# Derivation and analysis of nonlocal PDEs and Lattice systems from materials science

Peter W. Bates, Michigan State University

Collaborators:
F. Chen, X. Chen, A. Chmaj, P. Fife, X. Ren, X. Wang

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MODELING FROM FIRST PRINCIPLES

NONLOCAL DIFFUSION –
DISCRETE AND CONTINUUM EQUATIONS

CALCULUS OF VARIATIONS

INFINITE-DIMENSIONAL VECTOR CALCULUS

PATTERNS AND WAVES

WHY DO PATTERNS FORM?

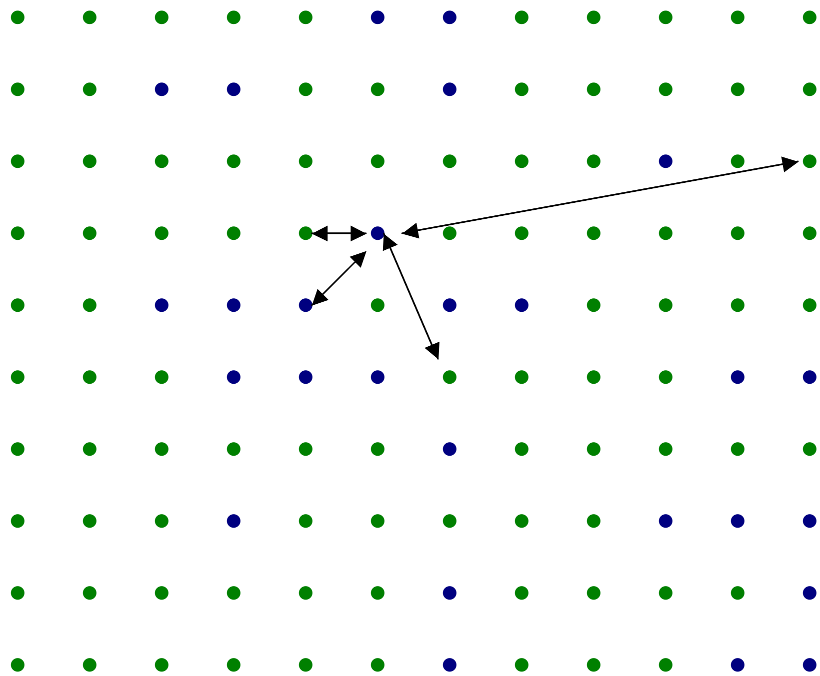

**FIGURE 1, LATTICE**

Spin system $u(r) \in \{\pm 1\}$ on a lattice $\Lambda$.

Thermal fluctuations cause random flipping, so use expected values $u(r) \in [-1, 1]$.

This distribution, $u$, of expected values will evolve with time, even without an externally applied field. Why is that?

## INTERACTION BETWEEN LATTICE SITES

## TENDENCY TO DISSIPATE ENERGY

What is energy?

"We shall obtain a complete solution of the problem ... if we can express *the free energy* at each point as a function of the density at that point and of the differences of density in the neighboring phases, out to a distance limited by the range over which the molecular forces act"
*J.D. van der Waals, 1893*

FREE ENERGY, $E(u)$ of a spatial state $u$ is

$$E = H - ST$$

where $H$ is potential energy of interaction, $S$ is entropy and $T$ is absolute temperature.

$$H(u) = -\frac{1}{2} \sum_{r,s \in \Lambda} j(r-s) u(r) u(s),$$

$j(r)$ is the (possibly anisotropic) interaction energy coefficient associated with displacement $r$.

$$S(u) =$$

$$-K \sum_{r \in \Lambda} [(1-u(r)) ln(1-u(r)) + (1+u(r)) ln(1+u(r))]$$

and so

$$E(u) = \frac{1}{4} \sum_{r,s \in \Lambda} j(r-s)[u(r)-u(s)]^2 +$$

$$\sum_{r \in \Lambda} \{TK[(1-u) ln(1-u) + (1+u) ln(1+u)] - \frac{\bar{j}}{2} u^2\}.$$

What is the minimizer?

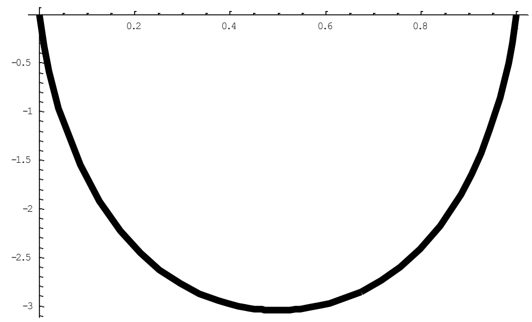


**FIGURE 2A, $T>T_c$**

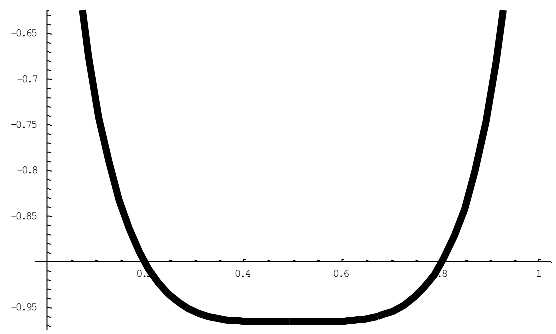


**FIGURE 2B, $T=T_c$**

At subcritical temp. the total free energy of a spin field $\{u(r) \in \mathbb{R} : r \in \Lambda\}$ has the form

$$E(u) = \frac{1}{4} \sum_{r,s \in \Lambda} j(r-s)(u(r)-u(s))^2 + \sum_{r \in \Lambda} W(u(r)), \tag{1}$$

where $W$ is a double-well potential having minima at the values $u = \pm\alpha$, say.

With an external field, the wells would not be of equal depth or symmetric about 0.

Scale and take $\alpha = 1$.

One may also consider a continuum version of this, in which case the free energy is

$$E(u) = \frac{1}{4} \int_{\mathbb{R}^{2n}} j(x-y)(u(x)-u(y))^2 dxdy + \int_{\mathbb{R}^n} W(u(x))dx. \tag{2}$$

Evolution?

SECOND LAW OF THERMODYNAMICS: REDUCE FREE ENERGY—EFFICIENTLY

$$\frac{\partial u}{\partial t} = -\ \mathrm{grad} E(u). \quad (*)$$

How do we interpret this? (Calc of Var.)
grad $E(u)$ is a linear functional on $X$ defined by

$$< \mathrm{grad}\ E(u), v >= \frac{d}{dh} E(u + hv)|_{h=0}$$

where $<, >$ is the duality pairing.

If $X = L^2$ then (*) becomes

$$\frac{\partial u}{\partial t} = j * u - ku - W'(u) \quad \text{(NAC)}$$

where $k = \int j$ and $*$ is convolution.

In the discrete case $j * u(r) = \sum_{s \in \Lambda} j(s) u(r - s)$.

Recall the first term in the free energy

$$\frac{1}{4}\iint j(x-y)(u(x)-u(y))^2 dxdy,$$

and make the approximation (good (?) for short-range interaction)

$$u(x)-u(y) \sim \nabla u(x)\cdot(x-y).$$

If $j$ is isotropic then this part of the energy can be written

$$\frac{\varepsilon^2}{2}\int |\nabla u(x)|^2 dx,$$

where $\varepsilon^2 = \int j(y) y_i^2 dy/2$.

The $L^2$ gradient flow is the Allen-Cahn equation:

$$\frac{\partial u}{\partial t} = \varepsilon^2 \Delta u - W'(u) \quad \text{in } \Omega \quad \text{(AC)}$$

with the natural boundary conditions

$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega.$$

How should (planar) interfaces move?

Traveling waves: $u(x,t) = u(x \cdot a + ct)$

where $a$ is a unit vector of direction and $c$ is the (unknown) speed.

Let $f \equiv W'$ e.g. $f(u) = (u - q)(u^2 - 1)$, and for this point we may as well rescale space so that $\epsilon = 1$.

There exists a unique speed and (monotone) wave-form $(c_0, u_0)$ satisfying

$$u'' - cu' - f(u) = 0, \;\; u(\pm\infty) = \pm 1, \;\; u(0) = 0.$$

What about TW's for (NAC)?
Write $J = \int_{a^\perp} j$ and take $\int J = 1$.

$$J * u - u - cu' - f(u) = 0, \;\; u(\pm\infty) = \pm 1, \;\; u(0) = 0.$$

This is truly an $\infty-$ dim'l (differential?) eqt.
Idea: Deform the second order ODE into this:

$$\lambda(J * u - u) + (1 - \lambda)u'' - cu' - f(u) = 0,$$

$u(\pm\infty) = \pm 1, \;\; u(0) = 0, \;\; \lambda \in [0, 1]$.

$$G(u, c, \lambda) \equiv (\lambda(J * u - u) + (1 - \lambda)u'' - cu' - f(u), u(0))$$

defined from $C^2 \times \mathbb{R} \times [0, 1]$ into $C \times \mathbb{R}$.

Use the I F T at $(u_0, c_0, 0)$ and the fact that 0 is an algebraically simple eigenvalue of $\phi \to \phi'' - c_0\phi' - f'(u_0)\phi$ with positive eigenfunction $u_0'$. This gets us started.

If $J \geq 0$ then, because $L\phi \equiv \phi - J * \phi$ is a positive operator, we can continue for all $\lambda \in [0, 1)$. Take the weak limit to $\lambda = 1$, getting $(c_1, u_1)$, then regularity using monotonicity.

Interesting features:

- $c_1$ may be 0 even when the depths of the wells of $W$ are not equal.
- $u_1$ may be discontinuous.

## II. WAVES ON A LATTICE

We have previously studied the Nonlocal Allen-Cahn equation on a continuum:

$$\frac{\partial u}{\partial t} = J * u - ku - W'(u) \quad \text{(NAC)}$$

Recall the last result:

**Theorem 1** *Let $J \in W^{1,1}$ be even with unit integral and let $f$ be a smooth bistable function with zeros at $\pm 1$ and an intermediate point $a$. There exists a unique solution $(c, u)$, with $u$ monotone and $u(0) = 0$, to*

$$J * u - u - cu' - f(u) = 0. \quad (TW)$$

On the integer lattice, the nonlocal Allen-Cahn equation may be written

$$\dot{u}_n = (J * u)_n - u_n - \mu f(u_n), \; n \in \mathbb{Z}, \quad (DAC)$$

where

$$(J * u)_n \equiv \sum_{i \in \mathbb{Z} \setminus \{0\}} J(i) u_{n-i}$$

and $\mu = \sum_{i \in \mathbb{Z} \setminus \{0\}} J(i)$.

Note that a special case of this equation is the discrete Nagumo equation,

$$\dot{u}_n = \frac{1}{2}(u_{n+1} - 2u_n + u_{n-1}) - \mu f(u_n),$$

studied by J. Keener and others in the context of myelinated nerve axons but is also interesting from a numerical analysis viewpoint.

Again, we seek traveling wave solutions to (DAC), i.e., solutions of the form $u_n(t) = u(n + ct)$ for some speed $c$ and profile $u$.

Change to independent variable $x = n + ct$.
To hide the discrete nature of the problem, write $J_\delta(x) = \sum_{|i|\geq 1} J(i)\delta(x-i)$ so that (DAC) in traveling wave coordinates becomes

$$J_\delta * u - u - cu' - \mu f(u) = 0, \quad (DTW)$$

where $J_\delta * u(x) = \int_{\mathbb{R}} J_\delta(x-y)u(y)dy$.

This traveling wave equation now looks remarkably like (TW) from the last theorem.

(Strange?) IDEA: Approximate the discrete equation by one in a continuum.

Let $\psi \geq 0$ be an even, compactly supported smooth function such that $\int_{\mathbb{R}} \psi(x)dx = 1$. Then $\delta_m(x) \equiv m\psi(mx)$ is a delta sequence, i.e.,

$(\delta_m * \phi)(x) \to \phi(x)$ as $m \to \infty$, for $\phi \in C_0^\infty(\mathbb{R})$. Let

$$J_m(x) \equiv \sum_{1\leq |i| \leq m} \frac{1}{w_m} J(i)\delta_m(x-i),$$

where $w_m \equiv \sum_{1\leq|k|\leq m} J(k)$.

From the main result above,

$$J_m * u - u - cu' - \mu f(u) = 0, \quad (SDTW)$$

has a unique solution $(c_m, u_m)$ with $u_m$ monotone and satisfying $u_m(\pm\infty) = \pm 1$, $u_m(0) = 0$.

Since $-1 \leq u_m \leq 1$ and $u_m$ is monotone, Helley's theorem allows one to take a pointwise convergent subsequence, converging to $u_\delta$, say.

One can easily show that $\{c_m\}$ is also bounded and we may assume that this sequence converges to some $c_\delta$.

However,the singular nature of the infinite sum of delta functions and the lack of control on the first derivatives prevents one from simply passing to the limit in the equation as $m \to \infty$.

Use Fubini's and Lebesgue's theorems with weak solutions.

If $c_\delta \neq 0$ then $u_\delta \in W^{1,1}$ and a bootstrapping argument shows that $u_\delta \in C^{r+1}$ if $f \in C^r$.

If $c_\delta = 0$, then $u_\delta$ need not be continuous and so $J_\delta * u_\delta(n)$ need not equal $\sum_{|i|\geq 1} J(i)u_\delta(n-i)$. However, since $u_\delta$ is monotone, it has at most countably many discontinuities and a sequence $u_n$ can be obtained satisfying

$$(J * u)_n - u_n - \mu f(u_n) = 0.$$

Using monotonicity of the approximating solutions $u_m$ one can show that our solution has the correct limits at $\pm\infty$.

Note that, if $g(u) = u + \mu f(u)$ has a null truncation, then $c_m = 0$ for all $m$ and hence $c_\delta = 0$.

However, in this case the converse is not true.
More pinning is possible in the discrete case than in the continuum.

## III PATTERNS

An important result obtained in the late 70's independently by Casten-Holland and Matano: Let $\Omega$ be a smooth convex domain and consider the nonlinear parabolic equation (the Allen-Cahn equation is an example) :

$$\frac{\partial u}{\partial t} = D\Delta u - f(u) \quad \text{in } \Omega \quad \text{(NPDE)}$$

with the Neumann boundary condition

$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega.$$

**Theorem 2** *If $u$ is a* **stable** *solution to (NPDE), then it is constant $u(x) \equiv C$ with $f(C) = 0$.*

We consider the evolution equation

$$\frac{\partial u}{\partial t} = D(J * u - u) - f(u) \quad \text{(NAC)}$$

where $D > 0$ (from the last part $D = 1/\mu$).

Let $M$ be a measurable set with complement $M^c$. Let $\alpha^- < 0$ be the local max of $f$ and $\alpha^+ > 0$ be the local min.

**Theorem 3** *For $D > 0$ sufficiently small there exists a unique stationary solution $\hat{u}$ to (NAC), such that*

$$\hat{u}(x) \begin{cases} \geq \alpha^+ & \text{for } x \in M, \\ \leq \alpha^- & \text{for } x \in M^c. \end{cases}$$

*Moreover, $\hat{u}$ is $C^0$ on $M$ and $M^c$, $C^2$ on $\operatorname{int}(M)$ and $\operatorname{int}(M^c)$ and (locally) asymptotically stable in the $L^\infty(\mathbb{R}^n)$ norm.*

MUCHAS GRACIAS