Asymptotic analysis of discrete systems

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From discrete to continuous energies

Discrete system: with discrete variables $u = \{u_i\}$ indexed on a lattice (e.g., $\Omega \cap \mathbb{Z}^d$)
Discrete energy: (e.g., pair interactions)

$$E(u) = \sum_{ij} f_{ij}(u_i, u_j)$$

Scaling arguments: derive

$$E_\varepsilon(u) = \sum_{ij} f^\varepsilon_{ij}(u_i, u_j)$$

indexed on a scaled lattice (e.g., $\Omega \cap \varepsilon\mathbb{Z}^d$)
Identification: identify u with some continuous parameter (e.g., its piecewise-constant interpolation)
Effective continuous theory: obtained by Γ-limit as $\varepsilon \to 0$.

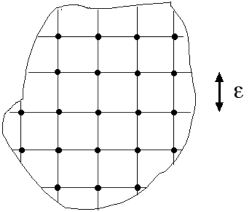
I present two case studies to highlight differences/mutual interactions with the continuous case

Part One: A prototypical model for defects

A "non-defected" simple model: the discrete membrane: quadratic mass-spring systems. $\Omega \subset \mathbb{R}^d$, $u : \varepsilon\mathbb{Z}^d \to \mathbb{R}$

$$E_\varepsilon(u) = \sum_{NN} \varepsilon^d \Big(\frac{u_i - u_j}{\varepsilon}\Big)^2$$

(NN = nearest neighbours (in Ω))



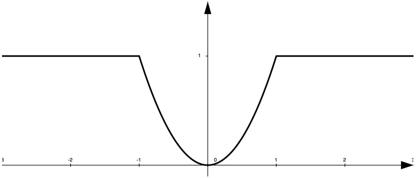
As $\varepsilon \to 0$ E_ε is approximated by the Dirichlet integral

$$F_0(u) = \int_\Omega |\nabla u|^2 \, dx$$

A prototypical 'defected' interaction:
at a 'defected spring'

substitute $\left(\frac{u_i - u_j}{\varepsilon}\right)^2$ by $\left(\frac{u_i - u_j}{\varepsilon}\right)^2 \wedge C_\varepsilon$

(*truncated quadratic potential*)



The spring 'breaks' when $\frac{u_i - u_j}{\varepsilon} = \sqrt{C_\varepsilon}$

The Blake-Zisserman weak membrane

The meaningful scaling for C_ε is (of order) $\frac{1}{\varepsilon}$, in which case the energy of a 'broken' spring scales as a surface: $\varepsilon^d \cdot \dfrac{1}{\varepsilon} = \varepsilon^{d-1}$.
When all springs are 'defected' the total energy

$$E_\varepsilon(u) = \sum_{NN} \varepsilon^d \Big(\Big(\frac{u_i - u_j}{\varepsilon} \Big)^2 \wedge \frac{1}{\varepsilon} \Big)$$

is then approximated as $\varepsilon \to 0$ by an *(anisotropic) Griffith fracture energy* (Chambolle 1995)

$$F_1(u) = \int_{\Omega \setminus S(u)} |\nabla u|^2 \, dx + \int_{S(u)} \|\nu\|_1 d\mathcal{H}^{d-1}$$

$S(u)$ = discontinuity set of u (crack site in reference config.)
$\nu = (\nu_1, \ldots, \nu_d)$ normal to $S(u)$, $\|\nu\|_1 = \sum_i |\nu_i|$ (lattice anisotr.)
$\mathcal{H}^{d-1}$ = surface measure; $u \in SBV(\Omega)$

G-closure theory for defects in discrete systems

Q: describe the overall effect of the presence of defects

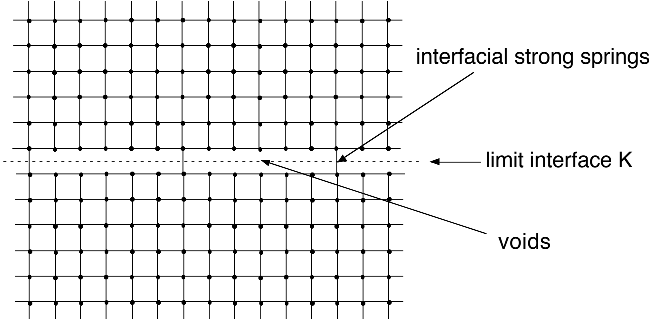
"G-closure" approach: Fix any family of distributions of defects $\mathcal{W}_\varepsilon$, and compute all the possible limits of the corresponding energies.
What type of energies do we get?
How does it depend on the local volume fraction of the defects?

NOTE: a possible limit energy is always sandwiched between F_0 (Dirichlet, from above) and F_1 (Blake and Zisserman, from below); in particular it equals F_0 if no fracture occurs.

Design of Weak Membranes

Contrary to usual continuous G-closure problems (bulk homogenization) it is essential to handle particular concentrations of defects on a single surface.

A side result: (quadratic) discrete transmission problems



$$E_\varepsilon(u) = \sum_{NN} \varepsilon^d c^\varepsilon_{ij} \left(\frac{u_i - u_j}{\varepsilon}\right)^2 \qquad c^\varepsilon_{ij} = \begin{cases} 1 \text{ (strong spring)} \\ 0 \text{ (void)} \end{cases}$$

Theorem (B-Sigalotti) Let p_ε be the percentage of strong springs over voids at the (coordinate) interface K. If

$$p_\varepsilon = \begin{cases} c\,\varepsilon|\log\varepsilon| & \text{if } d=2 \\ c\,\varepsilon & \text{if } d\geq 3 \end{cases}$$

then E_ε can be approximated by a "transmission energy"

$$F(u) = \int_\Omega |\nabla u|^2\,dx + b\int_K |u^+ - u^-|^2 d\mathcal{H}^{d-1},$$

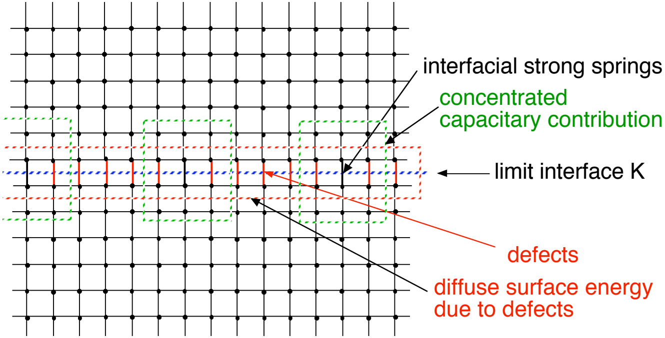
defined on $H^1(\Omega\setminus K)$, where

$$b = \begin{cases} c\,\frac{\pi}{2} & \text{if } d=2 \\ c\,\frac{C_d}{4+C_d} & \text{if } d\geq 3 \end{cases}$$

and C_d is the 2-capacity of a 'dipole' in $\mathbb{Z}^d$.

The Building Block for the design

Same geometry with voids substituted by defects



Proposition. The same p_ε give

$$F(u) = \int_\Omega |\nabla u|^2\, dx + \mathcal{H}^{d-1}(\{u^+ \neq u^-\}) + b \int_K |u^+ - u^-|^2 d\mathcal{H}^{d-1}$$

for $u \in H^1(\Omega \setminus K)$

Note:

(i) surface contribution of defects and capacitary contribution of strong springs can be decoupled as they live on different microscopic scales

(ii) the construction is local, and is immediately generalized to K a locally finite union of *coordinate hyperplanes* (i.e., hyperplanes with normal in $\{e_1, \dots, e_n\}$)

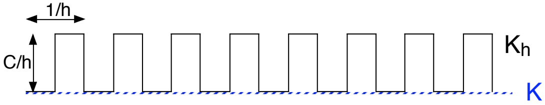
(iii) the limit functional F can be interpreted as defined on $SBV(\Omega)$ and can be identified with $F_{1,b,K}$, where

$$F_{a,b,K}(u) = \int_\Omega |\nabla u|^2\,dx + \int_{S(u)} (a + b|u^+ - u^-|^2)d\mathcal{H}^{d-1}$$

with the constraint $S(u) \subset K$

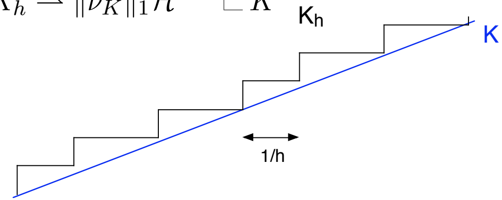
Limits of energies $F_{1,b,K}$

1. Weak approximation of surface energies (on coordinate hyperplanes) Suitable K_h s.t. $\mathcal{H}^{d-1} \llcorner K_h \rightharpoonup a\mathcal{H}^{d-1} \llcorner K$ $(a \geq 1)$



Then F_{1,b,K_h} Γ-converges to $F_{a,ab,K}$

2. Weak approximation of anisotropic surface energies. For non-coordinate hyperplanes K we find locally coordinate K_h s.t. $\mathcal{H}^{d-1} \llcorner K_h \rightharpoonup \|\nu_K\|_1 \mathcal{H}^{d-1} \llcorner K$



Then F_{a,b,K_h} Γ-converges to $F_{a\|\nu_K\|_1, b\|\nu_K\|_1, K}$

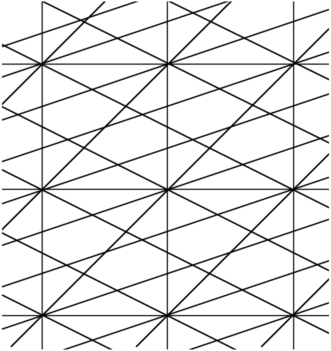
Summarizing 1 and 2: since all constructions are local, in this way we can approximate all energies

$$F_{a,b,K}(u) := \int_\Omega |\nabla u|^2\,dx + \int_{S(u)} (a(x) + b(x)|u^+ - u^-|^2)\|\nu\|_1 d\mathcal{H}^{d-1}$$

with $a \geq 1$, $b \geq 0$, K locally finite union of hyperplanes, and u s.t. $S(u) \subset K$.

3. Homogenization of planar systems

K_h $1/h$-periodic of the form



We can obtain all energies of the form

$$F_\varphi(u) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \varphi(\nu) d\mathcal{H}^{d-1},$$

with φ finite, convex, pos. 1-hom., $\varphi(\nu) \geq \|\nu\|_1$ on S^{d-1}

Note: The condition $\varphi \geq \|\cdot\|_1$ is sharp since we have the lower bound $F_\varphi \geq F_1 (= F_{\|\cdot\|_1})$.

Proof: choose (ν_j) dense in S^{d-1}, $\Pi_j := \{\langle x, \nu_j \rangle = 0\}$,

$$K_h = \frac{1}{h}\mathbb{Z}^d + \bigcup_{j=1}^{h} \Pi_j,$$

$b_h = 0$ and $a_h(x) = \varphi(\nu_j)$ on $\frac{1}{h}\mathbb{Z}^d + \Pi_j$. Then $F_{a_h,0,K_h} = F_\varphi$ on its domain, and the lower bound follows.

Use a direct construction if ν belongs to (ν_j) $\mathcal{H}^{d-1}$ a.e. on $S(u)$, and then use the density of (ν_j).

4. Accumulation of cracks (micro-cracking)

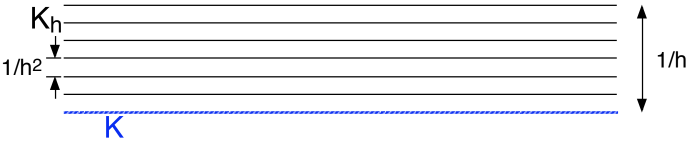
We can obtain all energies of the form

$$F_\psi(u) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \psi(|u^+ - u^-|) d\mathcal{H}^{d-1},$$

with ψ finite, concave, $\psi \geq \sqrt{d}$.

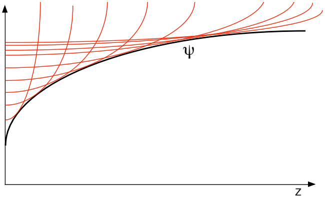
Note: $\psi \geq \sqrt{d}$ is sharp by the inequality $F_\psi \geq F_1$ and $\sqrt{d} = \max\{\|\nu\|_1 : \nu \in S^{d-1}\}$

K_h locally of the form



Proof. Choose $a_j \geq \sqrt{n}$, $b_j \geq 0$ such that

$$\psi(z) = \inf\{a_j + b_j z^2\}$$



1) For a planar K with normal ν, choose $K_h = \bigcup_{j=1}^{h}(K + \frac{j}{h^2}\nu)$ and $a(x) = a_j$, $b(x) = b_j$ on $K + \frac{j}{h^2}\nu$;

2) To eliminate the constraint $S(u) \subset K$ use the homogenization procedure of Point 3.

Homogeneous convex/concave limit energies

Theorem (B-Sigalotti) For all positively 1-hom. convex even $\varphi \geq \|\cdot\|_1$ and concave $\psi \geq 1$ there exists a family of distributions of defects $\mathcal{W}_\varepsilon$ such that the corresponding E_ε Γ-converge to

$$F_{\varphi,\psi}(u) := \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \varphi(\nu)\,\psi(|u^+ - u^-|) d\mathcal{H}^{d-1},$$

for $u \in SBV(\Omega)$.

Note: we can localize the construction to obtain all

$$F_{a,\varphi,\psi}(u) := \int_\Omega |\nabla u|^2 dx + \int_{S(u)} a(x)\varphi(\nu)\,\psi(|u^+ - u^-|) d\mathcal{H}^{d-1},$$

with $a \geq 1$ lower semicontinuous.

Some comments:

(1) This characterization is clearly not complete. It does not comprise, e.g.

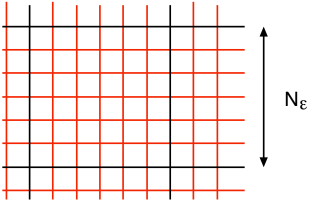
- F with constrained jump set: $S(u) \subset K$
- non-finite φ (as for layered defects)
- non-concave subadditive ψ such as $\sqrt{d}\,\mathrm{sub}(1+z^2)$; etc.

Partial conjecture: the reachable (isotropic) subadditive ψ are all that can be written as the subadditive envelope of $\psi(z) = \inf_j\{a_j + b_j z^2\}$ ($a_j \geq \sqrt{d}$, $b_j \geq 0$).

(2) The complete characterization seems to be out of reach. It would need e.g. approximation results for general lower semicontinuous surface energies (BV-elliptic densities); which is a more mysterious issue than approximation of quasiconvex functions (!)

(3) The result is anyhow sufficient for design of structures with prescribed failure set and resistance

(4) **(Prescribed limit defect density)** The theorem holds as is, also if we prescribe the local "limit volume fraction" θ of the defects. To check this it suffices to note that we may obtain the Dirichlet integral also with $\theta = 1$ (i.e., with a "negligible" percentage of strong springs)



(with $N_\varepsilon \to +\infty$, $\varepsilon N_\varepsilon \to 0$)

(5) **(Comparison with the random case)**

In that case $F_p(u) = \displaystyle\int_\Omega |\nabla u|^2\, dx + \int_{S(u)} \varphi_p(\nu) d\mathcal{H}^{d-1}$

($p =$ probability of a weak spring)

Part Two: Modeling of phase transitions

A multi-scale variational continuous model for phase transitions

$$F_\varepsilon(u) = \int_\Omega \Big(W(u) - c_1\varepsilon^2|\nabla u|^2 + c_2\varepsilon^4|\nabla^2 u|^2 \Big)\, dx$$

with W double-well potential.

• if $c_1 < 0$ and $c_2 = 0$ then it's good old "Modica-Mortola"
• if $c_1 = 0$ and $c_2 > 0$ Fonseca-Mantegazza prove a sharp-interface limit (MM-like result)
• if $c_2 > 0$ and $c_1 > 0$ **small enough** Cicalese-Spadaro-Zeppieri prove a sharp-interface limit
• if $c_2 > 0$ and $c_1 > 0$ **large enough** Mizel *et al.* prove that ground states are *periodic* (in particular no interface limit: all u_ε with $F(u_\varepsilon) = \min F_\varepsilon + o(\varepsilon)$ converge weakly to 0)

A discrete analog - dimension one

Ferromagnetic-anti-ferromagnetic spin systems in 1D

Substitute continuous u by discrete $u = \{u_i\}$ parameterized on $\varepsilon\mathbb{Z}$

$$W(u) \quad \to \quad u_i \in \{\pm 1\} \text{ (spin system)}$$

$$\nabla u \quad \to \quad \frac{u_i - u_{i-1}}{\varepsilon}$$

$$\nabla^2 u \quad \to \quad \frac{u_{i+1} - 2u_i + u_{i-1}}{\varepsilon^2}$$

Upon rearranging/renormalizing, we obtain a NNN energy of the form

$$E_\varepsilon(u) = \frac{1}{\varepsilon} F_\varepsilon(u) = \sum_i \Big(\alpha u_i u_{i-1} + u_{i-1} u_{i+1} \Big) + C_\varepsilon$$

The case "large c_1" corresponds to $|\alpha| < 2$

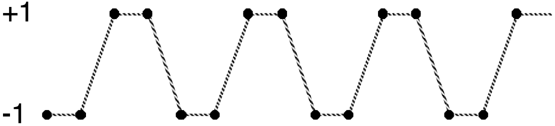
Rewrite

$$\sum_i \Big(\alpha u_i u_{i-1} + u_{i-1} u_{i+1}\Big) = \sum_i \Big(\alpha \frac{1}{2}(u_i u_{i-1} + u_{i+1} u_i) + u_{i-1} u_{i+1}\Big)$$

and note that for $|\alpha| < 2$ the integrand

$$\alpha \frac{1}{2}(u_i u_{i-1} + u_{i+1} u_i) + u_{i-1} u_{i+1}$$

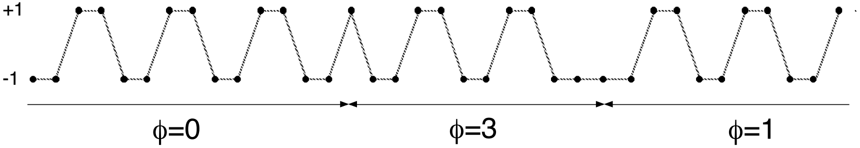
is minimal for $+,+,-$ -type configurations; i.e, in that case we have a 4-periodic ground state (and its translations)



The correct order parameter is the **phase** $\phi \in \{0, 1, 2, 3\}$ of the ground state.

Surface-scaling limit (B-Cicalese)

Functions u with $E_\varepsilon(u) = \min E_\varepsilon + o(1)$ have the form



$$F(\phi) = \sum_{t \in S(\phi)} \psi(\phi^+(t) - \phi^-(t))$$

defined on $\phi : \Omega \to \{0, 1, 2, 3\}$

$S(\phi)$ = phase-transition set

ψ given by an optimal-profile problem

NOTE: for $\alpha < 2$ we have flat ground states ± 1 (sharp interface limit); for $\alpha > 2$ we have 2-periodic oscillating minimizers (anti-phase interfaces)

Q: Is there a corresponding conjecture on the continuum?
Let

$$F_\varepsilon(u) = \int_\Omega \Big(W(u) - c_1\varepsilon^2|u'|^2 + \varepsilon^4|u''|^2 \Big)\, dt$$

with c_1 “large”

We may **conjecture** that there exists a continuous phase variable $\phi : \mathbb{R} \to S^1$ (we identify the period of the continuous ground states with S^1) and a scale ε^α such that sequences u_ε with

$$|F_\varepsilon(u_\varepsilon) - \inf F_\varepsilon| = O(\varepsilon^\alpha)$$

have the form (up to subsequences)

$$u_\varepsilon(x) = v\Big(\frac{x}{\varepsilon} + \phi(x)\Big) + o(\varepsilon)$$

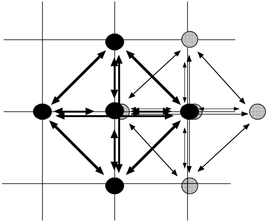
(v= periodic ground state).
In this way we can define a convergence $u_\varepsilon \to \phi$ and express the Γ-limit of $\frac{1}{\varepsilon^\alpha} F_\varepsilon$ in terms of ϕ

Q: is there a higher-dimensional analog?

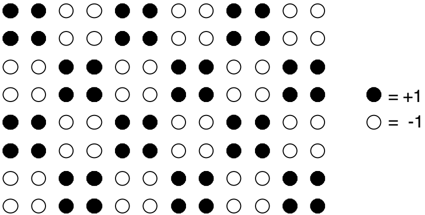
We can consider e.g. two-dimensional systems with NN, NNN (next-to-nearest), NNNN (next-to-next-...) interactions, $u_i \in \{\pm 1\}$ and

$$E_\varepsilon(u) = \sum_{NN} u_i u_j + c_1 \sum_{NNN} u_i u_j + c_2 \sum_{NNNN} u_i u_j$$

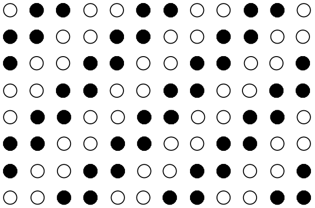
Again we can regroup the interactions to study ground states



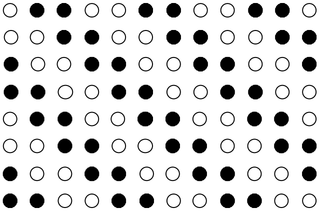
For suitable c_1 and c_2 again we have a non-trivial 4-periodic ground state



but also...



and also....



(counting translations 16 different ground states)
and a description for the surface-scaling Γ-limit similar to the 1-D case

Conclusion

The discrete setting

• on one hand with the additional ‘micro’ dimension may add interesting effects to discrete problems corresponding to continuous ones
• on the other hand can be a source of inspiration for continuous problems in simplifying technical details and supplying conjectures