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

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

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 $\Gamma$-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. $\Omega \subset \mathbb{R}^d$, $u : \varepsilon \mathbb{Z}^d \to \mathbb{R}$

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

(NN = nearest neighbours (in $\Omega$))

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

$$F_0(u) = \int_{\Omega} |\nabla u|^2 \, dx$$
A prototypical ‘defected’ interaction: 
at a ‘defected spring’

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

(*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 $C_\varepsilon$ is (of order) $\frac{1}{\varepsilon}$, in which case the energy of a ‘broken’ spring scales as a surface: $\varepsilon^d \cdot \frac{1}{\varepsilon} = \varepsilon^{d-1}$. When all springs are ‘defected’ the total energy

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

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 anisotro.)
$\mathcal{H}^{d-1} =$ surface measure; $u \in SBV(\Omega)$
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

\[ E_\varepsilon(u) = \sum_{NN} \varepsilon^d c_{ij}^\varepsilon \left( \frac{u_i - u_j}{\varepsilon} \right)^2 \]

\[ c_{ij}^\varepsilon = \begin{cases} 
1 & \text{(strong spring)} \\
0 & \text{(void)} 
\end{cases} \]
Theorem (B-Sigalotti) Let $p_\varepsilon$ be the percentage of strong springs over voids at the (coordinate) interface $K$. If

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

then $E_\varepsilon$ 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 \( p_\varepsilon \) 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 $\{e_1, \ldots, e_n\}$)
(iii) the limit functional $F$ can be interpreted as defined on $SBV(\Omega)$ and can be identified with $F_{1, b, K}$, where

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

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. $\mathcal{H}^{d-1} \sqsubseteq K_h \rightharpoonup a\mathcal{H}^{d-1} \sqsubseteq K$ ($a \geq 1$)

Then $F_{1,b,K_h} \Gamma$-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. $\mathcal{H}^{d-1} \sqsubseteq K_h \rightharpoonup \|\nu_K\|_1\mathcal{H}^{d-1} \sqsubseteq K$

Then $F_{a,b,K_h} \Gamma$-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 $\varphi$ 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 $(\nu_j)$ 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 $\nu$ belongs to $(\nu_j) \mathcal{H}^{d-1}$ a.e. on $S(u)$, and then use the density of $(\nu_j)$. 
4. Accumulation of cracks (micro-cracking)
We can obtain all energies of the form

\[ F_\psi(u) = \int_\Omega |\nabla u|^2 \, dx + \int_{S(u)} \psi(|u^+ - u^-|) \, dH^{d-1}, \]

with \( \psi \) 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

\[
\begin{array}{c}
K_h \\
\downarrow 1/h^2 \\
\downarrow 1/h
\end{array}
\]
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 $\nu$, 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 $E_\varepsilon$ $\Gamma$-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 $\varphi$ (as for layered defects)
- non-concave subadditive $\psi$ such as $\sqrt{d_{\text{sub}}(1 + z^2)}$; etc.

Partial conjecture: the reachable (isotropic) subadditive $\psi$ 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” $\theta$ 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) 

\[
\begin{array}{c}
\text{N}_\varepsilon \\
\end{array}
\]

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

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

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

($p = \text{probability of a weak spring}$)
Part Two: Modeling of phase transitions

A multi-scale variational continuous model for phase transitions

\[ F_\varepsilon(u) = \int_\Omega \left( W(u) - c_1 \varepsilon^2 |\nabla u|^2 + c_2 \varepsilon^4 |\nabla^2 u|^2 \right) \, dx \]

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 \( u_\varepsilon \) 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 $\varepsilon \mathbb{Z}$

$W(u) \rightarrow u_i \in \{\pm 1\}$ (spin system)

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

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

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

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

The case “large $c_1$” corresponds to $|\alpha| < 2$
Rewrite

\[
\sum_i \left( \alpha u_i u_{i-1} + u_{i-1} u_{i+1} \right) = \sum_i \left( \alpha \frac{1}{2} (u_i u_{i-1} + u_{i+1} u_i) + u_{i-1} u_{i+1} \right)
\]

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 $\phi : \Omega \rightarrow \{0, 1, 2, 3\}$

$S(\phi) = \text{phase-transition set}$

$\psi$ given by an optimal-profile problem

**NOTE:** for $\alpha < 2$ we have flat ground states $\pm 1$ (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 

\[ F_\varepsilon(u) = \int_\Omega \left( W(u) - c_1 \varepsilon^2 |u'|^2 + \varepsilon^4 |u''|^2 \right) \, dt \]

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 \( \varepsilon^\alpha \) such that sequences \( u_\varepsilon \) with

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

have the form (up to subsequences)

\[ u_\varepsilon(x) = v\left(\frac{x}{\varepsilon} + \phi(x)\right) + o(\varepsilon) \]

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