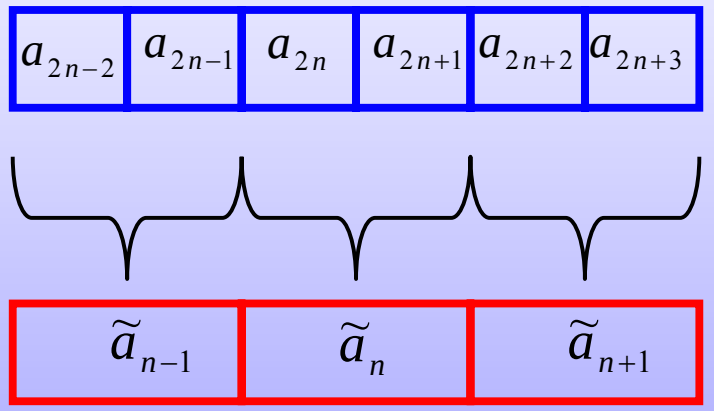
- Coarse-grain-able CA are ***predictable*** if they or their coarse-grained version are computationally reducible.

- We found that at least some ***computationally irreducible*** CA has ***predictable*** coarse-grained behavior.

Coarse-graining procedure

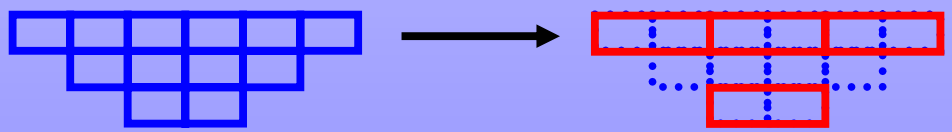
Step 1: Blocking with no information loss

Generate the *N*th block version $\widetilde{A}$ of *A*. Group every *N* cells of *A* into a super-cell $\widetilde{a}$.



The super-cells accept values from the alphabet $\{0,1\ldots 2^N-1\}$.

Calculate the transition function $f_{\widetilde{A}}$ for the super-cells by running *A* *N* time steps for all possible inputs of length *3N*.



Coarse-graining procedure

Step 2: Projection back on to the original alphabet with loss of information

Construct the coarse-grained CA B by projecting the alphabet of $\widetilde{A}$ on a subset of $\{0,1\ldots 2^N-1\}$.

The cell values of B are given by $b_n = P(\widetilde{a}_n)$

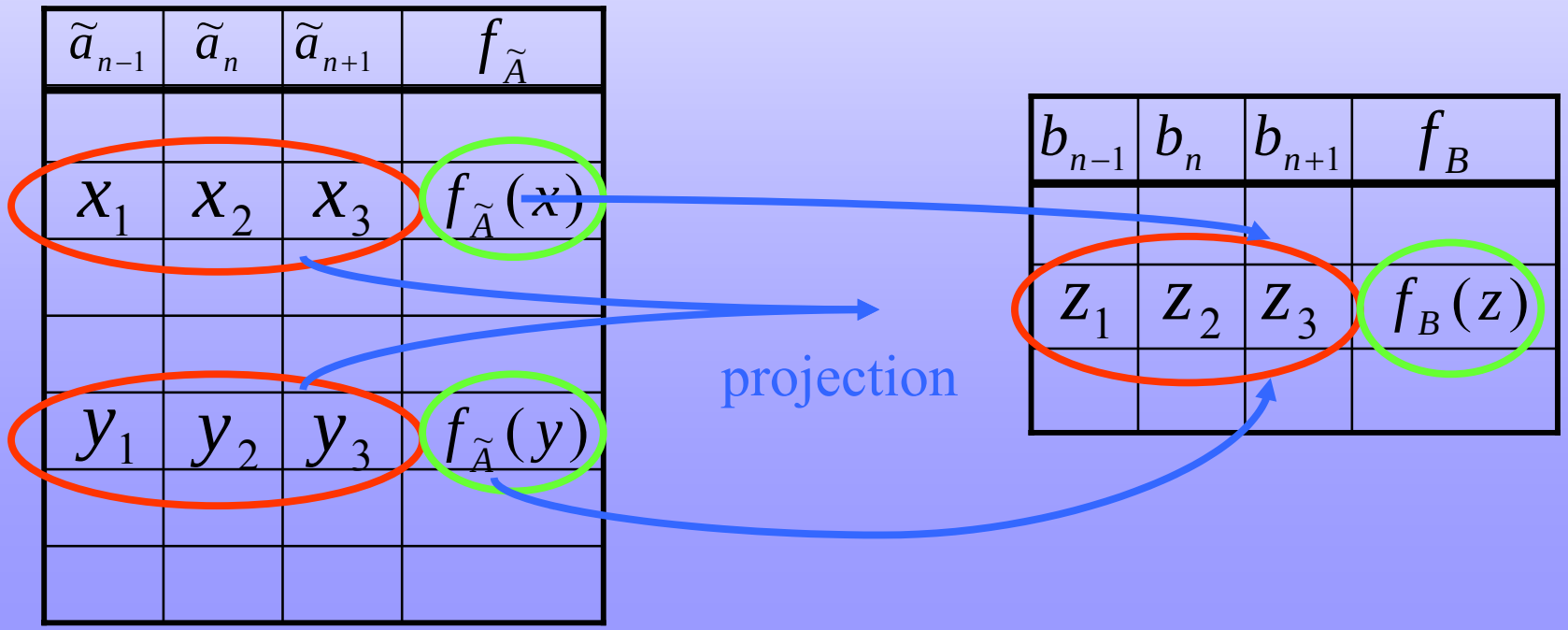
The transition function of B is given by projecting the arguments and outcome of $f_{\widetilde{A}}$

$$f_B[b_{n-1},b_n,b_{n+1}] = P\left(f_{\widetilde{A}}[\widetilde{a}_{n-1},\widetilde{a}_n,\widetilde{a}_{n+1}]\right) \quad , \quad b_k = P(\widetilde{a}_k)$$

This construction is possible only if:

$$P\left(f_{\tilde{A}}[x_1, x_2, x_3]\right) = P\left(f_{\tilde{A}}[y_1, y_2, y_3]\right), \quad \forall\left(x, y \middle| P(x_i) = P(y_i)\right).$$

Otherwise f_B is not single valued and the coarse-graining procedure fails for the choice (*N,P*).



When ★ is satisfied B is a coarse-graining of $\tilde{A}$ with a time constant $T = 1$.

For every step $\tilde{a}_n(t+1) = f_{\tilde{A}}\left[\tilde{a}_{n-1}(t), \tilde{a}_n(t), \tilde{a}_{n+1}(t)\right]$ that $\tilde{A}$ makes

B makes the move: $b_n(t+1) = f_B\left[b_{n-1}(t), b_n(t), b_{n+1}(t)\right]$

$$= P\left(f_{\tilde{A}}\left[P(\tilde{a}_{n-1}), P(\tilde{a}_n), P(\tilde{a}_{n+1})\right]\right)$$

use ★ ↓

$$= P\left(f_{\tilde{A}}\left[\tilde{a}_{n-1}(t), \tilde{a}_n(t), \tilde{a}_{n+1}(t)\right]\right)$$

$$= P\left(\tilde{a}_n(t+1)\right)$$

B is a coarse-graining of A with a time constant $T = N$

because $\tilde{A}$ computes N moves of A in a single time step.

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Computational Irreducibility and the Predictability of Complex Physical Systems

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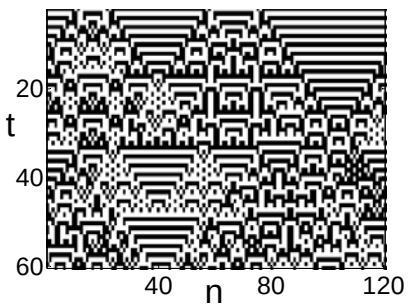
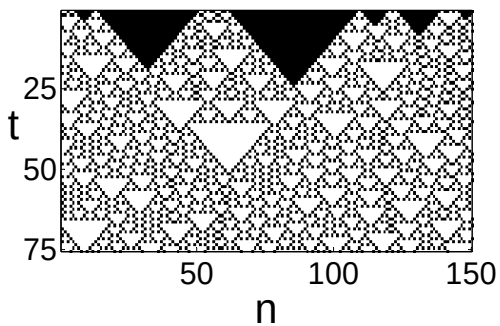
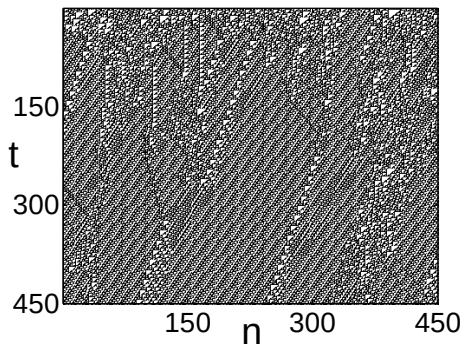
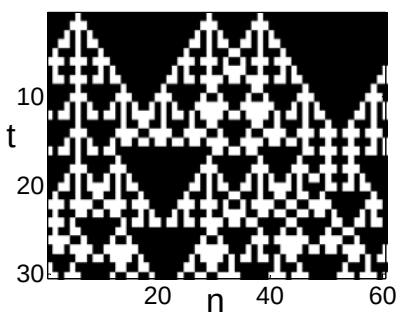
(Received 16 June 2003; published 20 February 2004)

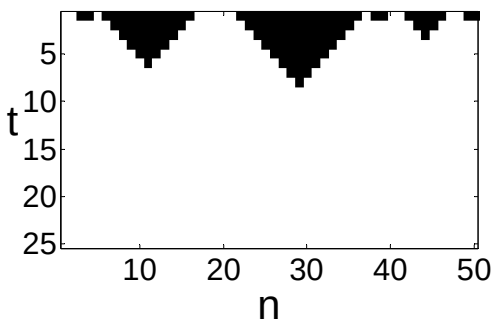
Using elementary cellular automata (CA) as an example, we show how to coarse grain CA in all classes of Wolfram's classification. We find that computationally irreducible physical processes can be predictable and even computationally reducible at a coarse-grained level of description. The resulting coarse-grained CA which we construct emulate the large-scale behavior of the original systems without accounting for small-scale details. At least one of the CA that can be coarse grained is irreducible and known to be a universal Turing machine.

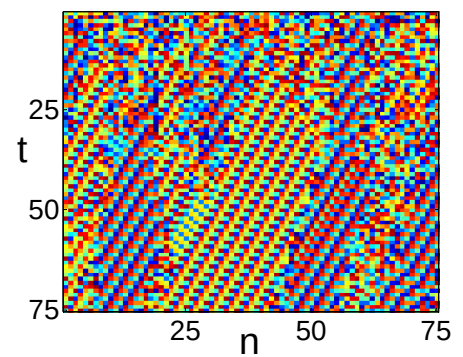












Results of coarse-graining elementary rules

- We were able to coarse-grain 240 out of the 256 elementary CA by trying different choices of super-cell sizes and projection operators.

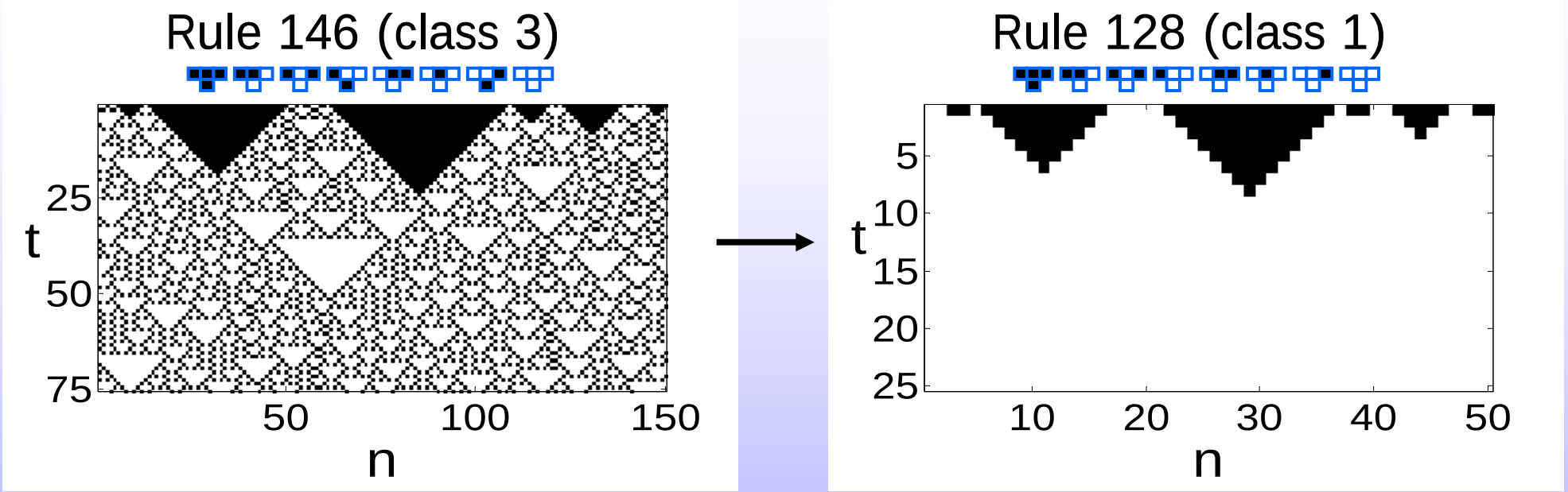
- It might be possible to coarse-grain the other 16 rules (30, 45, 106, 154 and their symmetries) by trying larger super-cell sizes.

- Many elementary CA can be coarse-grained by other elementary CA.

- Coarse-grained-able CA include members of all four classes.

- At least one ***computationally irreducible*** CA can be coarse-grained by a ***reducible*** CA and is therefore predictable on a coarse level.

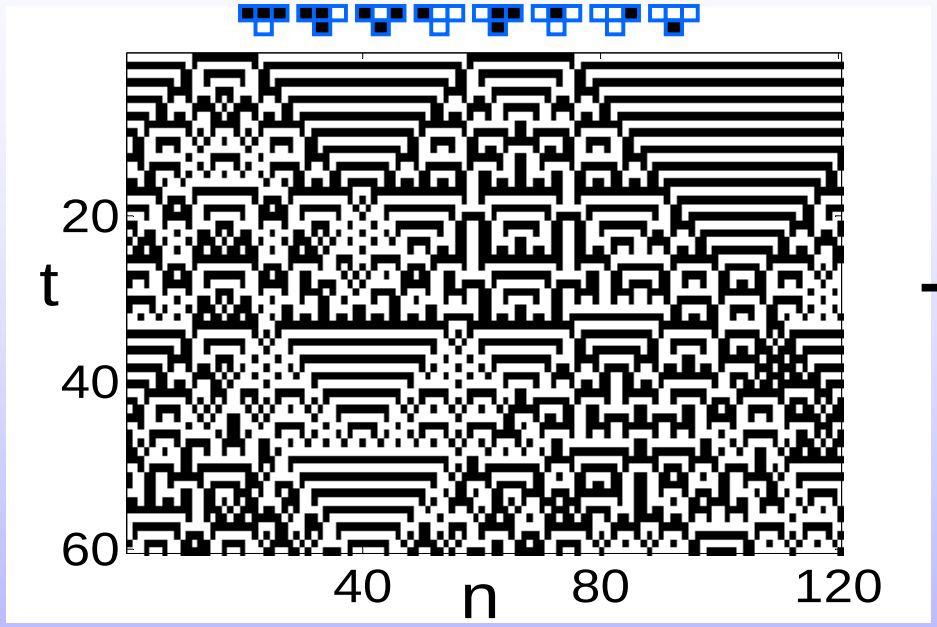
Example 1



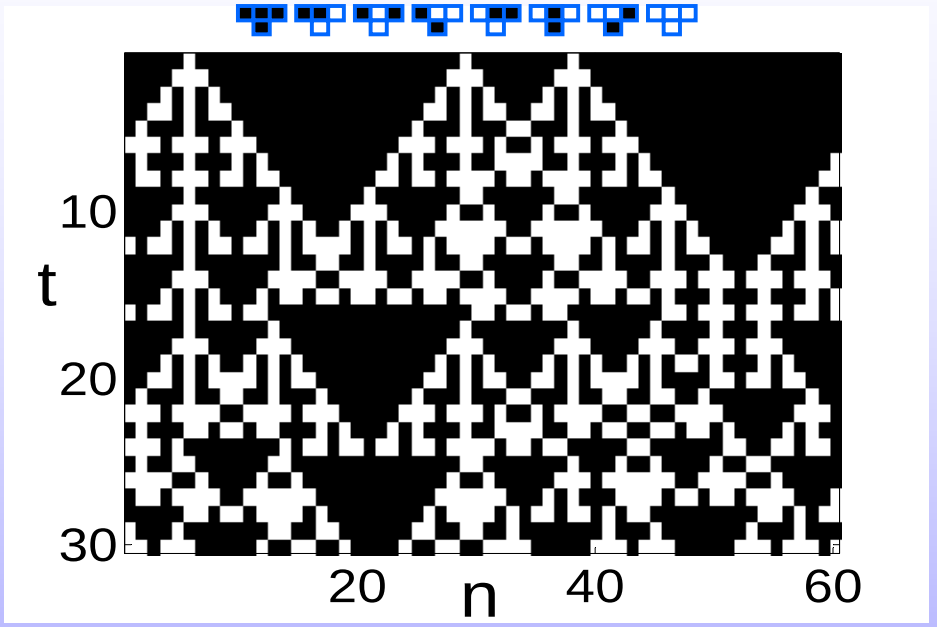
- super-cell size N=3.
- Projection: $P(\tilde{a}) = \begin{cases} \square\square\square & , \tilde{a} \neq \\ \blacksquare & , \tilde{a} = \blacksquare\blacksquare\blacksquare \end{cases}$
- Complex (potentially ***irreducible***) on the microscopic scale, ***predictable*** on the coarse scale.

Example 2

Rule 105 (class 2)



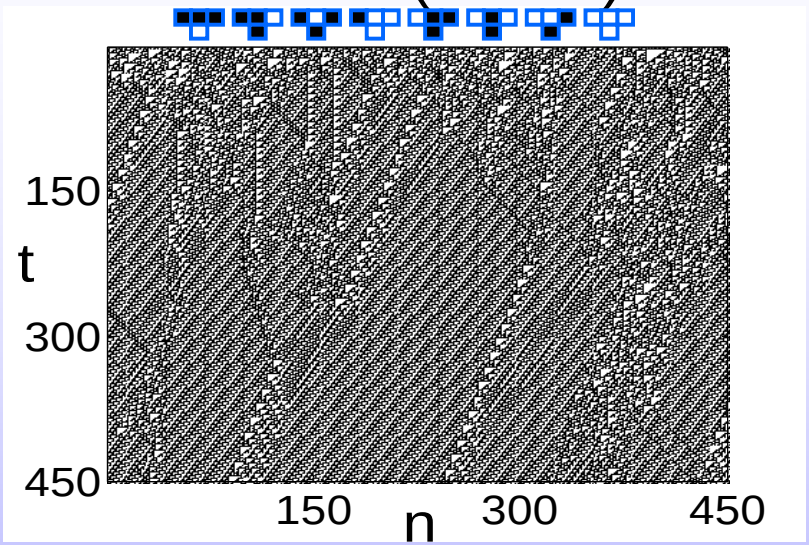
Rule 150 (class 2)



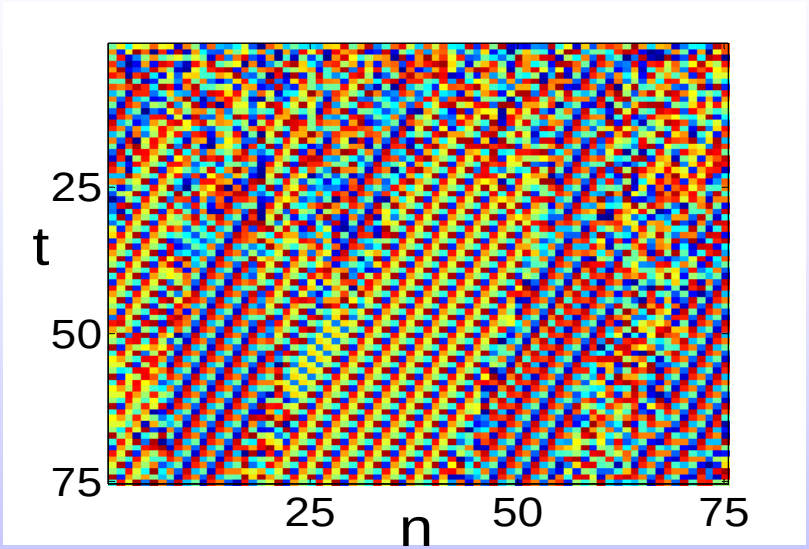
- super-cell size N=2.
- Projection: $P(\tilde{a}) = \begin{cases} \square\,, \tilde{a} = \square\blacksquare\,, \blacksquare\square \\ \blacksquare\,, \tilde{a} = \square\square\,, \blacksquare\blacksquare \end{cases}$

Example 3- an irreducible case

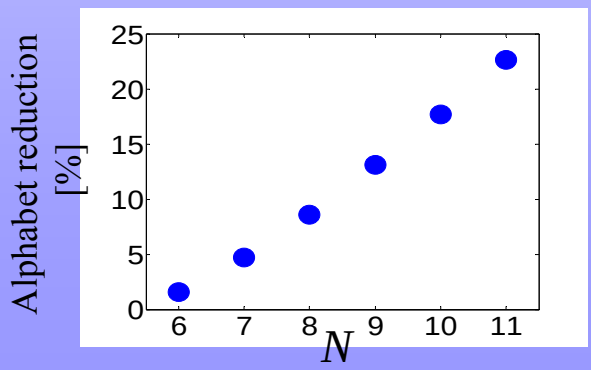
Rule 110 (class 4)



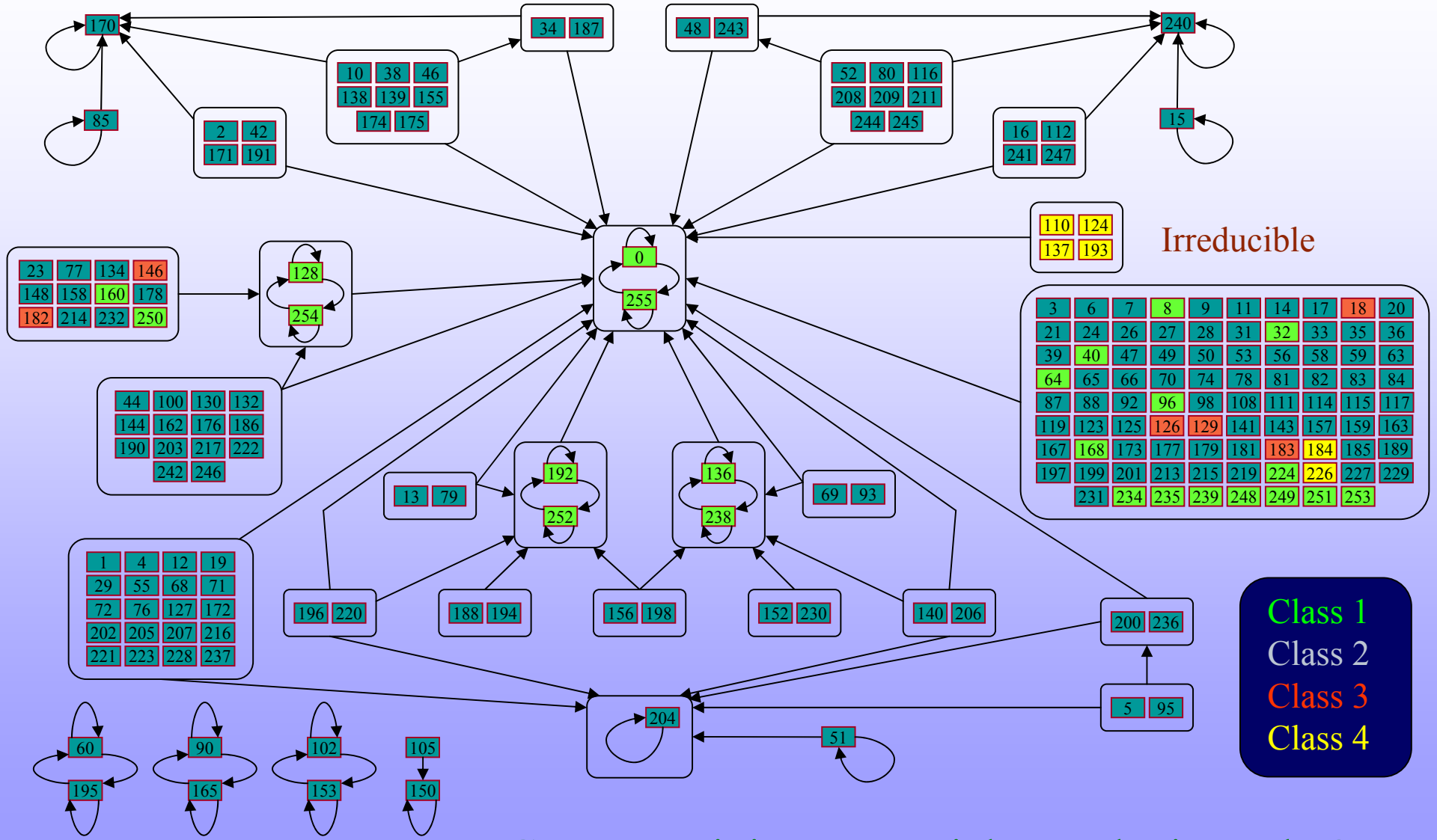
63 color CA



- Super-cell size: N=6. Projection: 64 colors → 63 colors.
- Rule 110 is a ***universal*** CA. Can emulate all other CA (Wolfram).
- A ***universal*** CA is ***computationally irreducible***.
- More impressive information loss with larger N:



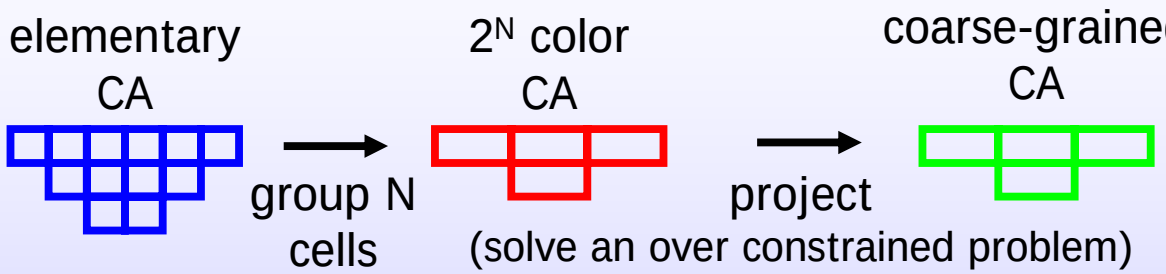
Coarse-graining transitions between elementary rules. with super-cell size N=2,3,4 (for rule 110 N=5)

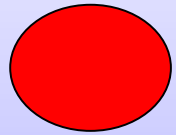
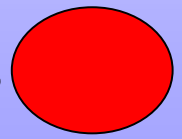


Coarse-graining → partial complexity order?

Why is it easy to coarse-grain CA?

Coarse-graining procedure:

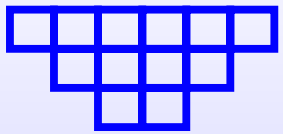


- When N=2 the success rate (among 256 elementary CA) is 
- 4 color CA which are the N=2 supercell version of elementary CA are a small fraction of all possible 4 color rules ($\approx 3 \cdot 10^{38}$).
- The probability of projecting a randomly chosen 4 color CA is 
- What is special about the CA rules that allows such a high probability of success in projecting on to the original alphabet?

Algorithmic complexity of local processes

4 color supercell version of an elementary CA.

$\tilde{a}_{n-1}$	$\tilde{a}_n$	$\tilde{a}_{n+1}$	$f_{\tilde{A}}$
0	0	0	0
0	0	1	3
0	0	2	2
0	0	3	2
⋮			
3	3	3	0



A short generating "program".

Small algorithmic complexity

General 4 color CA.

x_{n-1}	x_n	x_{n+1}	f_X
0	0	0	1
0	0	1	2
0	0	2	0
0	0	3	0
⋮			
3	3	3	3

random

Large algorithmic complexity

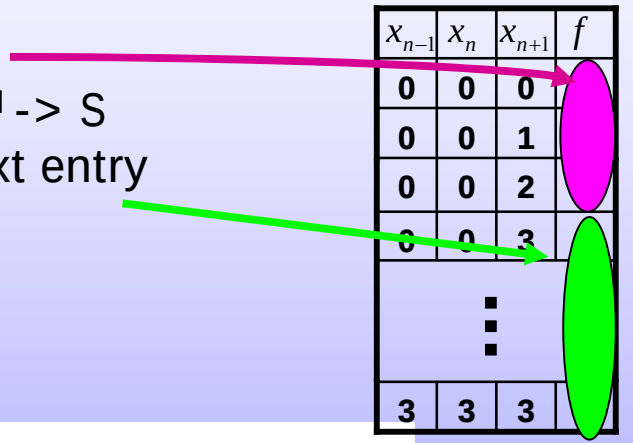
$$\text{Algorithmic complexity} = \frac{\text{length of minimal generating code}}{\text{length of string}}$$

Experiment: projection probability vs. algorithmic complexity

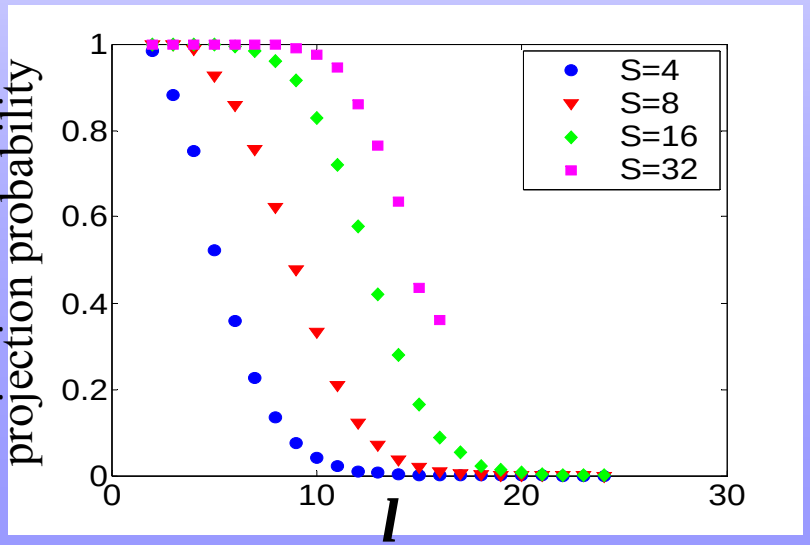
- Use short programs to generate random multicolor CA with definite algorithmic complexity.
- Measure the probability of a successful projection as a function of program length.

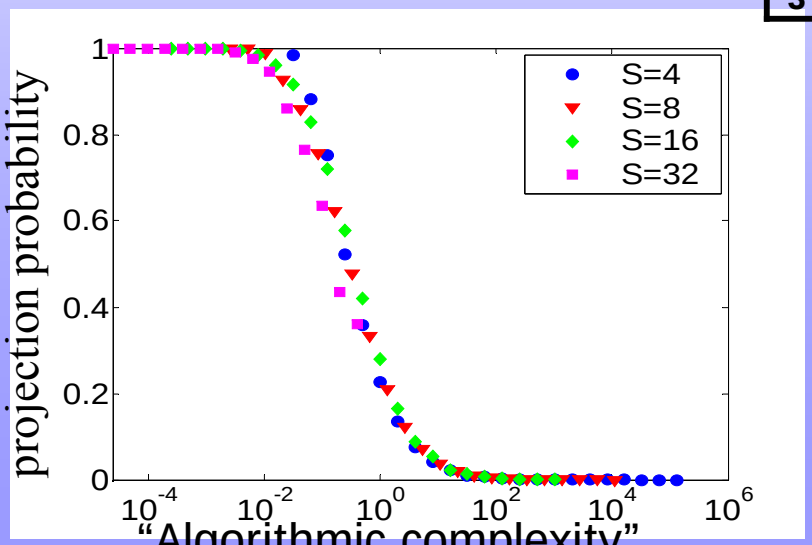
Program(***l***):

1. Randomly chose the first ***l*** entries of the rule table:
2. Pick a random ***generating function*** of ***l*** arguments: f: S^l -> S
3. Use the function f and the last ***l*** filled entries to fill the next entry
4. Repeat until all entries filled
5. Try to find a projection.



"Algorithmic complexity" $= \frac{l + S^l}{S^3}$





Relevant and Irrelevant degrees of freedom

Coarse-graining can loose two different types of dynamic information, depending on how the condition $P\left(f_{\tilde{A}}[x_1,x_2,x_3]\right)=P\left(f_{\tilde{A}}[y_1,y_2,y_3]\right)$ ★

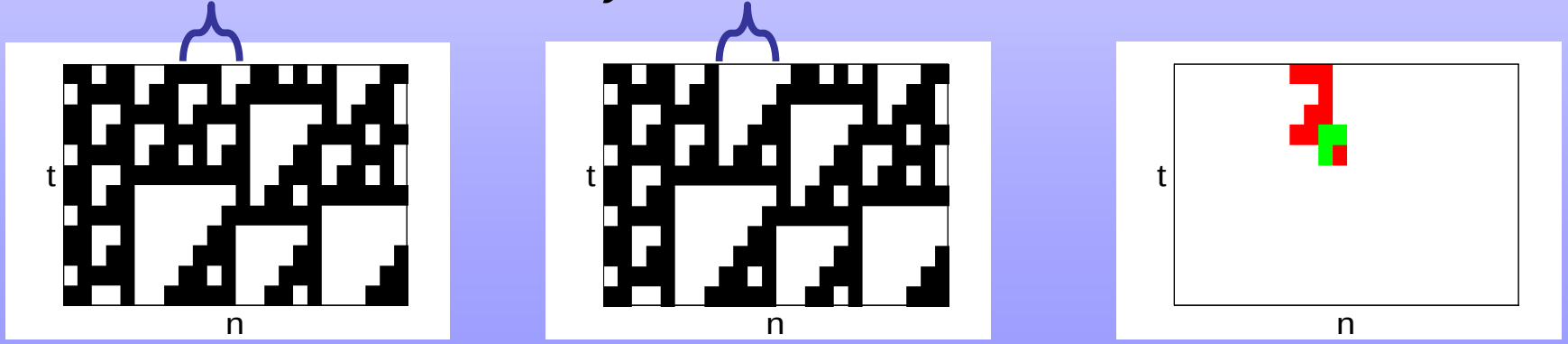
$\forall\left(x,y\middle|P(x_i)=P(y_i)\right)$ is satisfied:

1. Irrelevant DOF

★ is satisfied because $f_{\tilde{A}}[x_1,x_2,x_3]=f_{\tilde{A}}[y_1,y_2,y_3],\ \forall\left(x,y\middle|P(x_i)=P(y_i)\right).$

Replacing *x* by *y* is irrelevant to the long time behavior of *A*:

x in initial state | *y* in initial state | difference



The coarse-grained CA *B* accounts for all long time trajectories of *A*.

A and *B* fall in the same complexity class.

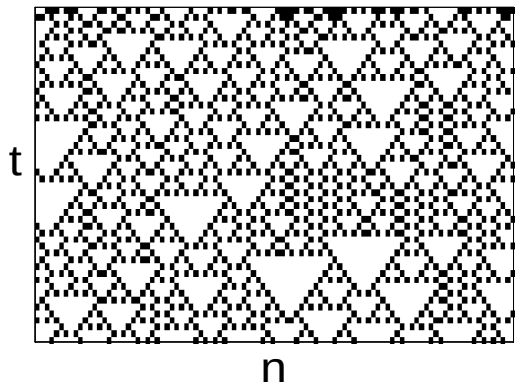
Relevant and Irrelevant degrees of freedom

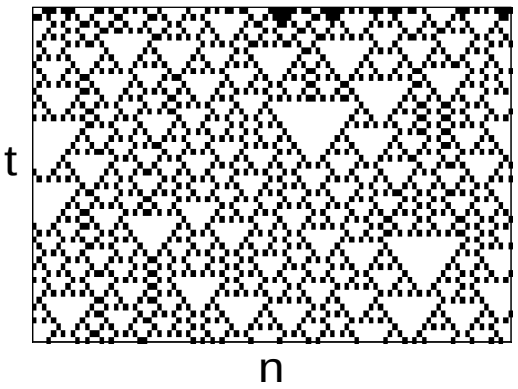
2. Relevant DOF

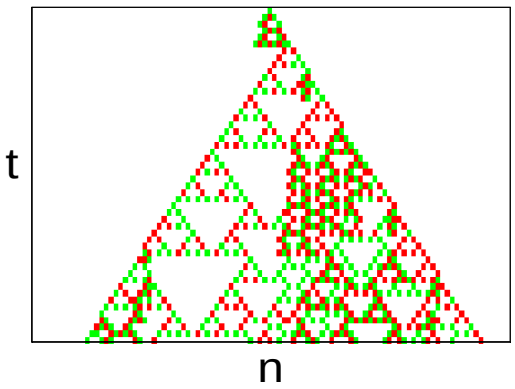
is satisfied even though $f_{\tilde{A}}[x_1, x_2, x_3] \neq f_{\tilde{A}}[y_1, y_2, y_3]$ for some $(x, y | P(x_i) = P(y_i))$.

Replacing *x* by *y* in the initial condition is relevant to the long time behavior of *A*.

x in initial state | *y* in initial state | difference







The coarse-grained CA *B* cannot account for all long time trajectories of *A.*

A and *B* may fall in different complexity classes (see example 1).

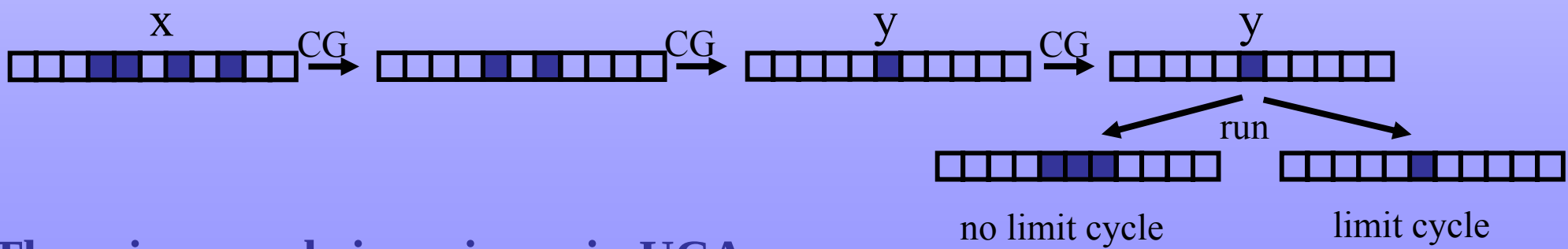
Coarse-graining and undecidability

- Universal cellular automata (UCA) are subject to undecidable questions.
- This puts constraints on possible coarse-grainings of UCA.
- For example, UCA cannot coarse-grain themselves (are not fixed points):

Proof sketch - Assume that a UCA U is a fixed point.

Question: Will U evolve to a limit cycle on input x?

Answer: Coarse-grain the input x several times to an “input fixed point” y, and run U on y.



There is no scale invariance in UCA.

Usually in physics, we do not seek exact predictions.

What happens if we coarse-grain computationally-irreducible dynamical systems?

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Week of March 20, 2004; Vol. 165, No. 12 , p. 189

Complexity by way of simplicity

Peter Weiss

In his controversial 2002 book *A New Kind of Science* (Wolfram Media), theoretical physicist Stephen Wolfram proposed that traditional science is incapable of fathoming many important phenomena in nature. The complexity of how galaxies formed or what the weather will be tomorrow is too much for mathematical formulas, he asserts (SN: 8/16/03, p. 106: http://ciencenews.org/articles/20030816/bob10.asp).

team of physicists has unveiled a new way to process pattern-iting algorithms called cellular automata, which Wolfram argues are a or way to model complex phenomena. The new study suggests that cellular automata can be simplified substantially yet retain the ial outlines of their patterns, says Navot Israeli of the Weizmann e of Science in Rehovot, Israel. He and Nigel D. Goldenfeld of the

Physical Review Focus

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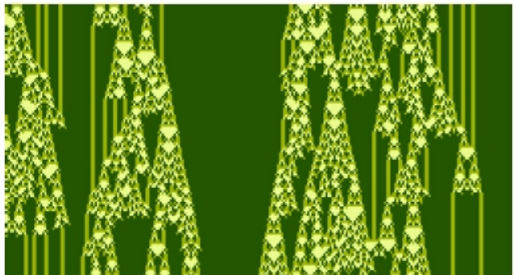
Phys. Rev. Lett. **92**, 074105
(issue of 20 February 2004)
Title and Authors

4 March 2004

Complexity is Elusive

Researchers need enormous computer power to forecast changes in the Earth's climate, but they can predict the speed of a ball rolling down a ramp with pencil and paper. Stephen Wolfram claimed in his 2002 best seller, *A New Kind of Science*, that there is a clear dividing line between complex problems that require



Conclusion: sometimes we can get good approximations to seemingly complex dynamical systems.

We do not need to abandon physics!

Renormalization group approach to multiscale modeling in materials science

Nigel Goldenfeld
Department of Physics
University of Illinois at Urbana-Champaign

Collaborators: Badri Athreya and Jon Dantzig
Project also involves Ken Elder and Nik Provatas

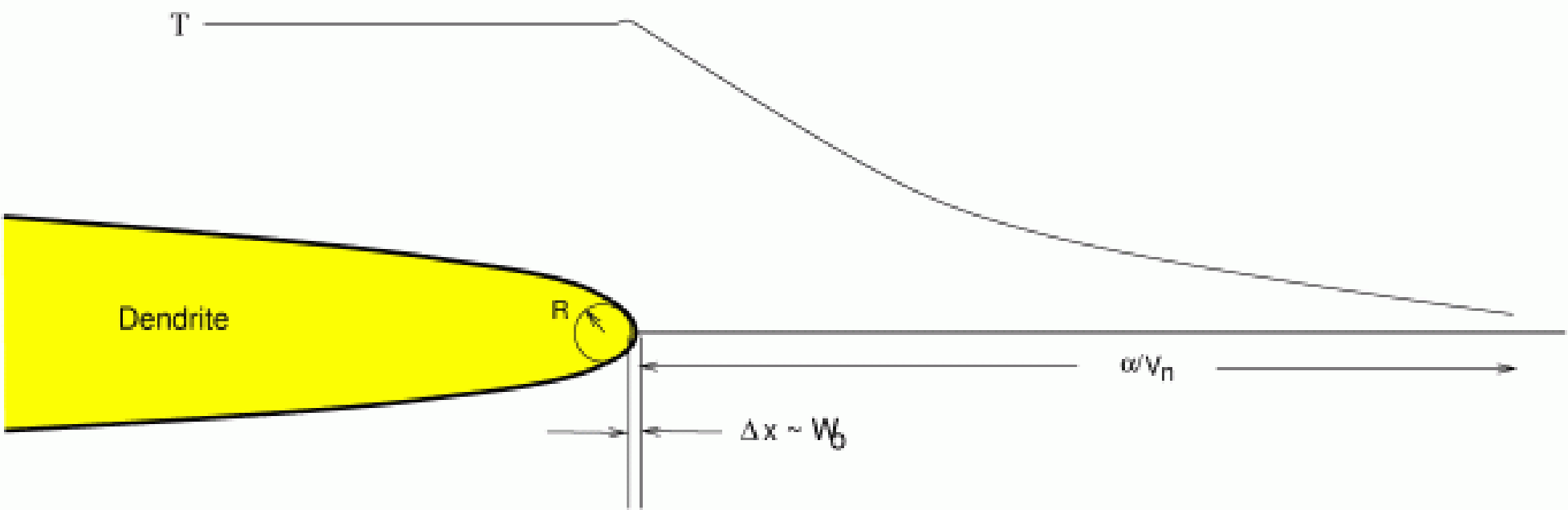
Work supported by the US National Science Foundation and NASA

ITR: Multiscale Models for Microstructure Simulation and Process Design
NSF DMR 01-21695

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
- **Can we make simple theories of complex phenomena?**
  - Computational irreducibility
- **Multiscale modeling of patterns**
  - Renormalization group approach to large-scale simulation of materials processes

Scale hierarchy problem

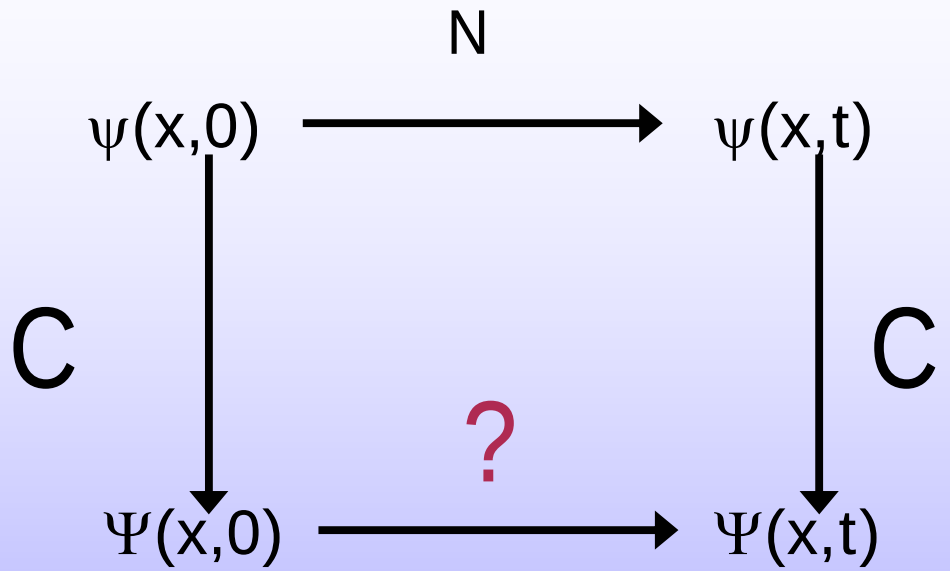


Outline

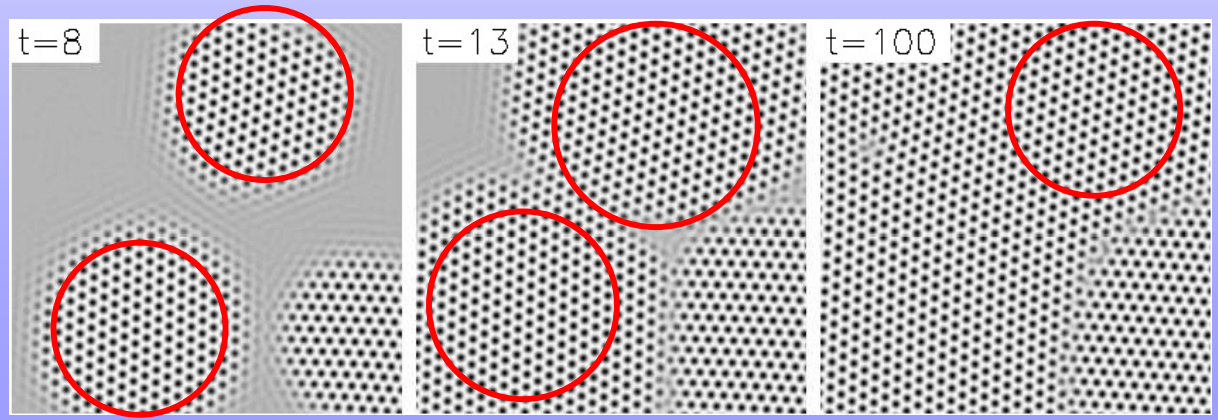
1. **What should a genuine multiscale method look like?**
   - Scale up
   - Adaptive mesh refinement
2. **Phase field crystal model (PFC)**
   - Advantages over molecular dynamics
   - Successful computation of macroscopic quantities
3. **Renormalization group**
   - Reductive perturbation theory & rotational covariance
   - RG equations for the PFC
4. **Preliminary results**
   - Adaptive mesh refinement

Goal of multiscale modeling

- **Given underlying dynamics, what is the effective dynamics at large scales?**

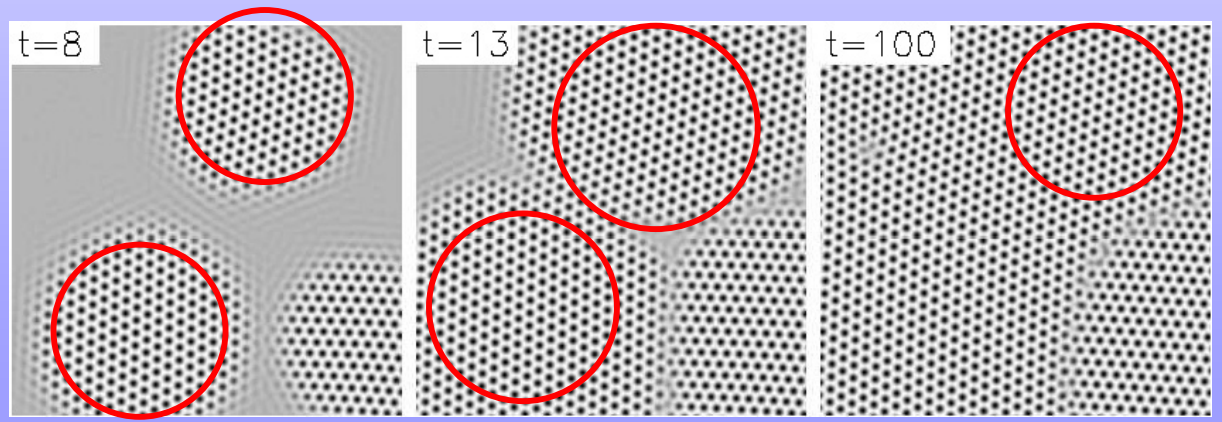


- **Representative behaviour of many degrees of freedom?**



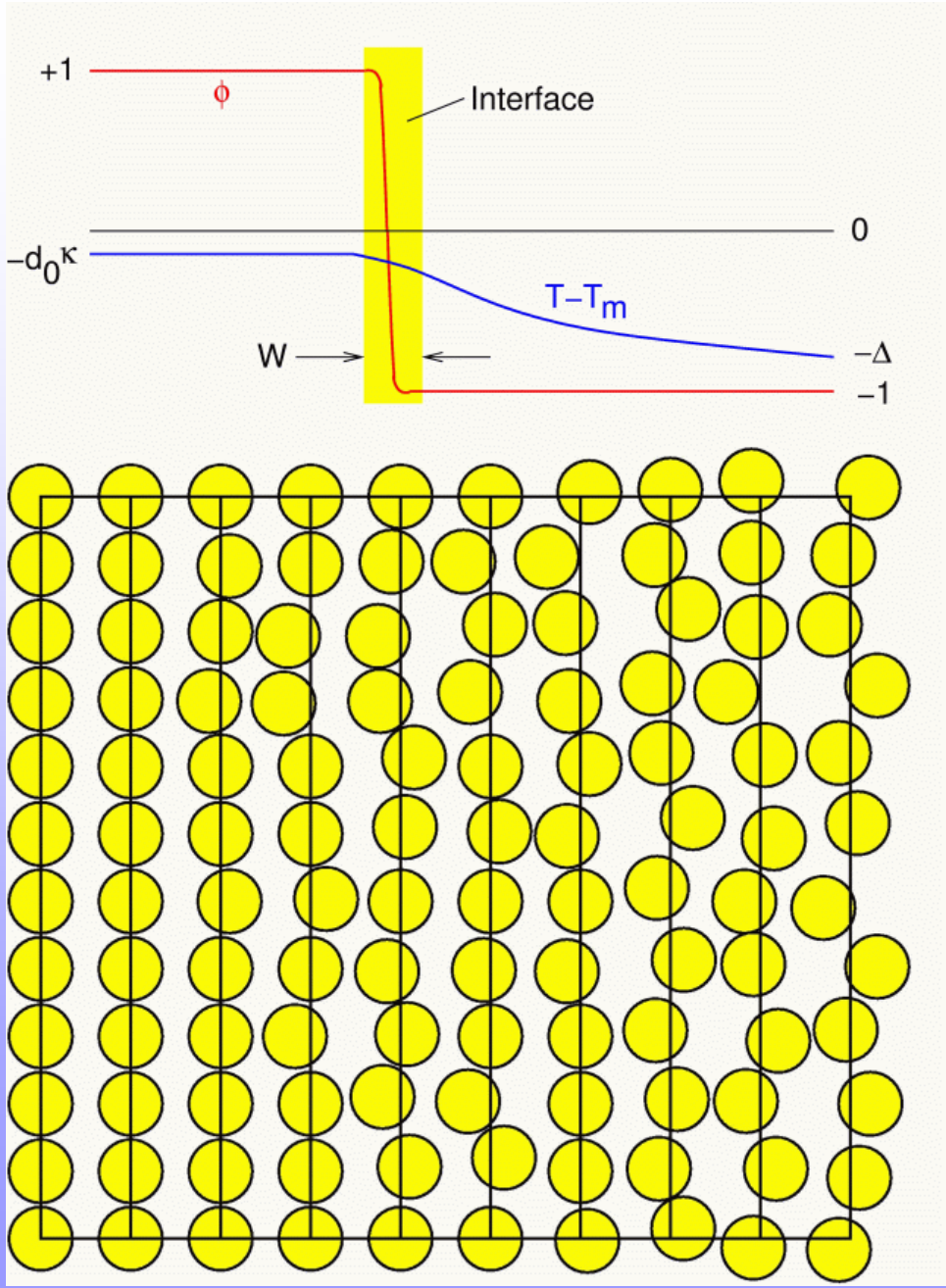
Goal of multiscale modeling

- **Basic idea: model large-scale, uniform regions by some representative variable**
  - Systematic reduction of number of degrees of freedom
- **Representative variable should be predominantly spatially uniform**
- **Significant variation only at boundaries**
  - Adaptive mesh refinement

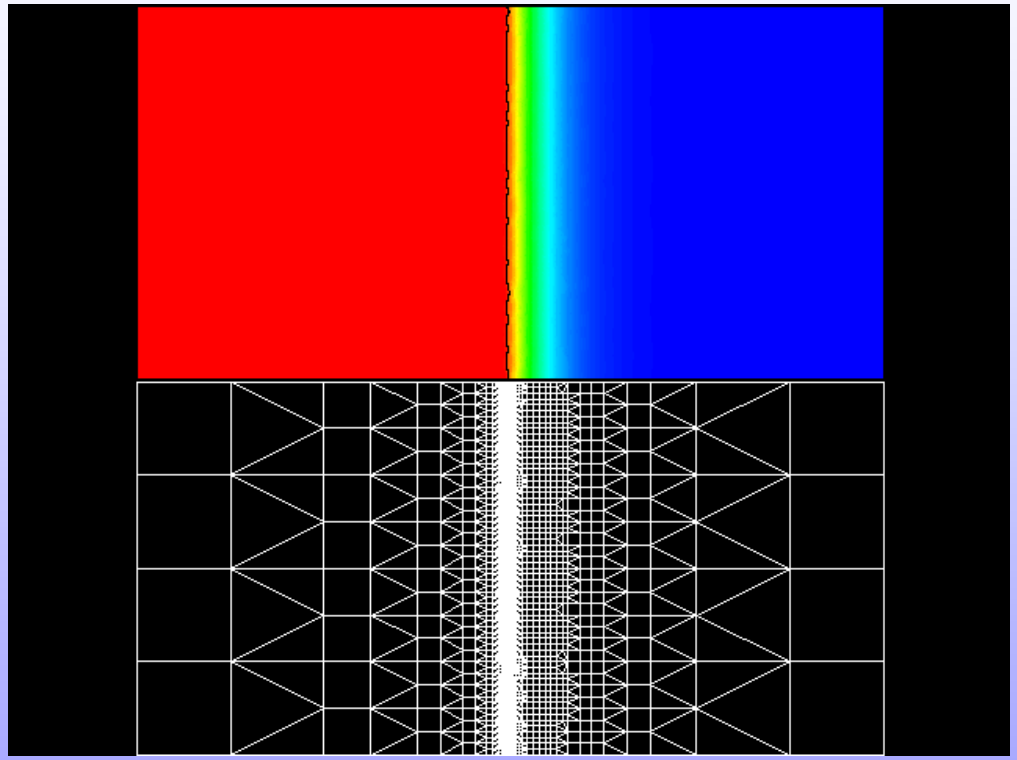


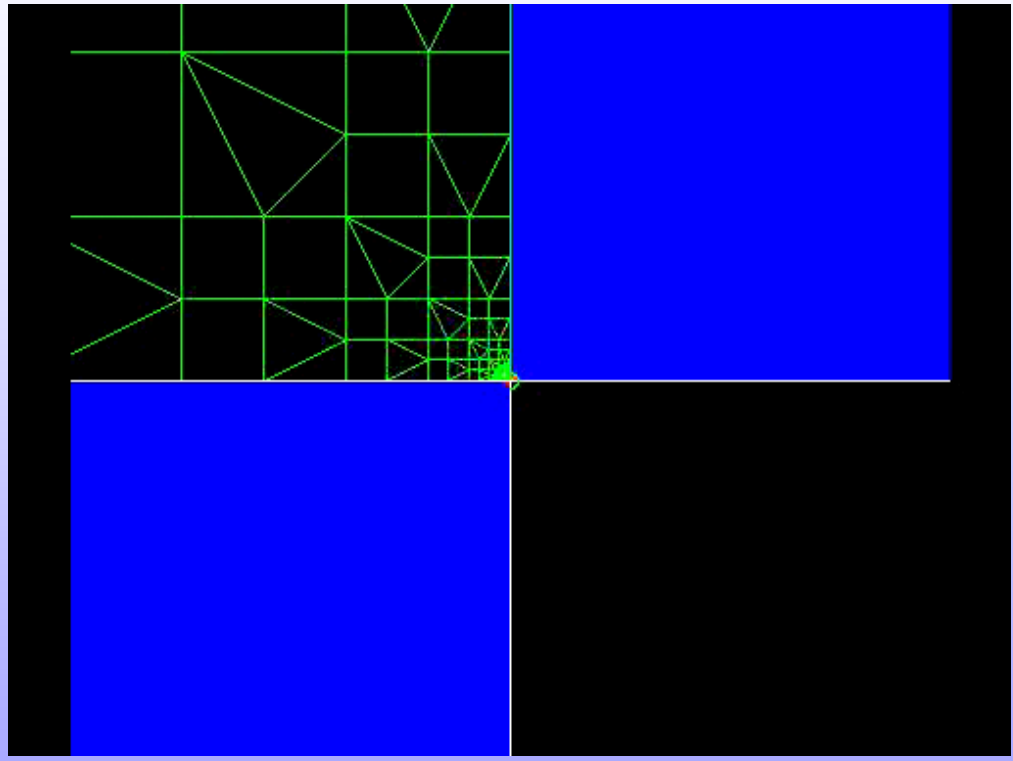
Phase field models

- **Coarse-grain spatial density to achieve a slowly-varying (on atomic scale) field that smoothly interpolates between phases**
- **Devise nonlinear PDE for the phase field so that it matches the Stefan problem for solidification**



Example: dendritic growth using phase field models



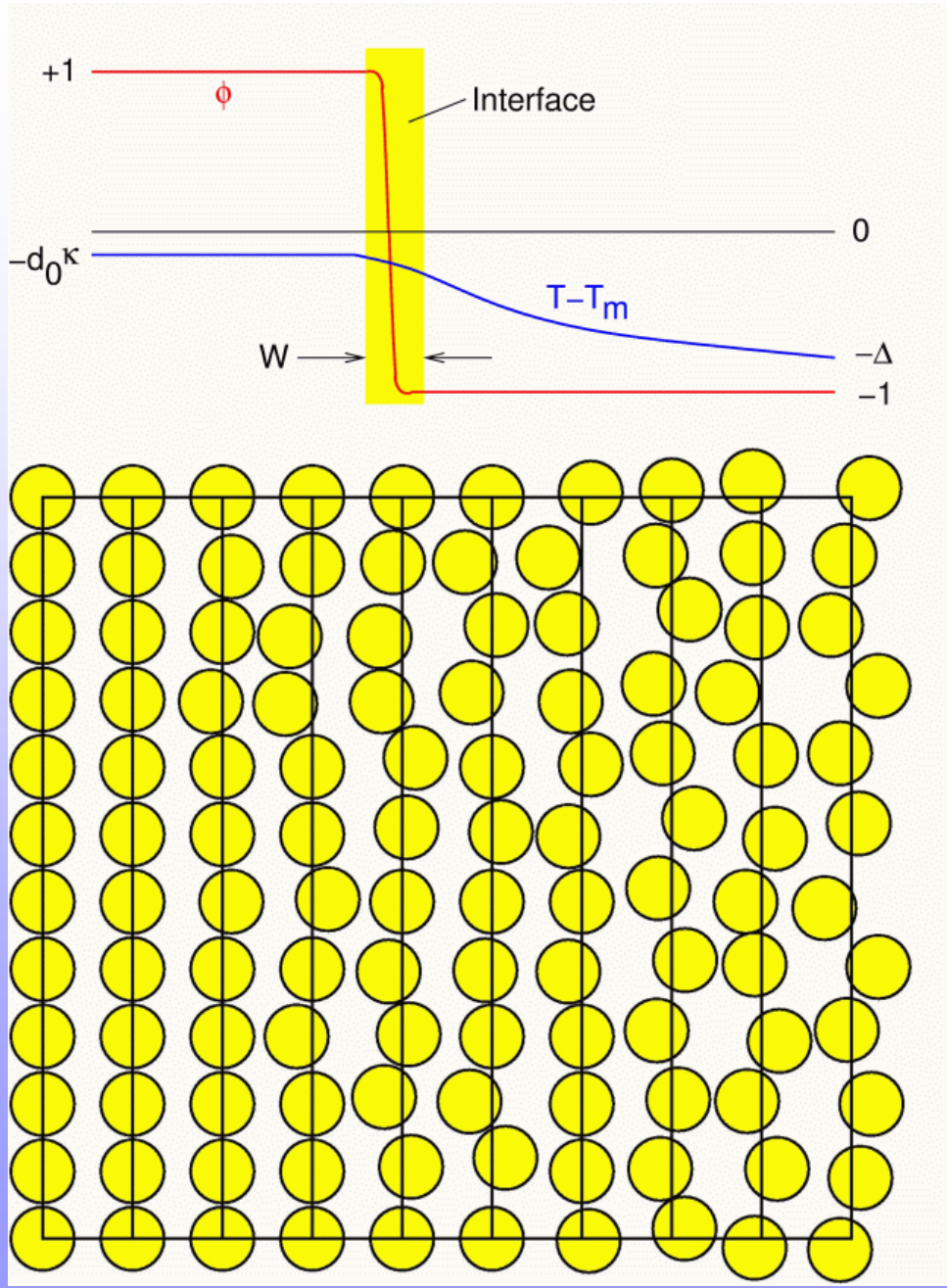


More mesh points in regions where phase field is varying rapidly

Computational load ~ $O(N^{2/3})$

Phase field models

- **Problem with phase field models is that they do not preserve crystallographic orientation**
  - Merging of domains is incorrectly captured
  - Modeling of complex material microstructure impossible



Phase field crystal

- **Phase field crystal (Elder et al. 2002, 2004)**
  - Dynamical variable has periodic solutions = atomic density

$$\mathcal{F} = \int [\rho \left(\alpha \Delta T + \lambda \left(q_o^2 + \nabla^2 \right)^2 \right) \rho/2 + u\rho^4/4] d^3x$$

Density

Periodic solutions

$$\frac{\partial \rho}{\partial t} = \Gamma \nabla^2 \left(\frac{\delta \mathcal{F}}{\delta \rho} \right) + \eta$$

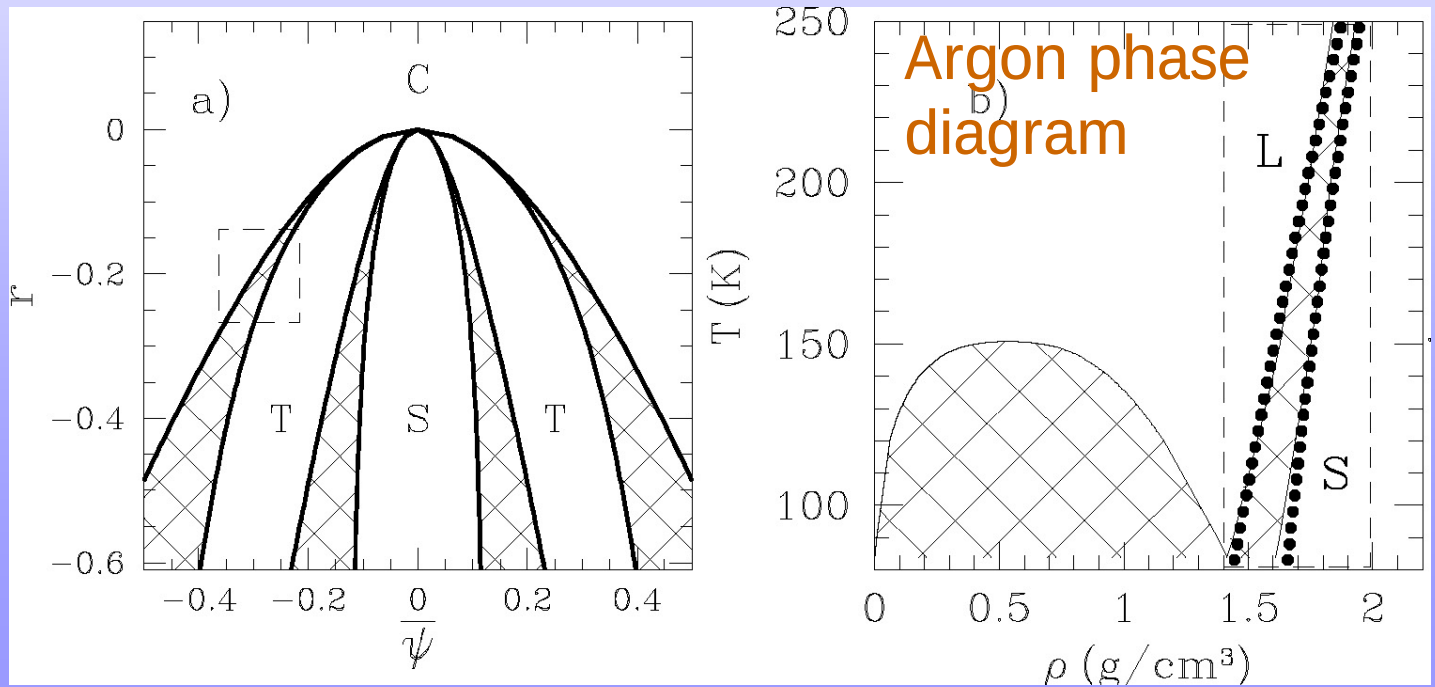
Conservation law

Phase field crystal

$$\partial\psi/\partial t = \nabla^2\left(\omega\,\psi + \psi^3\right) + \zeta$$

$$\omega \equiv r + (1+\nabla^2)^2$$

- **Constant solutions or periodic**
  - d=2 triangular lattice or stripes (smectic phase)



Phase field crystal

- **Properties**
  - Preserves crystallographic information
  - Representation of free boundaries
  - Captures defects
- **Incorporates elasticity natively!**

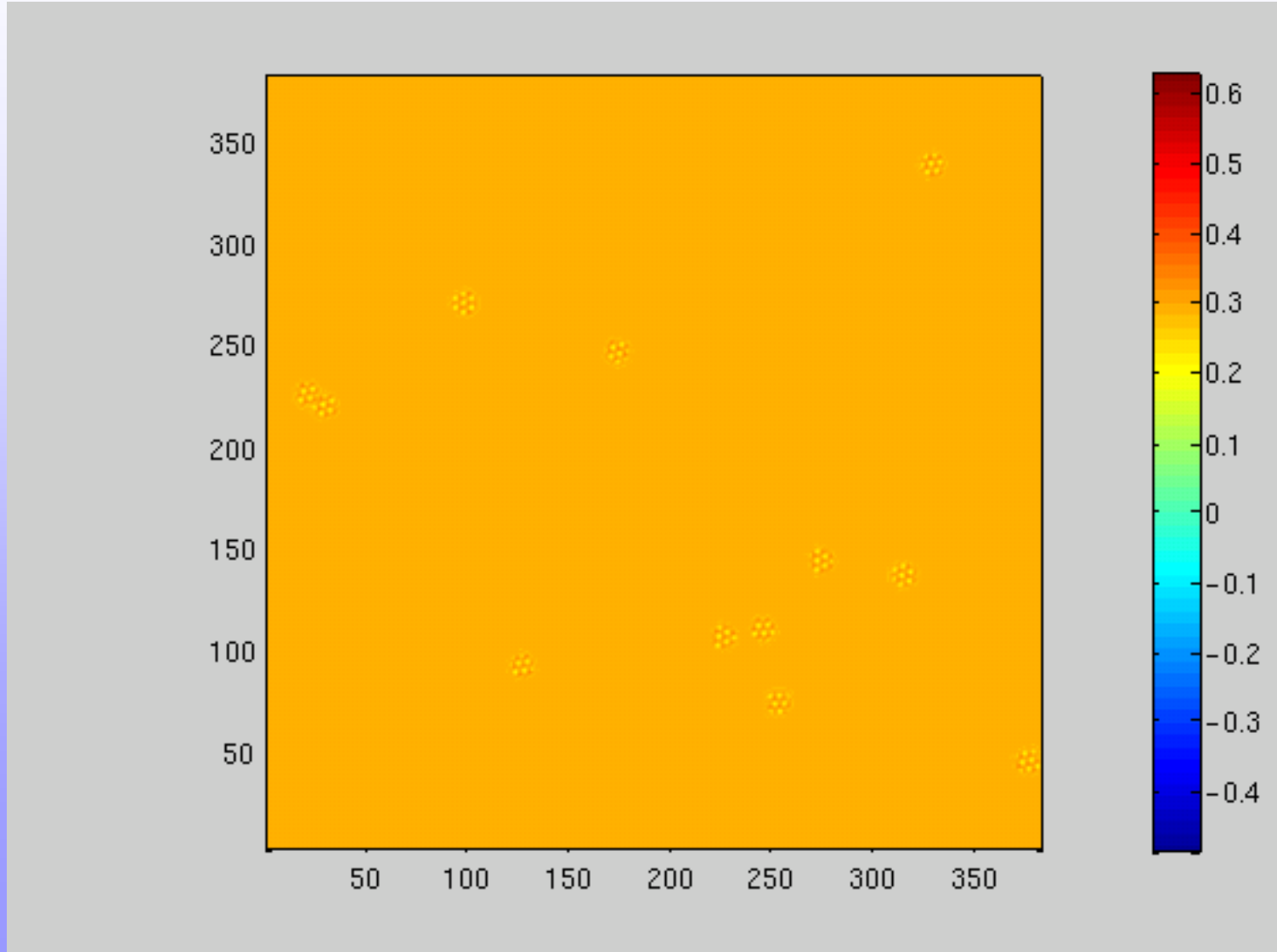
$$\psi = A_o \sin(2\pi x/a)$$

$$F/a - F_{eq}/a = (K/2)(a - a_{eq})^2 + \cdots$$

$$K \equiv -8(r + 3\bar{\psi}^2)/3$$

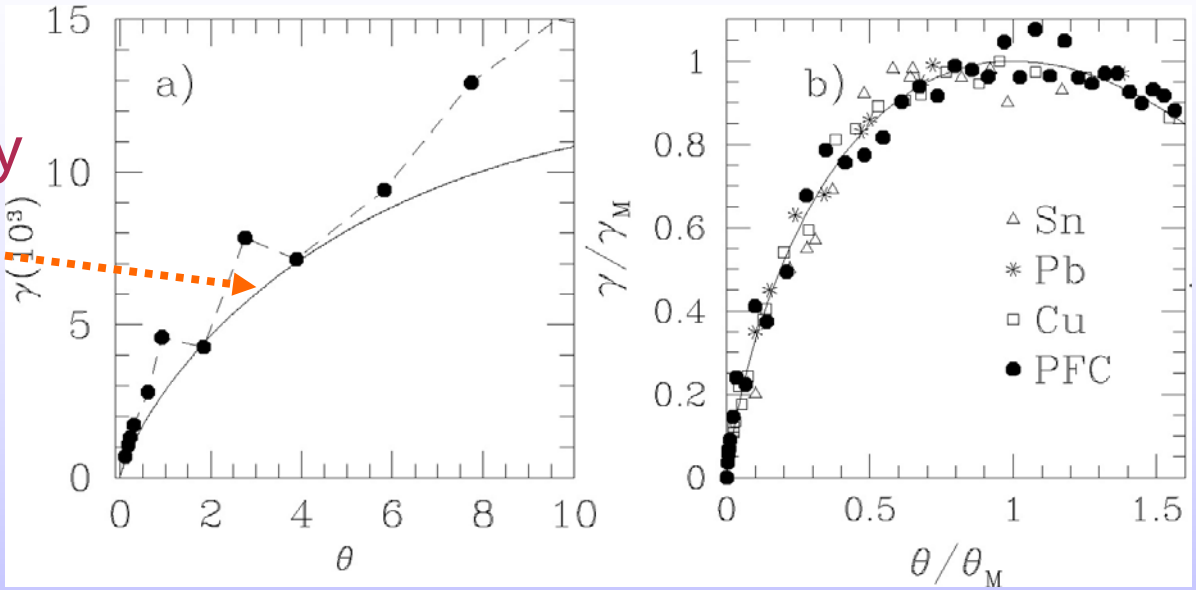
Phase field crystal

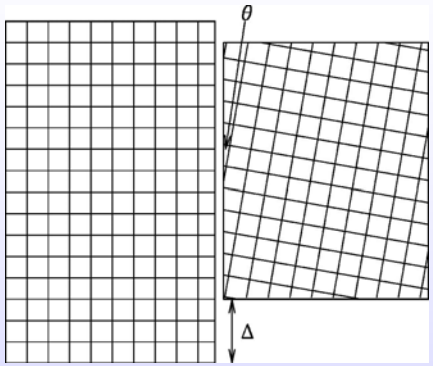
- **Dynamical solutions properly model grain growth**



Phase field crystal describes dislocations

Read-Shockley equation



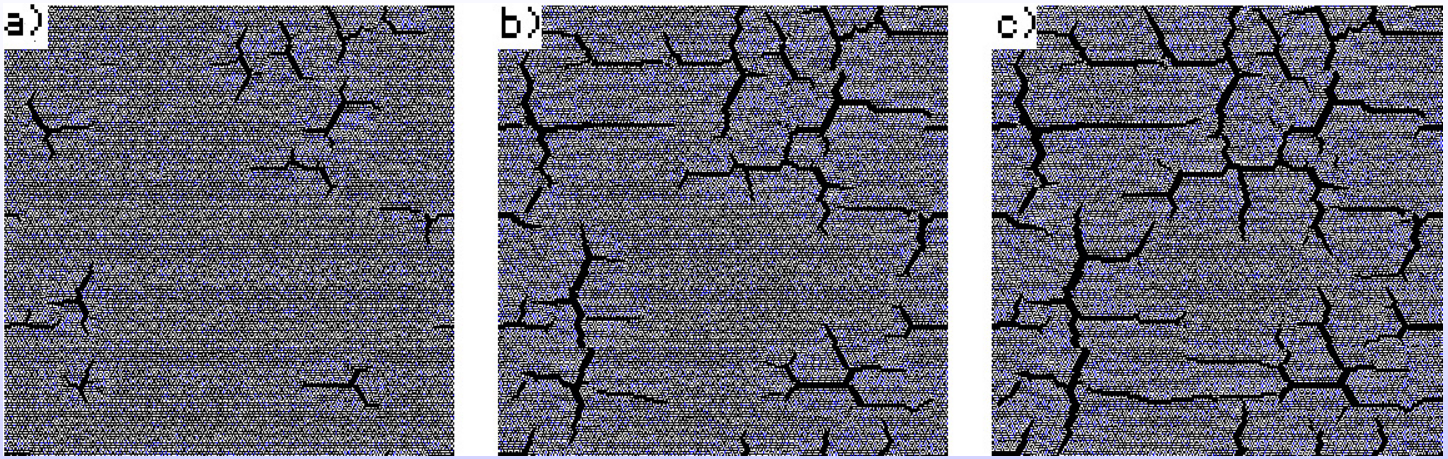


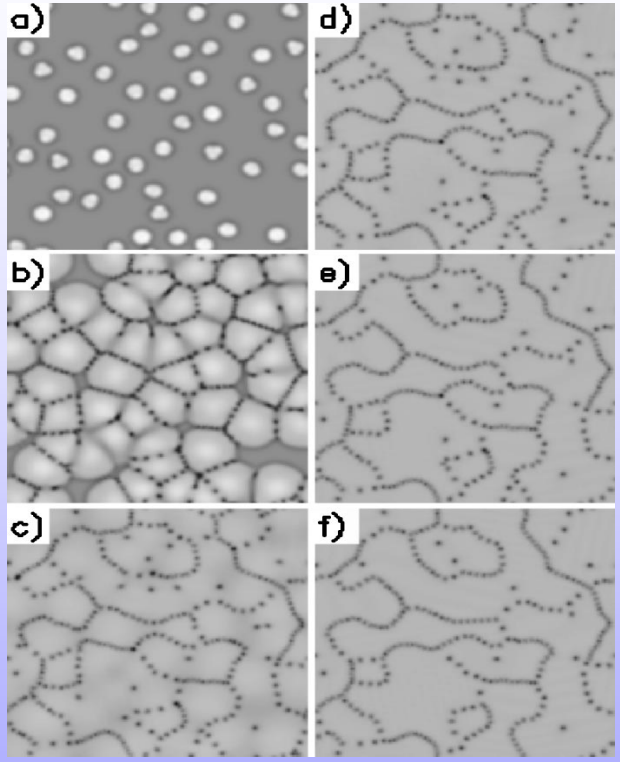
- **Dimensionless grain boundary energy as a function of angle**
- **Grain boundary energy normalised by maximum value compared with expt. data**

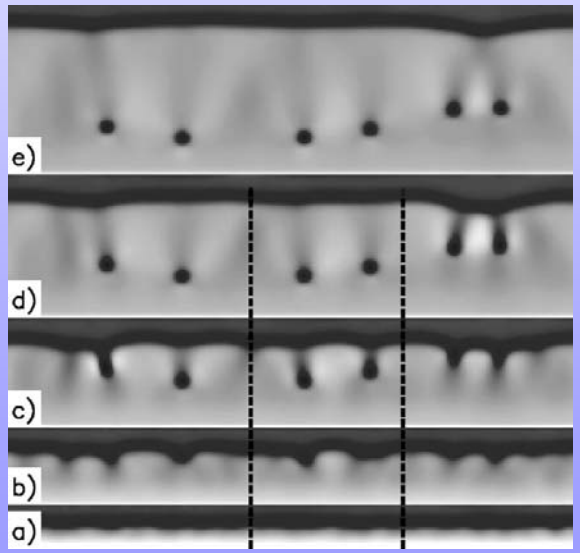
$$\gamma = (aY_2)/(8\pi)\,\theta\,[3/2 - \ln(2\pi\theta)]$$

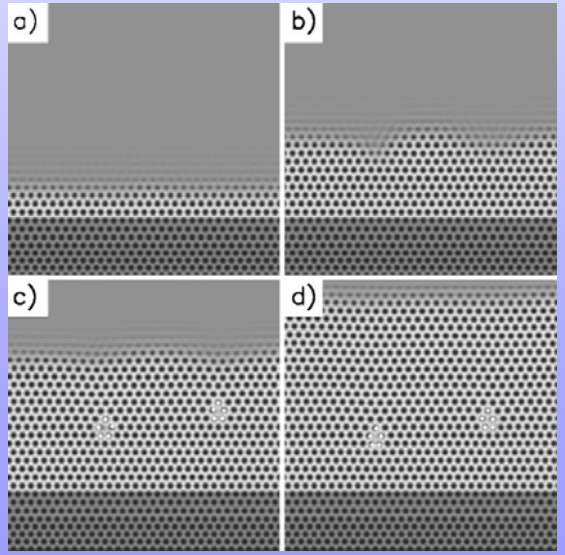
$$Y_2 = (4\sqrt{2}/15(\bar{\psi} + \sqrt{-15r - 36\bar{\psi}^2}))^2$$

PFC: Picture Gallery



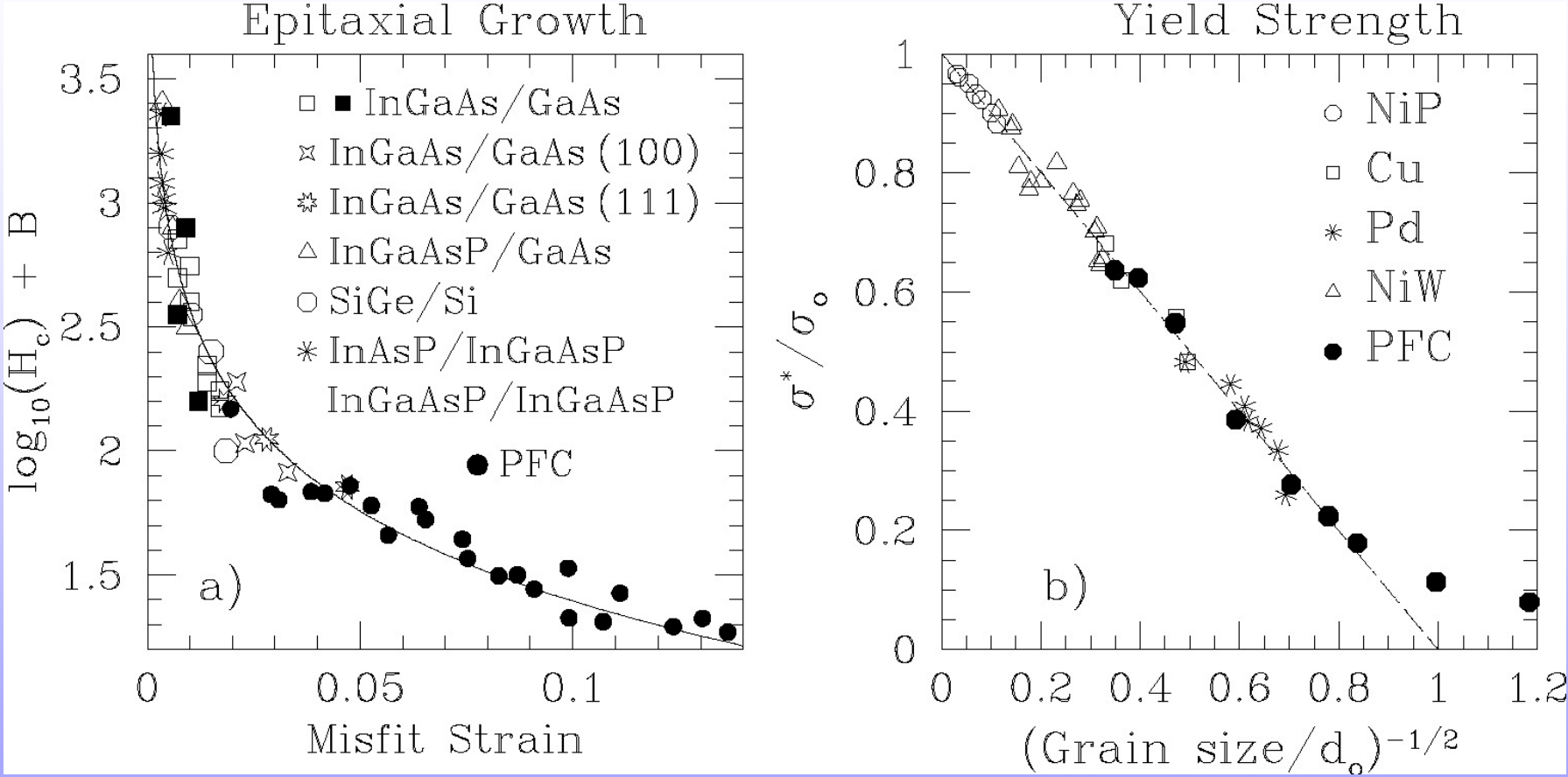






K. Elder and M. Grant, Modeling elastic and plastic deformation in nonequilibrium processing using phase field crystals, *Phys. Rev. E* **70**, 051605:1-18 (2004)

PFC: results gallery



Critical height for dislocation nucleation in strained epitaxial films

Yield stress of polycrystalline solid as a function of grain size

- **Quantitative scaling results in complex materials properties**

Phase field crystal

- **Comparison with molecular dynamics**
  - Fundamental time scale is diffusion time ~ DQ^2

$$D = 3\bar{\psi} + r + 1 + 9A_t^2/8$$

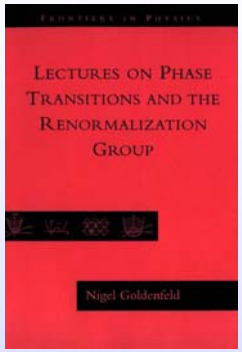
  - 1 diffusion time ~ thousand time steps
  - For Gold, diffusion time ~ 0.26 ms, 33 μs, 5 μs at T=800, 900, 1020 ^{o}C
  - Molecular dynamics: time step ~ 1 fs
  - **Conclusion: PFC ~ 10^6 – 10^9 times faster than MD!**

Phase field crystal

- **Big problem with the phase field crystal**
  - Modeling at the atomic scale means that it is computationally intensive
    - **Just like molecular dynamics**
  - Curse of dimensionality: $N \sim L^d$
- **Question**
  - How can we do multi-resolution analysis on the phase field crystal?
    - **Unlike the phase field model, do not have a simple kink structure describing interfaces**
- **Answer**
  - Use the renormalization group ...

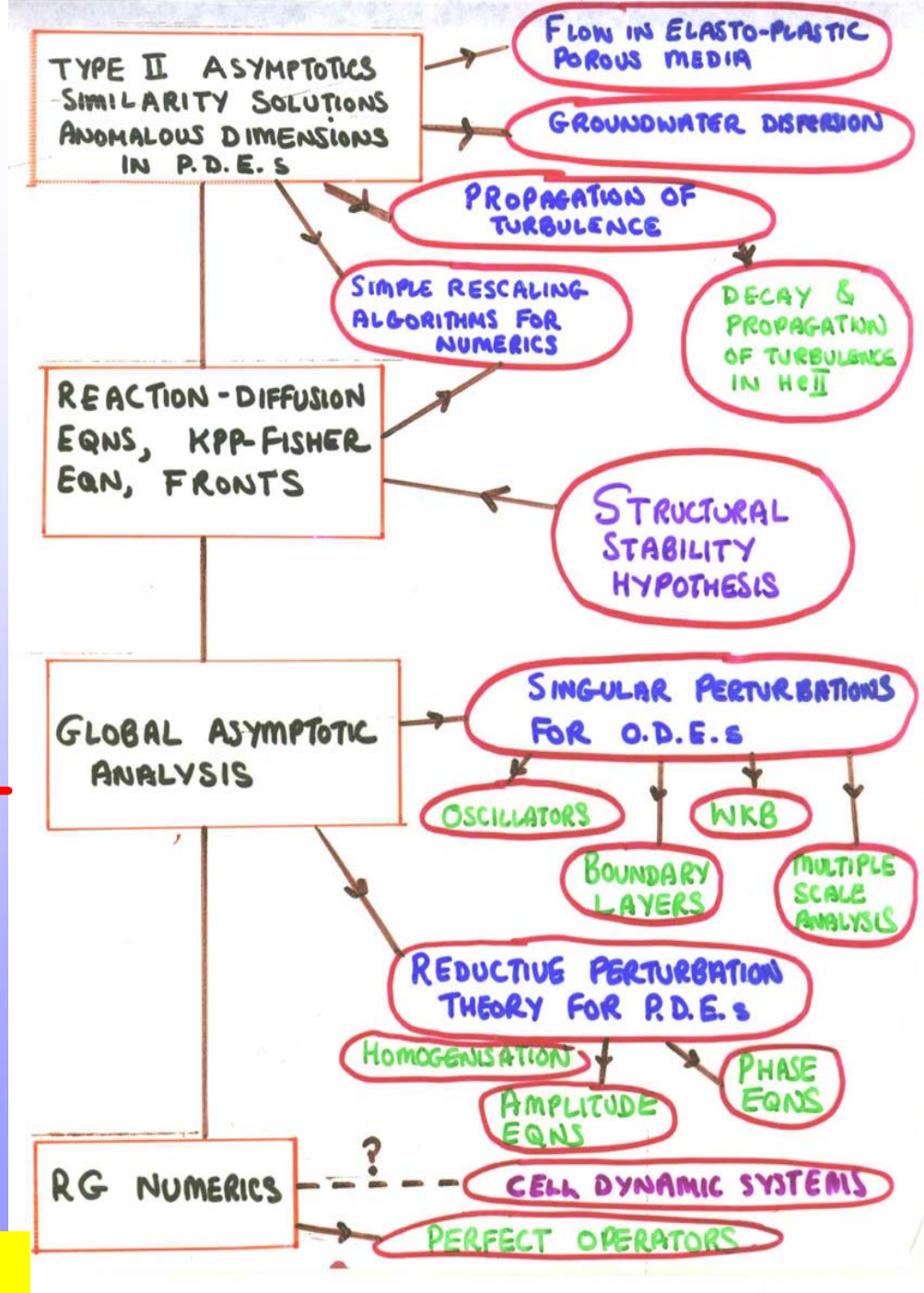
Renormalization group for PDEs

- Systematic program to extract universal, i.e. asymptotic features from PDEs



L. Chen, N. Goldenfeld, Y. Oono. Renormalization group theory for global asymptotic analysis. *Phys. Rev. Lett.* **73**, 1311-1315 (1994).

L. Chen, N. Goldenfeld and Y. Oono. The renormalization group and singular perturbations: multiple-scales, boundary layers and reductive perturbation theory. *Phys. Rev. E* **54**, 376-394 (1996).



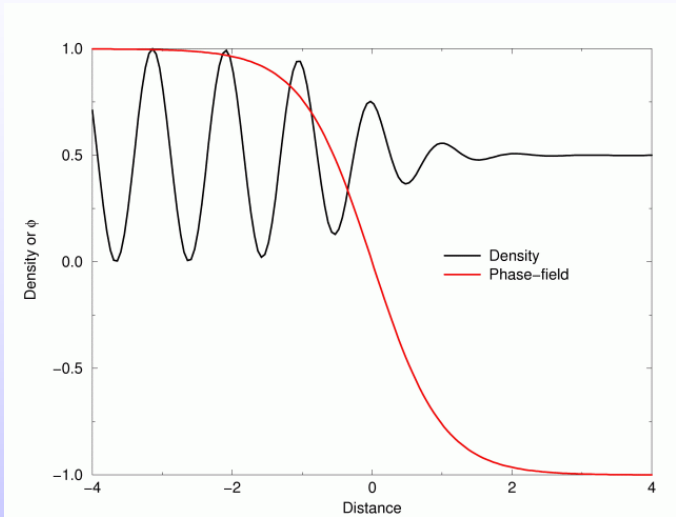
http://guava.physics.uiuc.edu/~nigel/articles/RG

How can RG help?

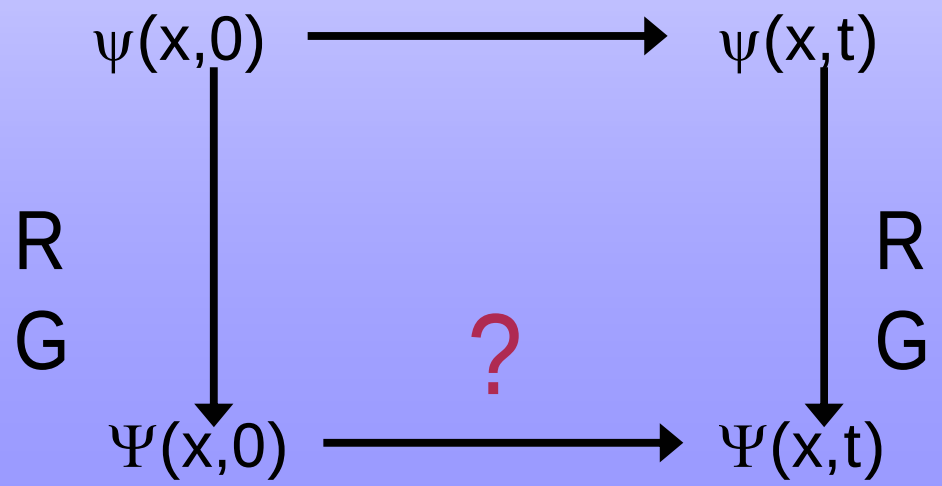
- On scales > lattice periodicity, amplitude and phase of density slowly varying, except near defects

- Derive dynamical equation satisfied by coarse-grained amplitude and phase
  - **Analogue of Newell-Whitehead and Cross-Newell equations in Rayleigh-Benard convection**
  - **Need rotational covariant form of the equations**
    - **Proposed by Gunaratne et al. (1994)**
    - **RG derivation by Graham (1996), Nozaki et al (2000).**

- **Amplitude and phase gradient vary slowly except near defects => can solve with adaptive mesh refinement!**
  - Then reconstruct the density



PFC



Example: Swift-Hohenberg

- **Swift-Hohenberg equation is a simplified model of convection in absence of mean flow**
  - Rolls

$$\partial_t \psi = [\epsilon - (1 + \nabla^2)^2]\psi - \psi^3$$

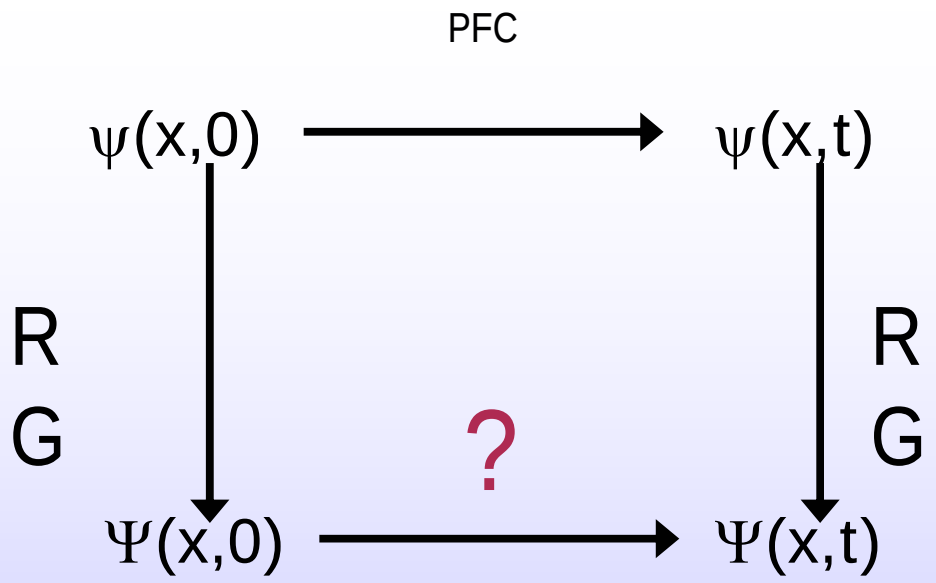
- **Rotationally-covariant complex amplitude equation near onset**

$$\partial_t A = \left(-r - 3|A|^2\right) A + 4k_0^2 \mathcal{L}^2 A$$

$$\mathcal{L} = \left(\hat{\mathsf{k}} \cdot \nabla - \frac{i}{2k_0}\nabla^2\right)$$

Example: Swift-Hohenberg

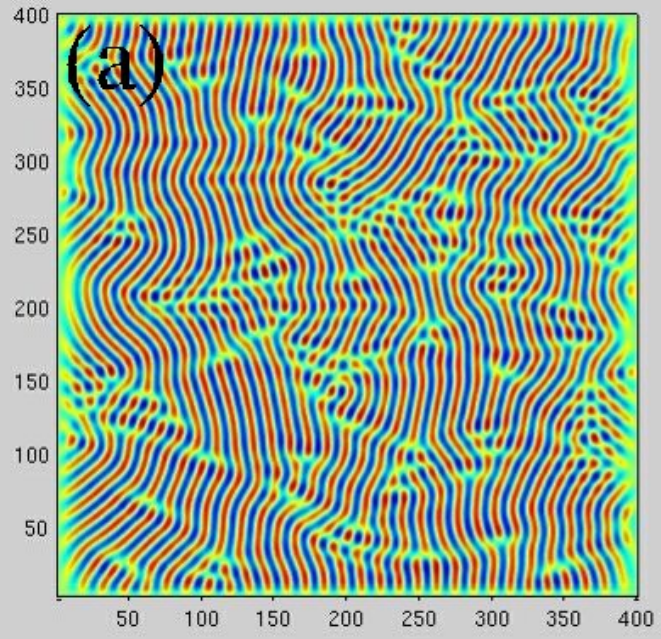
- **Solve SH by finite differences**
- **Solve RG-SH by finite differences**
- **Compare**

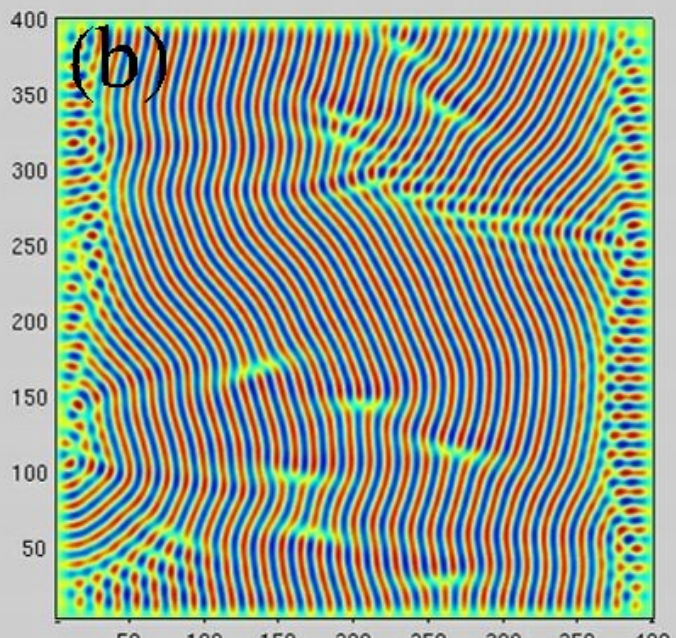


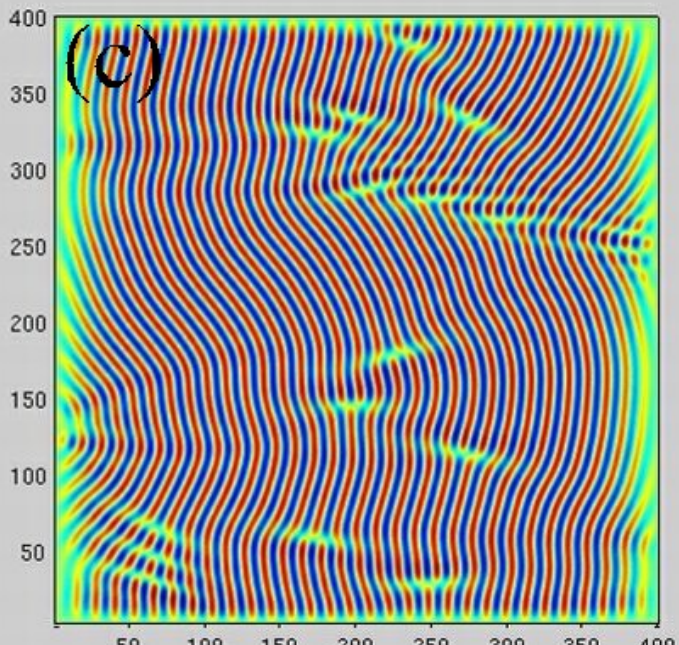
Initial condition

SH time evolution

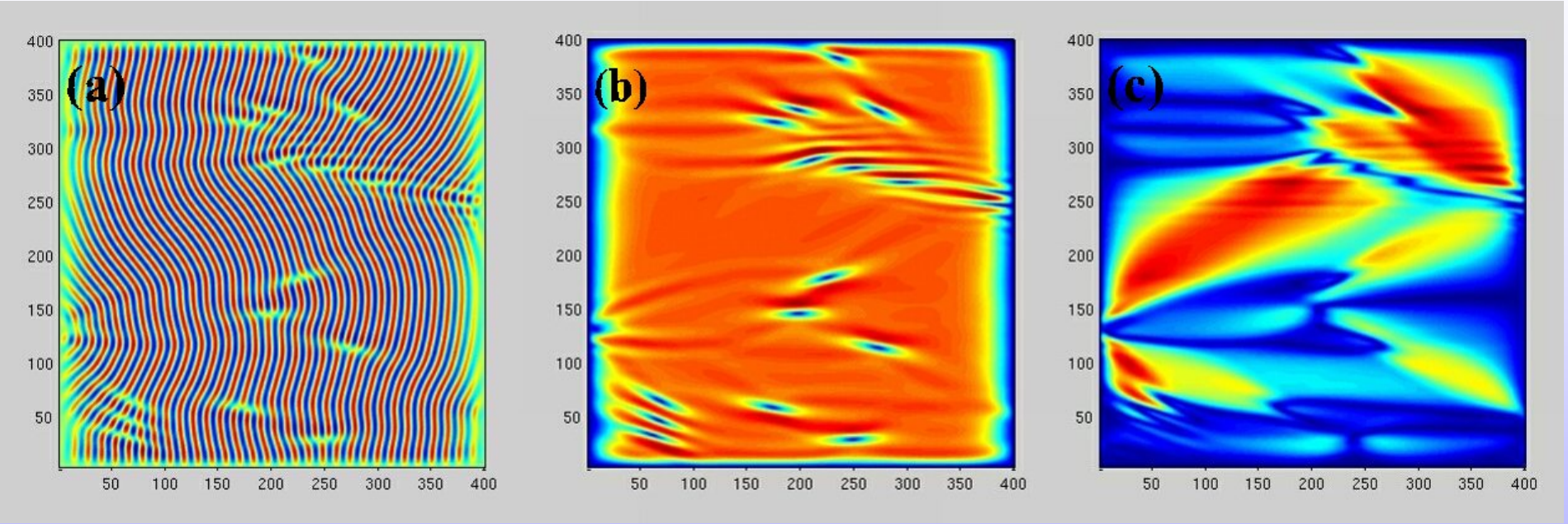
RG-SH time evolution







Example: Swift-Hohenberg



Order parameter Amplitude Phase

- **The amplitude and phase gradient are slowly varying everywhere, except in the vicinity of grain boundaries, topological defects etc.**
- **Exploit this property to do adaptive mesh refinement**

Phase field crystal

- **There are three density components giving rise to a triangular lattice**

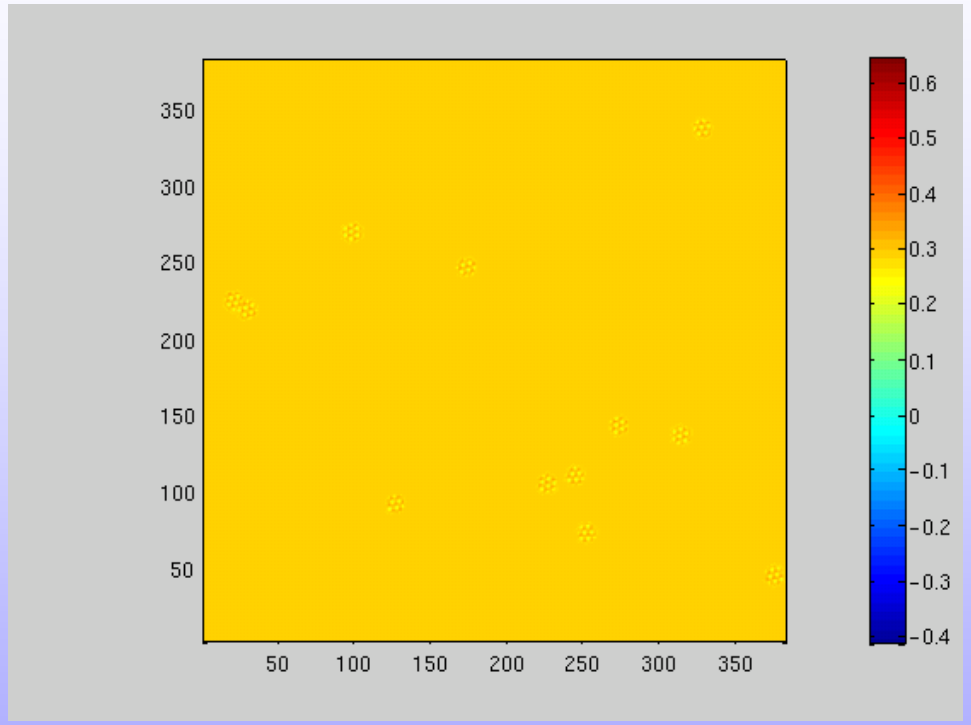
$$\psi(\vec{\mathbf{x}}) = \sum_j A_j(t) \exp(i\vec{\mathbf{k_j}} \cdot \mathbf{x}) + \bar{\psi}$$

- **Corresponding complex amplitude equation is**

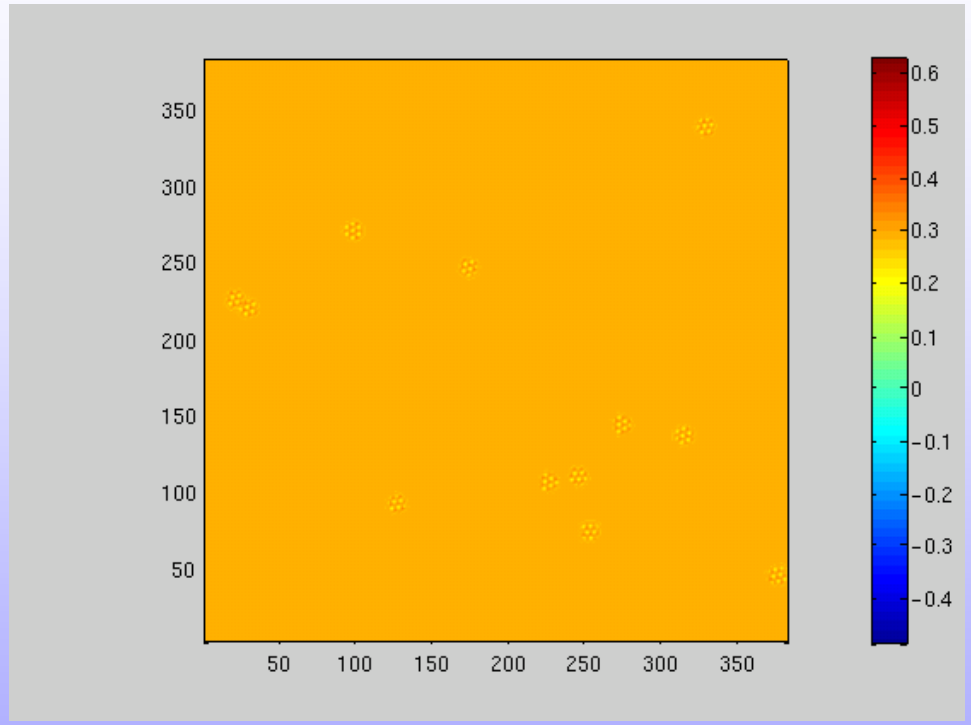
$$\mathcal{L}_j = [1 - \nabla^2 - 2i\mathbf{k}_j \cdot \nabla][\Gamma - (\nabla^2 + 2i\mathbf{k}_j \cdot \nabla)^2] \qquad \Gamma \equiv -(r + 3\bar{\psi}^2)$$

$$\begin{aligned}
\frac{\partial A_1}{\partial t} &= \tilde{\mathcal{L}}_1 A - 3A_1\left(|A_1|^2 + 2|A_2|^2 + 2|A_3|^2\right) - 6\bar{\psi}A_2A_3 \\
\frac{\partial A_2}{\partial t} &= \tilde{\mathcal{L}}_2 A - 3A_2\left(2|A_1|^2 + |A_2|^2 + 2|A_3|^2\right) - 6\bar{\psi}A_1A_3 \\
\frac{\partial A_3}{\partial t} &= \tilde{\mathcal{L}}_3 A - 3A_3\left(2|A_1|^2 + 2|A_2|^2 + |A_3|^2\right) - 6\bar{\psi}A_1A_2
\end{aligned}$$

Phase field crystal



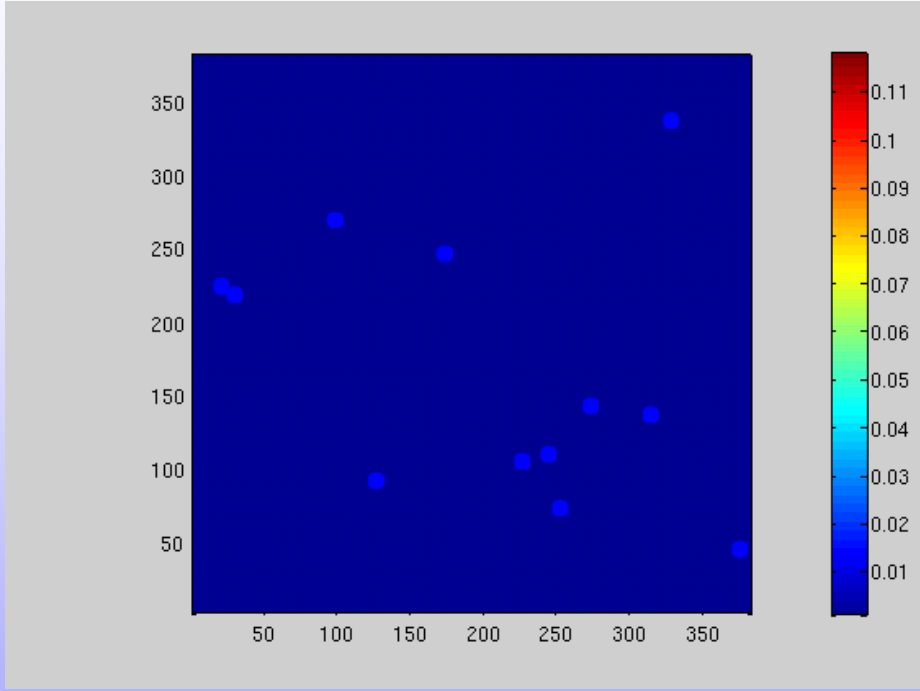
RG solution of PFC

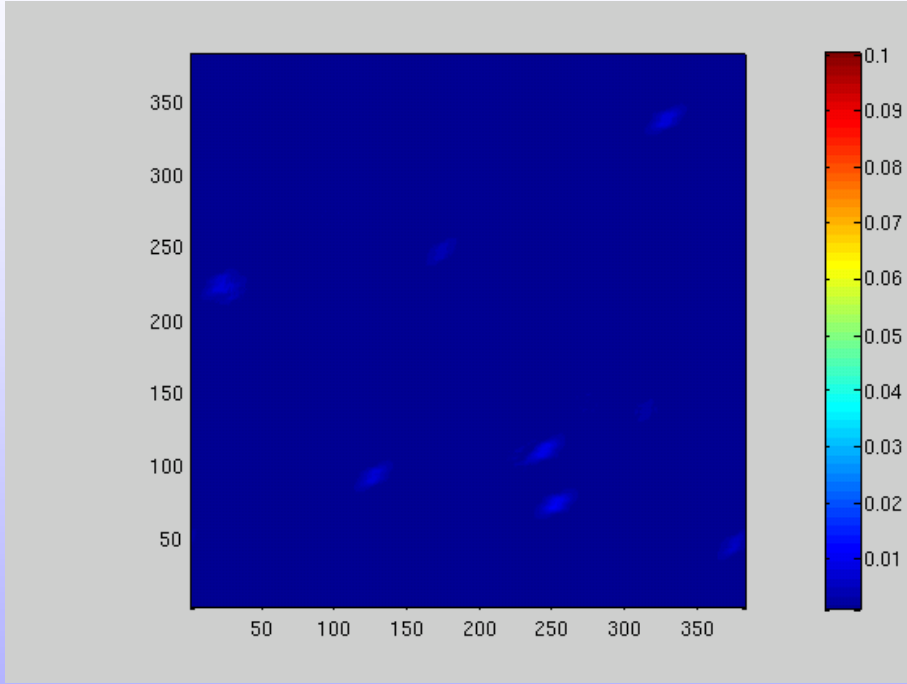


Brute force solution of PFC

Good agreement between solution reconstructed from RG and the actual solution

Phase field crystal





Amplitude

Phase gradient

- **The amplitude and phase gradient are constant everywhere, except in the vicinity of grain boundaries, topological defects etc.**
- **Exploit this property to do adaptive mesh refinement**

Ongoing work

- **Extensions of PFC model**
  - Taylor PFC to specific materials
    - **Fit correct 2-point correlations, using experimental structure factors**
    - **Fit correct dynamics, using experimentally-measured dynamic structure factor**
  - Multicomponent systems
  - Coupling to thermal and solute fields
- **Adaptive mesh refinement for RG formulation of the phase field crystal, in amplitude and phase formulation**
- **Extensions to 3D**
- **RG equations far from threshold: regularized version of Cross-Newell/Passot-Newell equations derived (Sasa 1996)**
  - Ill posed, due to enforcing of amplitude=constant.
  - Relaxation of constraint needed near defects
  - Match on to complex amplitude equation near threshold

Conclusions

1. **Phase field crystal models can capture realistic phenomenology of materials**

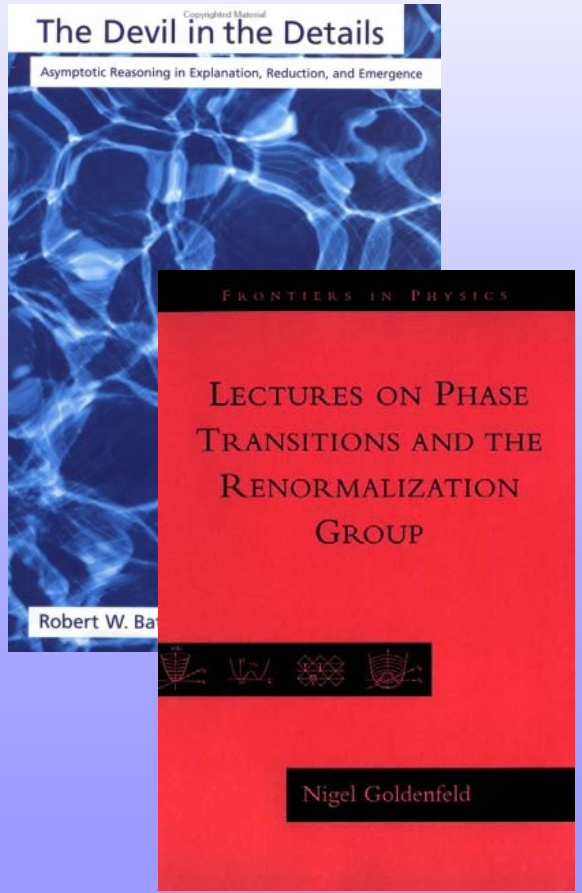
2. **Renormalization group methods, developed for pattern forming instabilities, can be used to derive effective mesoscale equations of motion**

3. **Adaptive mesh refinement can be used to optimize the computational efficiency**

4. **Multiscale modeling of realistic materials processing from the nanoscale is feasible, combining PFC, RG and AMR**

Further reading

All my RG papers can be obtained online
http://guava.physics.uiuc.edu/~nigel/articles/RG



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.