Discrete-to-Continuum Variational Methods

Andrea Braides (Roma *Tor Vergata*)

Tullio Levi Civita Lectures
Rome, October 12, 2015

An international connection

Connected results on variational methods by different research groups:

• (Italy/Norway) Alicandro, Braides, Gelli, Piatnitski, Solci, Scilla, Kreutz, Defranceschi, Vitali, Vallocchia, etc.

• (France) Le Bris, Lions, Truskinovsky, Blanc, Legoll, etc.

• (Germany/UK) Cicalese, Friesecke, Solombrino, Ruf, Theil, Ball, Schmidt, Friedrichs, Schlömerkemper, Ortner, etc.

• (US/China) E, Ortiz, Lew, Ming, etc.

+ interaction with related research (Presutti, Mielke, S. Müller, Kotecky, Luckhaus, Conti, Garroni, Peletier, Stefanelli, . . .)

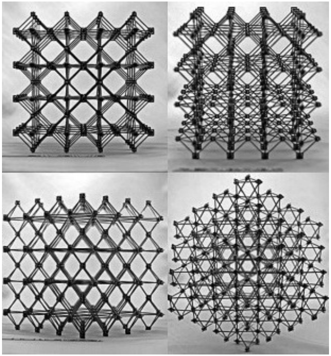
Motivations

Goal: develop methods for the study of interactions between many nodes of a network system.

Such systems may have different nature and field of application:
- numerical schemes
- computer vision models
- atomistic modelling
- design of reticular structure
- complex chemical interactions
- traffic flows
- biological systems

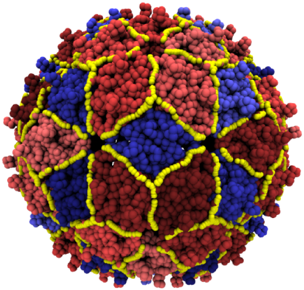
etc.

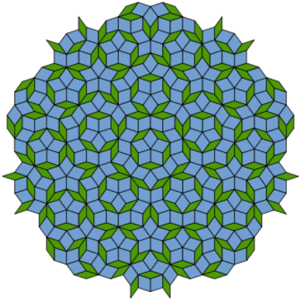
Examples: design of lattice structures



(K. Cheung, MIT)

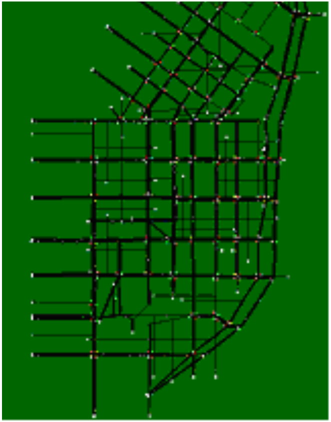
study of optimality properties of viruses





(Twarock et al.)

control of traffic flow on networks



(Daganzo)

Common general features

- **Underlying lattice reference** $\mathcal{L}$
This hypothesis can be a geometric design constraint (as in the design of networks), or justified by physical assumptions (as for crystalline solids), etc.

- **Variational setting**
We suppose that the systems are driven by an **energy**
Simplest energy: **pair interactions**
$u = \{u_i\}$ parameter defined on the nodes i of the lattice $\mathcal{L}$

$$E(u) = \sum_{i,j \in \mathcal{L}} \phi_{ij}(u_i, u_j)$$

Often: $u_i \in \mathbb{R}^m$ and $\phi_{ij}(u_i, u_j) = \phi_{ij}(u_i - u_j)$

Discrete-to-continuum analysis

Objective: description of the behaviour of **large systems** driven by E with a **continuum theory** characterized by some **continuum energy** $E_{\rm cont}$

- Introduction of a **scale parameter** $\varepsilon \to 0$
- Definition of a **scaled energy** $E_\varepsilon(u^\varepsilon) = \sum_{ij} \phi^\varepsilon_{ij}(u^\varepsilon_i - u^\varepsilon_j)$
- Definition of a **continuous limit parameter** u
  (and of a discrete-to-continuum convergence $u^\varepsilon \to u$)
- Definition of an **effective continuous energy** $E_{\rm cont}$.

The requirement for such energy is that: "**solutions to problems related to E_ε are close to solutions related to $E_{\rm cont}$**"

Major issues: choice of the *energy scalings defining* ϕ^ε_{ij}, and of the definiton of the *convergence* $u^\varepsilon \to u$

A multi-scale problem

The type of limit theory depends on the driving "energy level"

Example $\mathcal{L} = \mathbb{Z}^n$; identify each u^ε with (a suitable interpolation of) $U_\varepsilon(i) = u^\varepsilon(i/\varepsilon)$ defined on $\varepsilon\mathbb{Z}^n$

(*statistical scaling*) if $u^\varepsilon \to u \Leftrightarrow U_\varepsilon \to u$ weakly in L^1 then

$$\sum_{ij} \varepsilon^n \phi_{ij}(u_i^\varepsilon - u_j^\varepsilon) \sim \int_\Omega f_{\rm stat}(u)\,dx$$

(*bulk scaling*) if $u^\varepsilon \to u \Leftrightarrow U_\varepsilon \to u$ weakly in $W^{1,1}$ then

$$\sum_{ij} \varepsilon^n \phi_{ij}\Big(\frac{u_i^\varepsilon - u_j^\varepsilon}{\varepsilon}\Big) \sim \int_\Omega f_{\rm bulk}(\nabla u)\,dx$$

(*surface scaling*) if $u^\varepsilon \to u \Leftrightarrow U_\varepsilon \to u$ strong in L^1 and $u_i \in K$ finite, then

$$\sum_{ij} \varepsilon^{n-1} \phi_{ij}(u_i^\varepsilon - u_j^\varepsilon) \sim \int_{\partial\{u=k\}} f_{\rm surf}(u^+ - u^-)\,d\mathcal{H}^{n-1}$$

(*vortex scaling* /$n = 2$) if $u^\varepsilon \to \mu \Leftrightarrow$ Jac$(U_\varepsilon) \to \mu$ in the flat norm, then

$$\sum_{ij} \frac{\varepsilon^n}{|\log\varepsilon|} \phi_{ij}\Big(\frac{u_i^\varepsilon - u_j^\varepsilon}{\varepsilon}\Big) \sim \sum_x f_{\rm vortex}(k(x)), \text{ if } \mu = \sum_x k(x)\delta_x$$

(*etc.*)

In general we have a **superposition** of all such descriptions

(B-Truskinovsky)

Main points of the talk

1) **Variational Methods** developed in the last 30 years can be adapted to cover some problems in the passage **discrete-to-continuum**;

2) The **discrete nature** of the problems brings **additional effects** and provide **simpler models and answers**;

3) **New types of problems** can be addressed that differ to the usual continuum ones.

1. Application of

Continuum Variational Methods

to Lattice Problems

A paradigmatic analysis

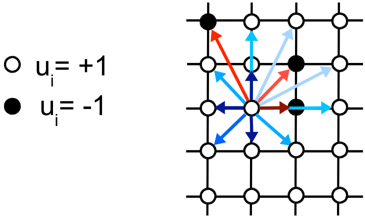
I will illustrate a **simplified situation** that nevertheless allows to **exemplify** the **general methods**:

- **two parameters:** $u_i \in \{+1, -1\}$ (*spin variable*)
- **pair interactions** $\phi_{ij} = \phi_{ij}(u_i - u_j)$
- **surface scaling** $\phi_{ij}^{\varepsilon} \sim \varepsilon^{n-1}$ (n = space dimension)

For the sake of illustration, mainly

- $\mathcal{L} = \mathbb{Z}^2$ (*square lattice*) or $\mathcal{L} = \mathbb{T}$ (*triangular lattice*)

Pictorial representation:



Up to additive/multiplicative constants

$$\phi_{ij}(u_i, u_j) \sim \sigma_{ij}(u_i - u_j)^2$$

We may have **two types of interactions**

ferromagnetic

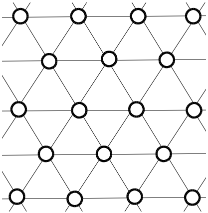
$\sigma_{ij} > 0$

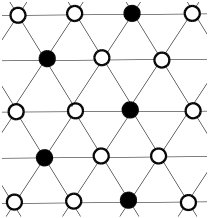
uniform ground states

antiferromagnetic

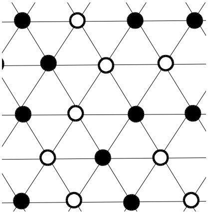
$\sigma_{ij} < 0$

microstructure





ordered

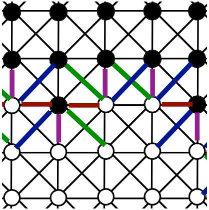


disordered

We first focus on **Ferromagnetic interactions** at the **surface scaling**

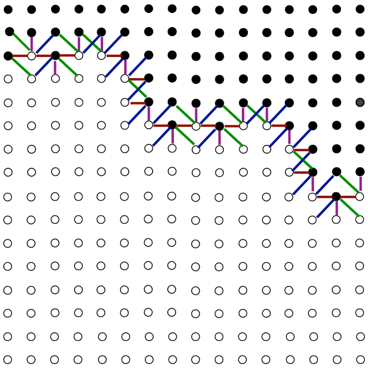
$$E_\varepsilon(u) = \sum_{ij} \varepsilon^{n-1} \sigma^\varepsilon_{ij} (u_i - u_j)^2$$

with $\sigma^\varepsilon_{ij} \geq 0$



Here we depict a next-to-nearest neighbour system.
The coloured segments highlight the 'active' interactions $(u_i \neq u_j)$, the different colours possible anisotropy and the dependence of σ^ε_{ij} on ij

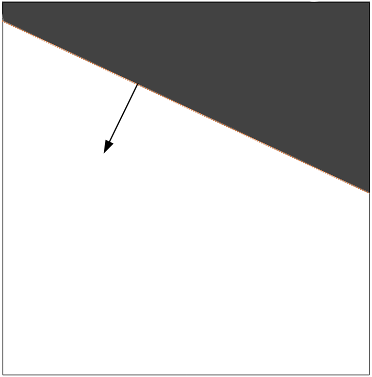
Passage from discrete to continuum - heuristics



As we ‘zoom out’, the energy tends to concentrate on an interface.

Convergence: L^1 convergence of the interpolates of u_i^ε on $\varepsilon\mathbb{Z}^n$

Passage from discrete to continuum - heuristics



The 'discrete interface' can be approximately described as a continuous one, smooth enough as to have a normal ν well defined

We expect to have a *continuum surface tension* which *approximately describes the behaviour of* E_ε.

Variational tools for the static analysis

For the behaviour of **minimum problems** the limit energy is described by the **Γ-limit** of E_ε (De Giorgi):

$$\textbf{Γ-convergence } E_\varepsilon \xrightarrow{\Gamma} E_{\rm cont}$$

$$\Updownarrow$$

$\forall u_\varepsilon \to u$ we have $E_\varepsilon(u^\varepsilon) \geq E_{\rm cont}(u) + o(1)$ (ansatz-free lower bound)
$\exists u_\varepsilon \to u$ such that $E_\varepsilon(u^\varepsilon) \leq E_{\rm cont}(u) + o(1)$ (constructive upper bound)

$$\Updownarrow$$

for all G_ε continuously converging to $G_{\rm cont}$ such that $E_\varepsilon + G_\varepsilon$ are equicoercive

$$\min\{E_\varepsilon + G_\varepsilon\} \to \min\{E_{\rm cont} + G_{\rm cont}\}$$

(**convergence of minimum values and minimizers**)

Continuum surface energies

We expect

$$E_{\text{cont}}(u) = \int_{\partial\{u=1\}} g(x,\nu)\,d\mathcal{H}^{n-1}$$

g = surface tension, ν = normal to the interface $\partial\{u=1\}$
Such a E_{cont} can be seen as a *perimeter functional* for the set $A = \{u = 1\}$

Rigorous treatments of variational theories for such energies require Geometric Measure Theory tools (Caccioppoli, Federer, De Giorgi).

A theory studying the Γ-convergence of such continuum energies has been developed as energies on (partitions of) sets of finite perimeter (Ambrosio-B)

Compactness and continuum description

Basic question: *existence of a limit surface energy?*

Theorem (Caffarelli-de la Llave '06, B-Piatnitsky '13, Alicandro-Gelli '14)
Suppose $\sigma_{ij}^{\varepsilon} \geq 0$ satisfy:
(i) (decay) e.g., $|\sigma_{ij}^{\varepsilon}| \leq C|i-j|^{-r}$ with $r > n+1$;
(ii) (coerciveness of NN interactions) $\sigma_{ij}^{\varepsilon} \geq \sigma_0 > 0$ if $|i-j| = 1$
(iii) (negligible long-range tail) $\lim_{T\to+\infty} \sum_{|i-j|>T} \sigma_{ij}^{\varepsilon} = 0$

Compactness and continuum description

Basic question: *existence of a limit surface energy?*

Theorem (Caffarelli-de la Llave '06, B-Piatnitsky '13, Alicandro-Gelli '14)
Suppose $\sigma^{\varepsilon}_{ij} \geq 0$ satisfy:
(i) (decay) e.g., $|\sigma^{\varepsilon}_{ij}| \leq C|i-j|^{-r}$ with $r > n+1$;
(ii) (coerciveness of NN interactions) $\sigma^{\varepsilon}_{ij} \geq \sigma_0 > 0$ if $|i-j| = 1$
(iii) (negligible long-range tail) $\lim\limits_{T\to+\infty} \sum\limits_{|i-j|>T} \sigma^{\varepsilon}_{ij} = 0$

Then (up to subsequences) there exists g with $g > 0$ on S^{n-1} and $g(x,\cdot)$ convex and positively 1-homogeneous such that $E_\varepsilon \to E_{\rm cont}$ where

$$E_{\rm cont}(u) = \int_{\partial\{u=1\}} g(x,\nu)\, d\mathcal{H}^{n-1}$$

is defined on $BV_{\rm loc}(\mathbb{R}^n; \{\pm 1\})$

Compactness and continuum description

Basic question: *existence of a limit surface energy?*

Theorem (Caffarelli-de la Llave '06, B-Piatnitsky '13, Alicandro-Gelli '14)
Suppose $\sigma^\varepsilon_{ij} \geq 0$ satisfy:
(i) (decay) e.g., $|\sigma^\varepsilon_{ij}| \leq C|i-j|^{-r}$ with $r > n+1$;
(ii) (coerciveness of NN interactions) $\sigma^\varepsilon_{ij} \geq \sigma_0 > 0$ if $|i-j| = 1$
(iii) (negligible long-range tail) $\lim\limits_{T\to+\infty} \sum\limits_{|i-j|>T} \sigma^\varepsilon_{ij} = 0$

Then (up to subsequences) there exists g with $g > 0$ on S^{n-1} and $g(x,\cdot)$ convex and positively 1-homogeneous such that $E_\varepsilon \to E_{\rm cont}$ where

$$E_{\rm cont}(u) = \int_{\partial\{u=1\}} g(x,\nu)\,d\mathcal{H}^{n-1}$$

is defined on $BV_{\rm loc}(\mathbb{R}^n;\{\pm 1\})$

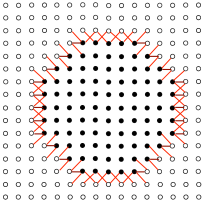
Note: (i) decay $\Rightarrow$ correctness of surface scaling
(ii) coerciveness $\Rightarrow$ existence of a interface (De Giorgi BV-compactness)
(iii) control of the tail $\Rightarrow$ 'locality' of the energy $\Rightarrow$ integral represent.

The Wulff problem (a good way to picture convergence)

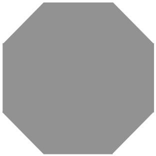
If $g = g(\nu)$ (homogeneous limit) then we deduce the convergence of *problems with* **volume constraint** ($C_\varepsilon \to C$)

$$\min\{E_\varepsilon(u) : \varepsilon^n \#\{i : u_i = 1\} = C_\varepsilon\}$$
$$\to \quad \min\Big\{\int_{\partial\{u=1\}} g(\nu)\, d\mathcal{H}^{n-1} : |\{u=1\}| = C\Big\} \quad \textbf{(Wulff problem)}$$

A minimizer of the latter (normalized e.g. to unit energy) is called a **Wulff shape**.



$\longrightarrow$



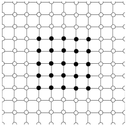
(for NNN interactions the Wulff shape is an octagon)

Conversely, the knowledge of the Wulff shape determines g and characterizes the Γ-convergence of E_ε.

Some Wulff shapes

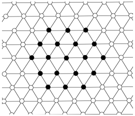
It is instructive then to look at the Wulff shape related to some simple discrete systems (and how it reflects the lattice structure)...

Square NN (**nearest-neighbour**) interactions $\longrightarrow$ square

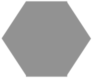


$\longrightarrow$

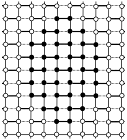
Triangular NN interactions $\longrightarrow$ hexagon



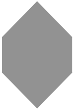
$\longrightarrow$



Inhomogeneous square NN interactions $\longrightarrow$ (irregular) polygon



$\longrightarrow$



Flexibility of the method

Relaxation of the control on the tail $\Rightarrow$ non local limits

If only $\sup_{\varepsilon,i} \sum_j c^{\varepsilon}_{ij} < +\infty$ then me may have an additional non-local term; e.g.,

$$E_{\rm cont}(u) = \int_{\partial\{u=1\}} g(x,\nu)\,d\mathcal{H}^{n-1} + \iint k(x,y)G(u(x),u(y))\,d\mu(x)\,d\mu(y)$$

(Alicandro-Gelli ’15)

Relaxation of the periodic lattice assumptions

- random lattices (Alicandro-Cicalese-Ruf 2014)
- aperiodic lattices (such as Penrose lattices, etc) (B-Solci 2011)

Relaxation of the ferromagnetic assumption

(replaced by the existence of two “uniform ground states”) E.g.,

- non-frustrated antiferromagnetic systems $\Rightarrow$ *anti-phase boundaries* (Alicandro-B-Cicalese 2006)
- models of phase segregation for chiral molecules (B-Garroni-Palombaro, in progress)

Extension to a larger (finite) set of parameters K

$$\Downarrow$$

1) functionals defined on partitions

$$E_{\rm cont}(u) = \sum_{l,k\in K_0} \int_{\partial\{u=l\}\cap\partial\{u=k\}} g^{lk}(x,\nu)\,d\mathcal{H}^{n-1}$$

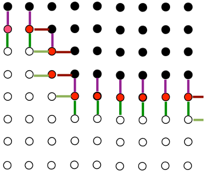
($K_0 \subset K$ the set of ground states)

$\Rightarrow$ BV-ellipticity of g^{lk} (surface analog of quasiconvexity for vector Sobolev maps (Federer, Ambrosio-B, White, Morgan))

$\Rightarrow$ relevant contribution of interfacial microstructure
In 2D applications to dislocations (Conti-Garroni-Massacesi 2014)

2) energies depending on measure concentration

Even if we have only two uniform ground states (± 1) the energy can depend on the concentration of a third phase (0-phase) on the interface (e.g., in the *Blume-Emery-Griffith model*)



$$E_{\text{cont}}(u,\mu) = \int_{\partial\{u=1\}} \varphi\Big(x,\nu,\frac{d\mu}{d\mathcal{H}^{n-1}}\Big)\,d\mathcal{H}^{n-1}$$

$\Longrightarrow$ surfactant energies (Alicandro-Cicalese-Sigalotti 2012)

Extension to "positive temperature"

In terms of Statistical Mechanics this is a "zero-temperature limit".

We may sometimes extend this procedure to positive temperature (Kotecky-Luckhaus 2014)

Variational tools in an 'evolutionary' framework

Variational evolution: an *implicit Euler scheme* (Almgren-Taylor-Wang 1993, De Giorgi 1995, Ambrosio-Gigli-Savaré 2005) can be adapted to study evolution of discrete systems: fix initial data u_0, time-step τ and space scale ε, define the *space/time-discrete evolution* of E_ε *at time-scale* τ as

- $u_0^{\tau,\varepsilon} = u_0$
- $u_{i+1}^{\tau,\varepsilon}$ **a minimizer** of

$$E_\varepsilon(u) + \frac{1}{\tau} D(u, u_i^{\tau,\varepsilon})$$

(D = "dissipation" measuring the "L^2 interfacial distance")
Up to subsequences, we define a **space/time-continuum limit**

$$u(t) = \lim_{\varepsilon \to 0} u_{\lfloor t/\tau \rfloor}^{\tau,\varepsilon}$$

as $\tau, \varepsilon \to 0$ (**Minimizing movement** of E_ε at scale τ from u_0)

Connections with the static analysis

If E_ε Γ-converge to $E_{\rm cont}$ and D is a continuous perturbation then

$$E_\varepsilon(\cdot) + \frac{1}{\tau} D(\cdot, \overline{u}^\varepsilon)$$

Γ-converge to

$$E_{\rm cont}(\cdot) + \frac{1}{\tau} D(\cdot, \overline{u})$$

if $\overline{u}^\varepsilon \to \overline{u}$, from which we deduce that *if $\varepsilon \to 0$ fast enough with respect to* τ then $u(t)$ *is the minimizing movement of the* Γ*-limit* $E_{\rm cont}$ from u_0

Theorem. "for slow time" the Γ-limit gives also a description of the evolution.

In general, the limit $u(t)$ *does depend on the mutual behaviour of ε and τ* (B Lecture Notes Math 2013)

An Example: Flat Flow

Example. If we take NN ferromagnetic interactions in $\mathbb{Z}^2$ then the Γ-limit is the crystalline perimeter with a coordinate-square Wulff shape. Its evolution (flat flow) is **motion by crystalline curvature** (Almgren-Taylor 1995)

$$v = \kappa, \qquad \kappa = \text{ crystalline curvature}$$

where e.g. each side of a rectangle moves inwards with velocity

$$v = \frac{2}{L} \qquad \text{i.e., } \kappa = \frac{2}{L} \text{ (crystalline curvature of the side)}$$

($L =$ length of the side).

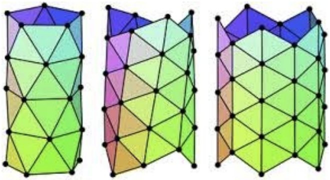
This evolution is also as the minimizing movement for E_ε at scale τ if $\varepsilon << \tau$

2. Additional Effects of Discreteness - Some Examples

a) Flexible Modeling

• **Complex Materials.** Thanks to the "non-local" aspect of discrete interactions we can easily model problems that in the continuum require complex assumptions; e.g.,
• multiphase materials
• surfactants
• double-porosity media, etc.

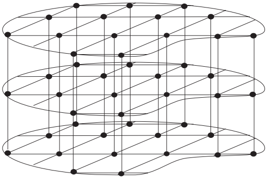
• **"Low-dimensional" Objects.** Discrete modeling can be extended to thin films, nanotubes, etc.



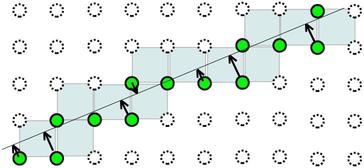
(figure by Lee-Cox-Hill)

adapting a dimension-reduction procedure (Le Dret-Raoult 1995, B-Fonseca-Francfort 2000, Friesecke-James-Müller 2002, etc)

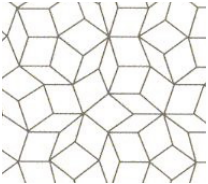
The models involve “microscopic design parameters” as **number of layers** of a thin film, **chirality** of a nanotube, etc.
The resulting low-dimensional model may depend effectively from such parameters (Alicandro-B-Cicalese 2008)



• **Quasicrystals.** They can be modeled as “irrational discrete thin films” in higher-dimension through a ‘cut-and-proiect’ procedure



$\Longrightarrow$



b) Discrete Optimal Design Problems

Optimal design problems = construction of structures with "**extreme properties**" subject to design constraints.
Discrete structures $\Rightarrow$ **more flexible design constraints** with respect to the continuum case

Example: composites of two ferromagnetic materials
This translates in the computation of all possible limits of

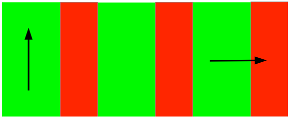
$$E_\varepsilon(u) = \sum_{ij} \varepsilon^{n-1} \sigma_{ij} (u_i - u_j)^2$$

with periodic $\sigma_{ij} \in \{\alpha, \beta\}$ with given proportions.

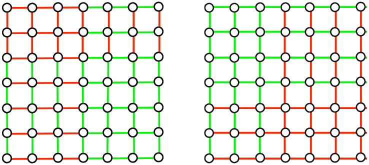
In this case we can give exact bounds on the limit energy densities (*contary to the analog continuum problem*)
(B-Kreutz in progress)

Optimal discrete geometries

In the continuum often extremal properties are obtained by “laminates”, which “extremize” different properties in different directions



In a discrete setting we can extremize *the same* property in different directions by discrete lamination



(even more surprising constructions for long-range interactions)

c) Variational Percolation Problems

The discrete setting is a perfect environment to include a *random distribution* of coefficients $\sigma_{ij} = \sigma_{ij}^\omega$ and consider energies

$$E_\varepsilon^\omega(u) = \sum_{ij} \varepsilon^{n-1}\sigma_{ij}^\omega(u_i - u_j)^2$$

depending on the realization ω of a random variable

Model case: $\sigma_{ij}^\omega = \alpha$ (resp., β) with probability p (resp., $1-p$) (e.g., modeling a random distribution of defects).

• We characterize $E_{\rm cont} = E_{\rm cont}^p$ in terms of p and suitable *percolation formulas* (first-passage percolation for $\alpha, \beta > 0$ finite)

• In the degenerate (limit) cases $\alpha = 0$ (*dilute spins*) or $\beta = +\infty$ (*rigid spins*) prove that we have different behaviours above/ below a *percolation threshold*

(B-Piatnitski 2012, Scilla 2014)

Variational Percolation Questions

Proof of probabilistic representation theorems	$\Longleftrightarrow$	Understanding of geometric and 'measure theoretic' properties of percolation clusters
Proof of random homogenization formulas	$\Longleftrightarrow$	Estimates of metric properties of percolation clusters

$$\Downarrow$$

New *variational questions* in Percolation Theory
Modeling of new variational problems in terms of percolation issues

d) Pinning and Evolutionary Homogenization

The time/space-discrete (τ/ε) evolution generally gives

• convergence to the evolution of the static Γ-limit for *slow time*; i.e., $\varepsilon \to 0$ fast enough

• completely pinned motion for *fast time*; i.e., $\tau \to 0$ fast enough

Hence we have **existence of one or more *critical time scales* with non-trivial evolution**. In particular at such scales we obtain the evolution of a *"corrected"* Γ-limit (ε and τ-dependent)

Example (B-Gelli-Novaga 2010) For NN ferromagnetic interactions in $\mathbb{Z}^2$ the *critical scale* is $\varepsilon/\tau \to \gamma$ for which the motion is

$$v = \frac{1}{\gamma}\lfloor \gamma\kappa \rfloor \qquad (\lfloor t \rfloor \text{ is the integer part of } t)$$

• large sets (of size depending on γ) are **pinned**; in particular
 as $\gamma \to 0$ all initial sets are pinned
 as $\gamma \to +\infty$ we recover motion by crystalline curvature

Differently from the continuum case
• velocity is "quantized" (due to rows of microscopic energy barriers)
• (*partial pinning*) we may have non-trivial motions of compact sets existing for all time (and not always finite-time existence)

Example (B-Scilla 2013) The geometry of discrete interactions may give evolutionary effects that are **not detected by the Γ-limit**. For NN ferromagnetic interactions in $\mathbb{Z}^2$ with "defects" the limit motion may be of the form

$$v = \frac{1}{\gamma} f_{\rm hom}(\gamma\kappa)$$

where $f_{\rm hom}$ is a *homogenized velocity* obtained implicitly by showing the existence of "asymptotically periodic" orbits of an auxiliary problem.

Note. Even for simple distributions of defects the computation of $f_{\rm hom}$ raises non-trivial combinatorial issues

Related questions in homogenization by minimizing movements of ODE (Ansini-B-Zimmer), geometric motions (B-Malusa-Novaga, in prog.)

3. New Problems - Patterns and Microgeometries*

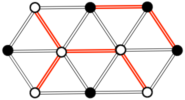
* unless otherwise stated the results of this part are in collaboration with Alicandro and Cicalese

Lattice Microstructure

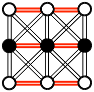
For (mixtures of ferromagnetic and) **antiferromagnetic interactions** ground states may be **frustrated**; i.e., not all interactions are minimized $\Longrightarrow$ **lattice microstructure**

Examples (all antiferromagnetic interactions)
ground states with frustrated interactions (in red)

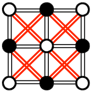
NN Triangular lattice
('disordered' ground states)



NNN square lattice
(periodic ground states)

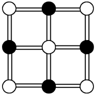


or



(depending on σ_{ij})

NN square lattice
(periodic ground states)

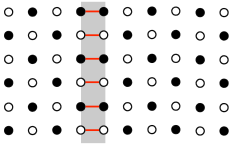


(not frustrated)

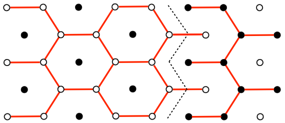
Limit analysis

Q.: can we still describe the Γ-limit? with resp. to what convergence?
Note: L^1 convergence $u^\varepsilon \to u$ in general is meaningless (e.g., for NN and NNN square lattice all ground states have 0 average)

Example (NN antiferrom. square lattice $\Longrightarrow$ anti-phase boundaries)



(NN antif. triangular lattice $\Longrightarrow$ no interfacial energy - **"total frustration"**)



Limits parameterized on ground states

A positive convergence result

Theorem. Suppose σ_{ij} periodic, **no sign hypothesis**
Suppose that there exist $u_1, \dots, u_N$ periodic discrete functions s.t.
(i) u_k are the "ground states" of E
(ii) "between different u_k we have an energy barrier"
(iii) "surface-type decay of the interactions" with the distance

Limits parameterized on ground states

A positive convergence result

Theorem. Suppose σ_{ij} periodic, **no sign hypothesis**
Suppose that there exist $u_1, \dots, u_N$ periodic discrete functions s.t.
(i) u_k are the "ground states" of E
(ii) "between different u_k we have an energy barrier"
(iii) "surface-type decay of the interactions" with the distance

Then

(a) if $\sup_\varepsilon E_\varepsilon(u^\varepsilon) < +\infty$ then locally $u^\varepsilon = \sum_{k=1}^N \chi_{A_k^\varepsilon} u_k$, with (WLOG) $\varepsilon A_k^\varepsilon \to A_k$ and $\{A_k\}$ is a partition of sets of finite perimeter, and we may define the convergence $u^\varepsilon \to (A_1, \dots, A_N)$
With an abuse of notation we may say that the limit value is u_k on A_k

Limits parameterized on ground states

A positive convergence result

Theorem. Suppose σ_{ij} periodic, **no sign hypothesis**
Suppose that there exist $u_1, \dots, u_N$ periodic discrete functions s.t.
(i) u_k are the "ground states" of E
(ii) "between different u_k we have an energy barrier"
(iii) "surface-type decay of the interactions" with the distance

Then

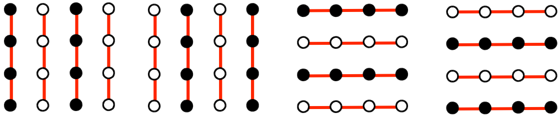
(a) if $\sup_\varepsilon E_\varepsilon(u^\varepsilon) < +\infty$ then locally $u^\varepsilon = \sum_{k=1}^N \chi_{A_k^\varepsilon} u_k$, with (WLOG) $\varepsilon A_k^\varepsilon \to A_k$ and $\{A_k\}$ is a partition of sets of finite perimeter, and we may define the convergence $u^\varepsilon \to (A_1, \dots, A_N)$
With an abuse of notation we may say that the limit value is u_k on A_k

(b) E_ε Γ-converge to $E_{\rm cont}$ of the form

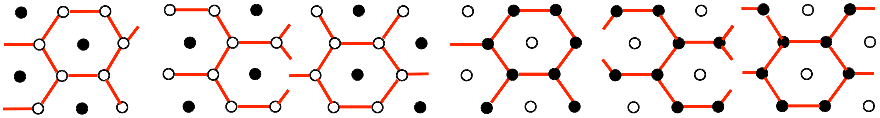
$$E_{\rm cont}(A_1, \dots, A_N) = \sum_{i \neq j} \int_{\partial A_i \cap \partial A_j} g_{ij}(x, \nu) d\mathcal{H}^{n-1}$$

Examples: (all σ_{ij} of period 1)

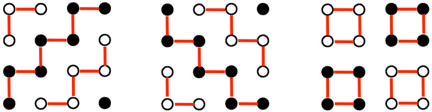
NNN antif. square lattice – 4 “striped” ground states



NN antif.+ NNN ferrom. triangular lattice – 6 “hexagonal” gr. states



NNNN squ. lattice - 16 gr. states “slanted stripes” and “checkerboard”



(and translations)

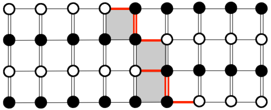
etc.

Homogenization and G-closure Problems

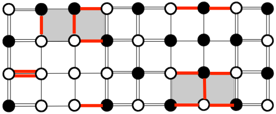
Q: compute the possible limits of mixtures of (periodic) ferromagnetic + antiferromagnetic interactions (with given proportions)

Partial answer With NN, $\sigma_{ij} = \pm 1$ and equal proportions we may obtain 2 param. and all interfacial energies not greater than $|\nu_1| + |\nu_2|$
(in the picture: single line = ferrom., double line = antiferrom.)

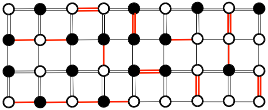
non-frustrated



frustrated/
degenerate surface energy



totally frustrated/
no surface energy



Note: question must be correctly put (equivalence by Γ-convergence)
It is not clear if with only NN we may have more than 2 parameters

Many (open) problems

E.g.,

Deterministic setting

• can we give a bound on the number of ground states from the periodicity and the range of interactions?
• can we give a description of the type of ground states in terms of percentage of interactions?

Partial results (NN): the percentage of T-periodic geometries with "essentially" two ground states tends to 100% if we have percentage of antiferromagnetic interactions below some $p_0 > 0$ (B-Causin-Piatnitski-Solci, in preparation)

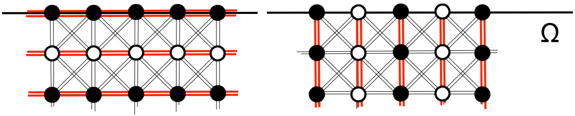
Probabilistic setting

• if we replace the percentage with the *probability* of having antiferromagnetic interactions, can we keep the limit description away from $p = 0$ or 1?
• if so, how does the number of ground state changes with p?
• is there a limit variational formulation at $p = 1/2$? (spin glass?)

Boundary effects for finite domains

For finite domains the energetic description is not complete.
We have a *non-trivial boundary effect*.

E.g.,



(second configuration energetically convenient)

$\Longrightarrow$ effective energy of the form

$$E_{\text{cont}}(A_1,\ldots,A_N) = \sum_{i\neq j}\int_{\partial A_i\cap\partial A_j\cap\Omega} g_{ij}(x,\nu)\,d\mathcal{H}^{n-1} + \sum_k \int_{\partial A_k\cap\partial\Omega} \widetilde{g}_k(x,\nu)\,d\mathcal{H}^{n-1}$$

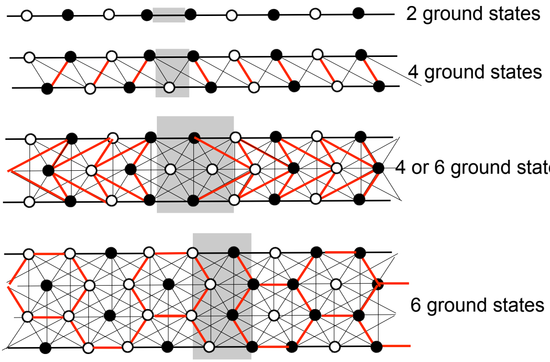
("wetting" term)

$\Longrightarrow$ Ω is an additional "design parameter"

Boundary effects for thin films - I

Boundary effects are particularly important for thin objects such as thin films.

Example (dependence of $\#$ of parameters on the thickness)
The number of parameters of N-layer thin films may depend on N and 'stabilize' to those of the 'bulk' limit
E.g., for triangular NN antiferrom. + NNN ferromagnetic,

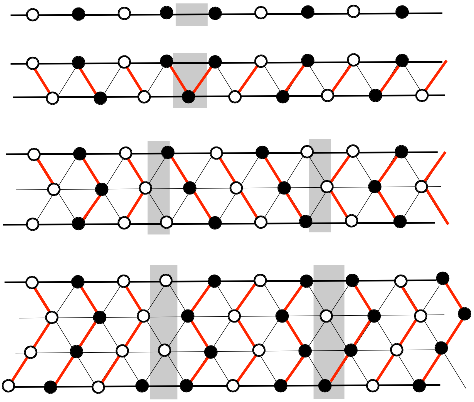


(Note: the $\#$ is not always increasing with the thickness)

Boundary effects for thin films - II

Example (rigidity by boundary effects)
"Total frustration" may only occur as the number of layers $N \to +\infty$

E.g., for triangular NN antiferromagnetic,



2 ground states

4 ground states

8 ground states

16 ground states

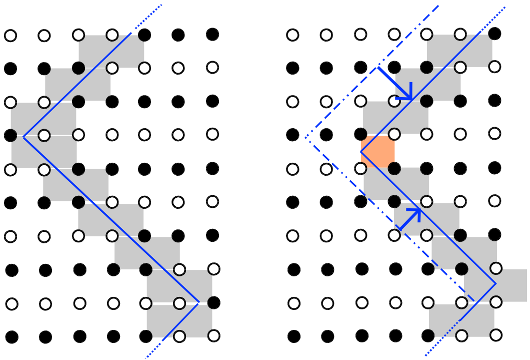
… N layers

2^N ground states

Motions by microstructures

New features in the motion of interfaces. E.g.,

(a) Motions by creation of defects (surface microstructures)

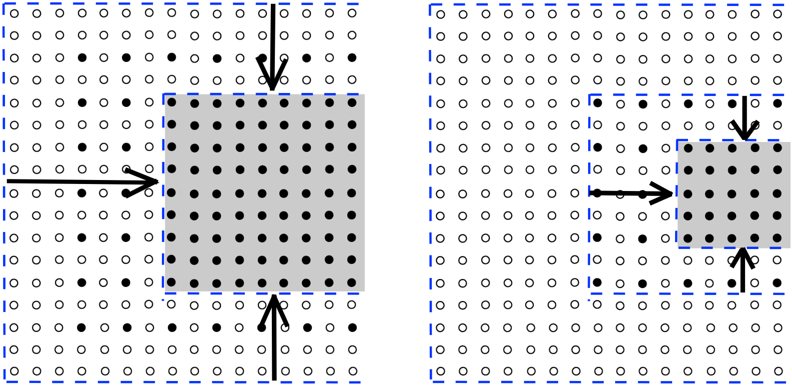


(of interfaces otherwise pinned for the Γ-limit)

(B-Cicalese-Yip, in progress)

(b) Motions by "mushy layers" (bulk microstructure)

(connection with Fluid Mechanics; (Grae Worster 1991))



$\Longrightarrow$ additional terms to motion by crystalline curvature

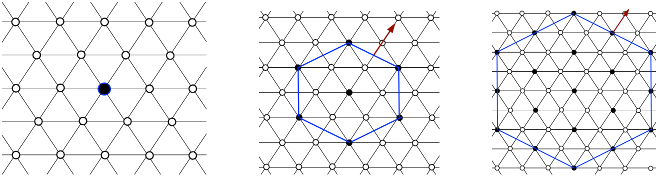
(B-Solci, 2015)

$\Longrightarrow$ "failure" of the "Slow-time Theorem"

"Backwards evolution" by crystalline curvature

Approximation of crystalline perimeters by (anti-)ferromagnetic interactions may give a meaningful definition of backward motion (otherwise **ill-defined** in the continuum) by minimizing movements.

Example (nucleation in a triangular lattice driven by local maximization of the perimeter, with "hexagonal dissipation")



Continuum limit: hexagon expanding at constant velocity (after scaling time)

In general the motion depends on the "dissipation-distance", and may give rise to complex patterns (linked to the problem of couting integer points inside a ball) and homogenization of the velocity (B-Scilla 2013)

Conclusions

I have illustrated the simplest (only two parameters) passage discrete-to-continuum for variational lattice theories, and only in the surface regime

Nevertheless we have seen interesting effects with applications in optimal design of discrete structures, percolation, modeling, etc., and a range of new problems coming from the role of lattice microstructure

Analogous effect can be analyzed at other scales. Applications have been given to problems in Computer Vision, Optimal Design, Fracture Mechanics, Continuum Mechanics, Liquid Crystals, etc. and some proposals have been made for the overall problem of matching scales

At all scales new and challenging issues appear, and many more are to come

Thank you for your attention!