Stochastic and deterministic analysis of models of defects in discrete systems

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Mathematical challenges motivated by multi-phase materials: analytic, stochastic and discrete aspects

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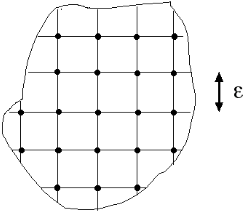
A prototypical model for defects

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))



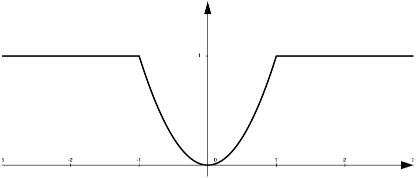
As $\varepsilon \to 0$ E_ε is approximated by the Dirichlet integral

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

A prototypical ‘defected’ interaction:
at a ‘defected spring’

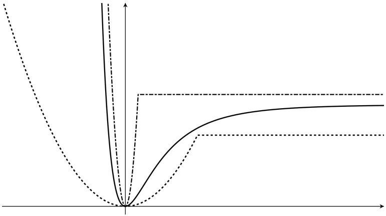
substitute $\left(\frac{u_i - u_j}{\varepsilon}\right)^2$ by $\left(\frac{u_i - u_j}{\varepsilon}\right)^2 \wedge C_\varepsilon$

(*truncated quadratic potential*)



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

Note: Truncated quadratic potentials capture the main features of classes of discrete potentials. For example (asymmetric) truncated quadratic potentials can be used to derive limit energies for Lennard-Jones interactions by a comparison and scaling argument



$$\min\Big\{\alpha' z^2, \beta'\Big\} \le J(z) \le \min\Big\{\alpha'' z^2, \beta''\Big\} \qquad (z > 0)$$

NOTE: $\sup \alpha' = \inf \alpha'' = \frac{1}{2} J''(0) =: \alpha$ (Taylor expansion at 0)
$\sup \beta' = \inf \beta'' = J(+\infty) =: \beta$ (depth of the well)
(B-Truskinovsky, B-Lew-Ortiz, etc.)

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: $\varepsilon^d \cdot \dfrac{1}{\varepsilon} = \varepsilon^{d-1}$.
If only 'defected' springs are present 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.)
$\nu = (\nu_1, \dots, \nu_d)$ normal to $S(u)$, $\|\nu\|_1 = \sum_i |\nu_i|$ (lattice anisotr.)
$\mathcal{H}^{d-1}$ = surface measure; $u \in SBV(\Omega)$

Models of defects in discrete systems

Q: describe the overall effect of the presence of defects

1. (**Probabilistic setting**) Assume that the distribution of defects is random, and the probability of a defected interaction is $p \in (0, 1)$. Is the limit deterministic? What is its form? How does it depend on p?

2. (**"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.

Random defects: a model for variational problems with percolation

(We restrict to dimension $d = 2$)
Let $\omega : \{(i,j) \text{ NN in } \mathbb{Z}^2\} \to \{\text{strong, defected}\}$ be a realization of an *i.i.d.* random variable such that

$$\omega(i,j) = \begin{cases} \text{strong} & \text{with probability } p \\ \text{defected} & \text{with probability } 1-p \end{cases}$$

Define for i, j NN in $\varepsilon\mathbb{Z}^2$

$$f^{\varepsilon}_{ij}(z) = \begin{cases} z^2 & \text{if } \omega\left(\frac{i}{\varepsilon}, \frac{j}{\varepsilon}\right) = \text{ strong} \\ z^2 \wedge \frac{1}{\varepsilon} & \text{if } \omega\left(\frac{i}{\varepsilon}, \frac{j}{\varepsilon}\right) = \text{ defected} \end{cases}$$

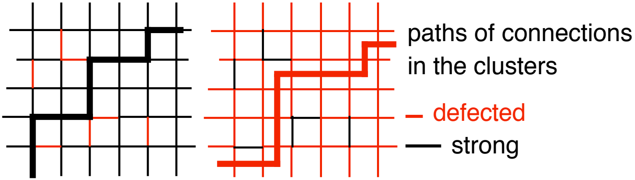
and the energy

$$E^{\omega}_{\varepsilon}(u) = \sum_{NN} \varepsilon^d f^{\varepsilon}_{ij}\left(\frac{u_i - u_j}{\varepsilon}\right)$$

Tools for variational problems with percolation

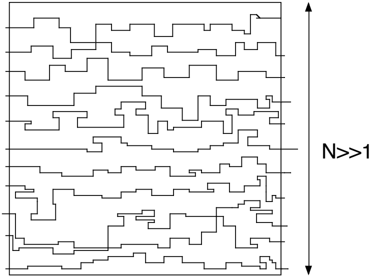
Clusters of strong/defected connections

If $p < 1/2$ (resp., $p > 1/2$) *almost surely* there exists a (unique) infinite connected component (*cluster*) of strong (resp., defected) connections in $\mathbb{Z}^2$.



“Measure-theoretical” properties of clusters

Each cluster is **uniformly distributed**: for all (large) cubes $\#$ disjoint paths connecting opposite sides is proportional to the area of the side



Consequence: if $p < 1/2$ then the functionals E_ε^ω are equi-coercive on $H^1(\Omega)$ (use Poincaré’s inequality on strong paths).

Metric properties of clusters
We define a distance on the cluster as

$$d_\omega(x,y) = \min\{\text{length of path in the cluster joining } x \text{ and } y\}$$

This distance can be *homogenized*: a.s. (in ω)

$$d_\omega\Big(\frac{x}{\varepsilon},\frac{y}{\varepsilon}\Big) \to \varphi(x-y),$$

with $\varphi = \varphi_p$ deterministic, convex and one-homogeneous (**asymptotic chemical distance**).

Consequence: if $p > 1/2$ cracks will follow a minimal path in the defected cluster (the proof uses the property that long paths not in the defected cluster contain a proportion of strong links).

The Percolation Theorem

(i) **(subcritical regime)** if $p < 1/2$ then defects are a.s. negligible and the energy is approximated by

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

defined in $H^1(\Omega)$;
(ii) **(supercritical regime)** if $p > 1/2$ then a.s. the discrete energy is approximated by a fracture energy governed by the chemical distance; i.e.,

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

defined in $SBV(\Omega)$.
(B-Piatnitski 2008)

Notes

• other types of distributions of random defects $\Rightarrow$ different percolation thresholds

• asymptotic expansion close to $p = 1/2$ not known

• analysis limited to $d = 2$ for the supercritical case

• similar variational formulation for other problems: dilute spin systems, “spin glass”, etc.

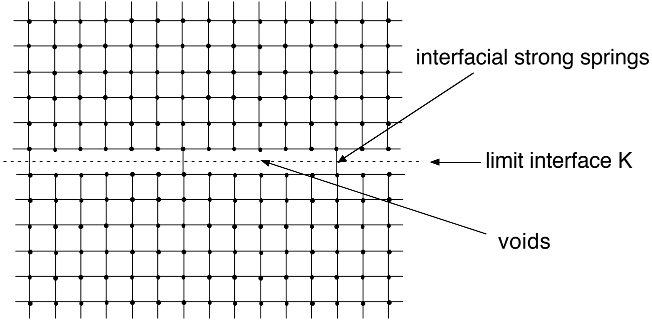
• definition and asymptotic properties of distances d_ω depend on the problem – little studied by the percolation community

• *i.i.d.* random variables essential to have energies defined on surfaces

The deterministic case: design of weak membranes

Contrary to the random case it is essential to handle particular concentrations of defects on a single surface.

A side result: 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"

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

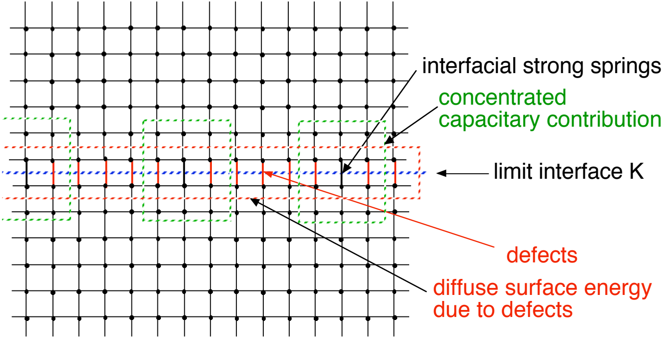
defined on $H^1(\Omega\setminus K)$, where

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

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

The Building Blocks 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 $u \in H^1(\Omega \setminus K)$

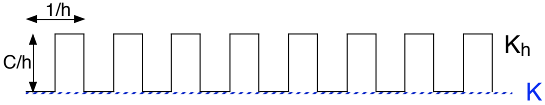
Note:
(i) surface contribution of defects and capacitary contribution of strong springs can be decoupled as they live on different microscopic scales
(ii) the construction is local, and is immediately generalized to K a locally finite union of *coordinate hyperplanes* (i.e., hyperplanes with normal in $\{e_1, \dots, e_n\}$)
(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 $S(u) \subset K$

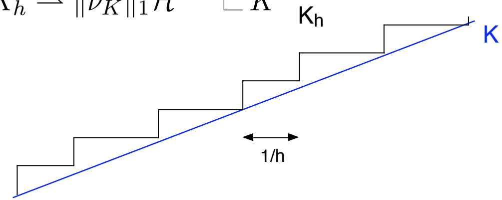
Limits of energies $F_{1,b,K}$

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 $F_{a\|\nu_K\|_1, b\|\nu_K\|_1, K}$

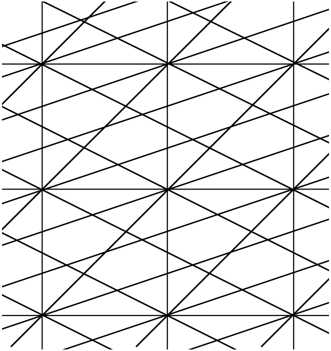
Summarizing 1 and 2: since all constructions are local, in this way we can approximate all energies

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

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., $\varphi \geq \|\cdot\|_1$

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}, $\Pi_j := \{\langle x, \nu_j \rangle = 0\}$,

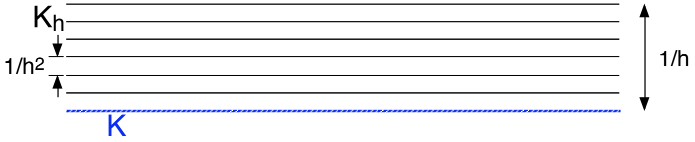
$$K_h = \frac{1}{h}\mathbb{Z}^d + \bigcup_{j=1}^{h} \Pi_j,$$

$b_h = 0$ 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)

K_h locally of the form



We can obtain all energies of the form

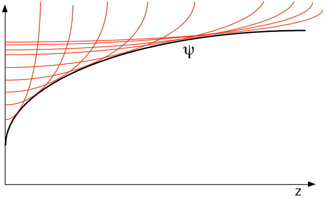
$$F_\psi(u) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \psi(|u^+ - u^-|) d\mathcal{H}^{d-1},$$

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

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

Proof. Choose $a_j \geq \sqrt{d}$, $b_j \geq 0$ 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 $\varphi \geq \|\cdot\|_1$ 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.

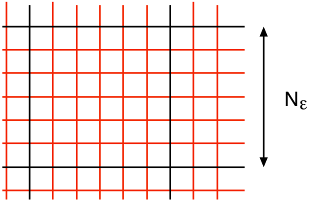
- F with constrained jump set: $S(u) \subset K$
- non-finite φ (as for layered defects)
- non-concave subadditive ψ such as $\sqrt{d}\,\mathrm{sub}(1+z^2)$; etc.

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 prescribed 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 $N_\varepsilon \to +\infty$, $\varepsilon N_\varepsilon \to 0$)

Conclusions

Defects can be modeled as two-phase discrete interactions
• **random setting** (*prototype of variational problems with percolation*): requires independent random variables to avoid uncontrolled effects on exceptional surfaces.
Leading to a wide range of open questions for “variational” percolation problems, completely unexplored for $d \geq 3$

• **G-closure setting** (*prototype of design problems for materials with different scales*): requires construction of surface energies using homogenization, capacitary and subadditive arguments.
A variety of complex energies can be obtained, but that is only a partial description due to lack of general approximation results for surface energy densities.