Local minimization, variational evolution and Γ-convergence

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Multi-Scale Modeling and Characterization
of Innovative Materials and Structures

General Issue:

the description of the limit behavior of energy-driven systems involving a small parameter

Model problems

Gradient theory of phase transitions (scalar Ginzburg-Landau)

$$F_\varepsilon(u) = \int_\Omega \Big(\varepsilon^2 |\nabla u|^2 + (1-u^2)^2\Big)dx, \qquad u : \Omega \to \mathbb{R}$$

(Lennard-Jones) atomistic systems

$$F_\varepsilon(u) = \sum_{i\neq j} J\Big(\frac{|u_i - u_j|}{\varepsilon}\Big) \qquad u_1, \ldots, u_{N_\varepsilon} \in \mathbb{R}^n$$

Homogenization (of surface energies)

$$F_\varepsilon(A) = \int_{\partial A} a\Big(\frac{x}{\varepsilon}\Big) d\mathcal{H}^1 \qquad A \subset \mathbb{R}^2$$

Global minimization:

can be stated in terms of De Giorgi's **Γ-convergence**. Up to technicalities,

$$F_\varepsilon \xrightarrow{\Gamma} F_0 \qquad \Longleftrightarrow \qquad \min\{F_\varepsilon + G\} \to \min\{F_0 + G\}$$

(+ convergence of minimum points) for all G continuous perturbations

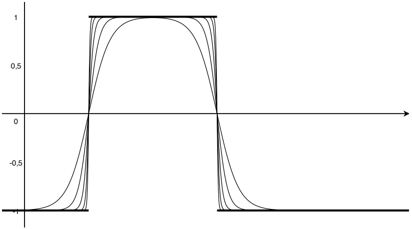
Model problems

Scalar Ginzburg Landau. after scaling the energies by $\dfrac{1}{\varepsilon}$ we have a *sharp-interface limit*

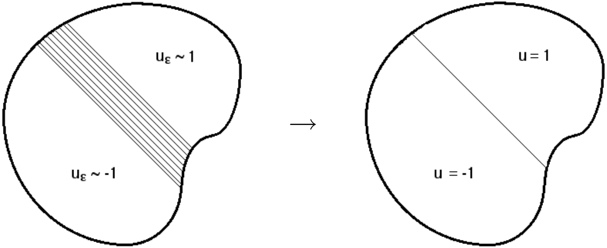
$$F_0(u) = \frac{4}{3}\mathcal{H}^{n-1}(\partial\{u=1\}\cap\Omega) \qquad u \in BV(\Omega;\{\pm 1\})$$

(Modica-Mortola 1977)

1D picture: $\#$ of interfaces for piecewise-constant limit



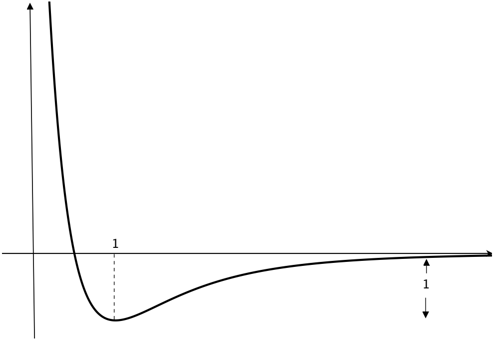
2D (and higher) picture: minimal-interface limit problems



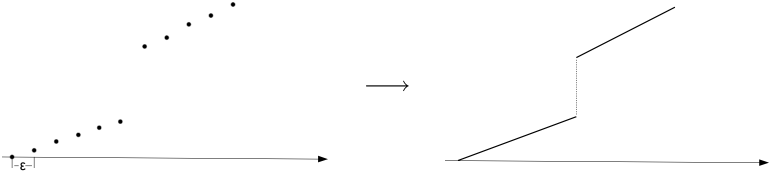
1D atomistic systems (nearest-neighbour interactions)

$$F_\varepsilon(u) = \sum_i J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big)$$

L-J potential



We regard u_i as values of a function defined in $\varepsilon\mathbb{Z}$ and identify it with its piecewise-affine interpolation $u : [0,1] \to \mathbb{R}$



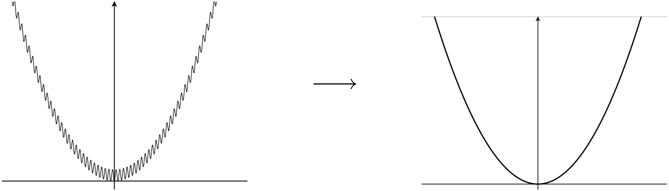
After scaling the variable $v = \sqrt{\varepsilon}(u - id)$ we have

$$F_0(v) = \int_0^1 |v'|^2 \, dx + \#(S(v))$$

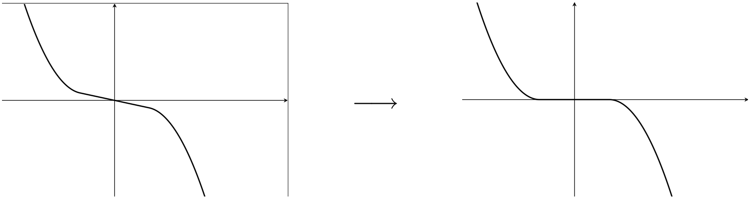
with the constraint $v^+ > v^-$ (defined on piecewise-Sobolev functions)
(**Griffith Fracture Energy**/ Mumford-Shah Functional **with unilateral constraint on the jump opening**)
(B-Lew-Ortiz ARMA 2006)

Local minimization

In general Γ-convergence does not imply any relation between local minimizers of F_ε and F_0 (as for functions in $\mathbb{R}$)



(loss of local minimizers)



(appearance of local minimizers)

Examples

• In 1D **all functions** $u \in BV(\Omega; \{\pm 1\})$ are local minimizers for the sharp-interface model, but the scalar Ginzburg-Landau energy has **no** non-trivial local minimizers.

• In 1D the **Griffith fracture energy** with boundary conditions $v(0) = 0$, $v(1) = L$ has local minimizers:

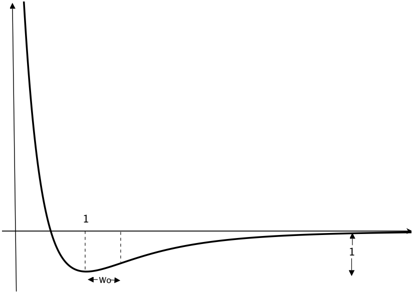
1) the uniform state $u(x) = Lx$ (with energy L^2)

2) *all* (increasing) piecewise-constant functions (with energy k = number of jumps)

Note that the global minimizer is the uniform state if $L^2 \leq 1$.

Local minima for 1D Lennard-Jones systems

$$F_\varepsilon(u) = \sum_i J\left(\frac{u_i - u_{i-1}}{\varepsilon}\right)$$



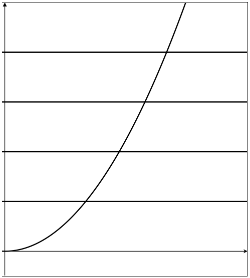
In scaled variables $v = \sqrt{\varepsilon}(u - \mathrm{id})$

1) the uniform state : (discretization of) $v = Lx$ (*up to the inflection point* $L = w_0/\sqrt{\varepsilon}$)

2) a uniform state except for **one** interaction exceeding the inflection point (corresponding to one limit jump)

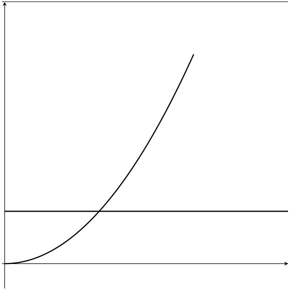
Comparison of patterns of local minima for Lennard-Jones systems, in terms of the total displacement L,

of F_0



(uniform states + *states with* n *jumps)*

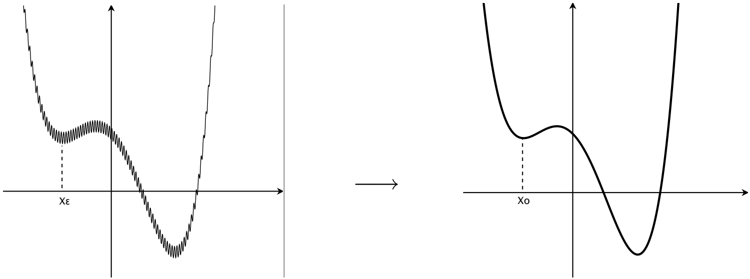
and of F_ε



(uniform states *up to (scaled) inflection point* + minimizer with 1 jump)

Kohn-Sternberg variational principle

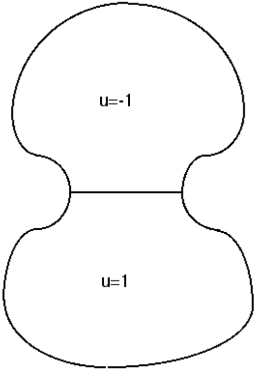
If x_0 is an **isolated** local minimizer for $F_0 = \Gamma\text{-}\lim_\varepsilon F_\varepsilon$ then there exist $x_\varepsilon \to x_0$ local minimizers of F_ε.



This is an immediate consequence of the 'local' character of Γ-convergence

An application (Kohn-Sternberg)

Existence of non-trivial solution of the Allen-Cahn equation (Euler-Lagrange equation for the scalar Ginzburg-Landau energy) in domains with a ‘neck’. Proved by showing the existence of a local-minimizing interface

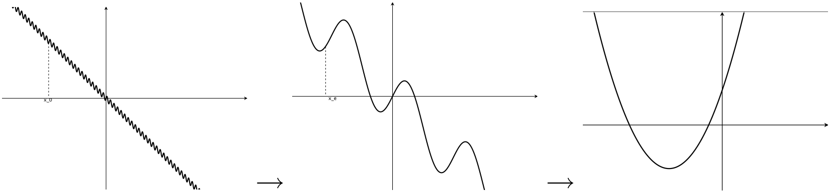


Generalizations

The same principle can be applied if we have an isolated local minimizer of the Γ-limit of the *scaled* functionals

$$G_\varepsilon(v) = \frac{1}{\lambda_\varepsilon}\Big(F_\varepsilon(\rho_\varepsilon v_\varepsilon + x_\varepsilon) - m_\varepsilon\Big)$$

with $x_\varepsilon \to x_0$, $\rho_\varepsilon \to 0$, $\lambda_\varepsilon \to 0$, $m_\varepsilon \in \mathbb{R}$



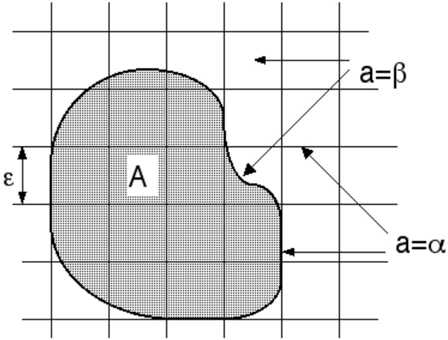
This can be used to prove the existence of multiple local minimizers

Example of application

Density of local minimizers for the inhomogeneous perimeter functionals

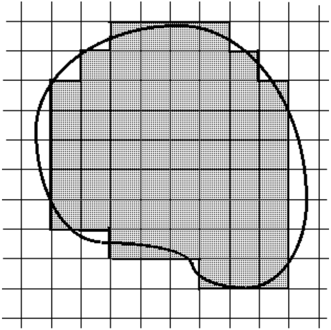
$$F_\varepsilon(A) = \int_{\partial A} a\Big(\frac{x}{\varepsilon}\Big) d\mathcal{H}^1$$

a 1-periodic with $a(y_1, y_2) = \alpha$ if $y_1 y_2 = 0$,
$a(y_1, y_2) = \beta > 2\alpha > 0$ otherwise in $(0,1)^2$



$$F_0(A) = \alpha \int_{\partial A} \|\nu\|_1 d\mathcal{H}^1$$

($\|\nu\|_1 = |\nu_1| + |\nu_2|$, ν normal to ∂A) (**crystalline perimeter**)



F_0 has no non-trivial local minimizer, but for all A there exists $A_\varepsilon \to A$ and A_ε local minimizer of F_ε

Local minimization as a choice criterion

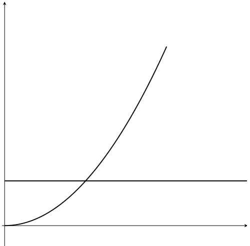
Γ-equivalence: $G_\varepsilon \approx F_\varepsilon$ if "they have the same Γ-limits"
(cf. the notion of Γ-expansion, B-Truskinovsky CMT 2010)

Choice criterion: among equivalent theories of a *desired form* choose the one(s) *maintaining the pattern of local minima*

Example: cohesive fracture from Lennard-Jones potentials

$$F_\varepsilon(u) = \sum_i J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big)$$

Pattern of local minima for F_ε
in terms of boundary condition



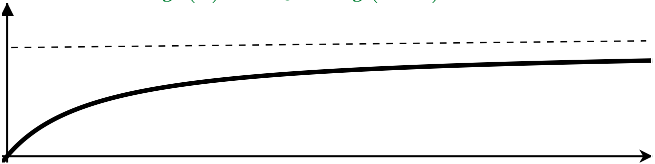
The same pattern can be achieved with *fracture energies*

$$G_\varepsilon(v) = \int_0^1 |v'|^2\,dt + \sum_{S(v)} g_\varepsilon(v^+ - v^-) \qquad v^+ > v^-$$

(this is the "desired form")

Possible g_ε: $g_\varepsilon(z) = g(z/\sqrt{\varepsilon})$ with g strictly concave and

$$g'(0) = w_0 \qquad g(+\infty) = 1$$



(**Barenblatt cohesive-fracture energy density**)

This argument provides a "validation" of a widely used Fracture Mechanics model

(B-Dal Maso-Garroni ARMA 1999, revisited)

Evolution by local minimization: Minimizing Movements

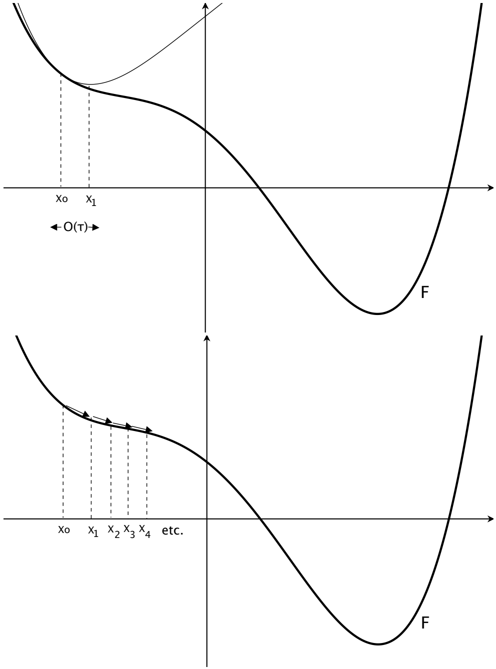
For a single energy F (*Hilbert-space setting*)
(1) (**time-discrete scheme**) fix $\tau > 0$ time-discretization parameter, and initial datum u_0 define u^τ_{k+1} recursively as a minimizer of

$$\min\Big\{F(u) + \frac{1}{2\tau}\|u - u^\tau_k\|^2\Big\}$$

(dissipation $D(u) = \frac{1}{2\tau}\|u\|^2$)

(2) (**passage to the limit**) define $u^\tau(t) = u^\tau_{\lfloor t/\tau \rfloor}$ and pass to the limit as $\tau \to 0$ (up to subsequences).

Each limit u is called a **minimizing movement** for F from u_0 (Almgren-Taylor-Wang, De Giorgi, Ambrosio, etc.)



xo
x1
O(τ)
F
xo
x1
x2
x3
x4
etc.
F

Remarks

1. (**approximation of gradient flow**) If F is differentiable from the E-L equation

$$\frac{\partial u}{\partial t} \approx \frac{u^\tau_{k+1} - u^\tau_k}{\tau} = -\nabla F(u^\tau_{k+1}) \approx -\nabla F(u(t))$$

2. F need not be differentiable, just lower semicontinuous and coercive

3. (**trivial motions from local minima**) if u_0 is a local minimum for F then $u(t) = u_0$ for all t

4. We can add a forcing term by considering $F = F(t, u)$ and compare with quasistatic motion (obtained by global minimization at all t, with no dissipation)).

Example: 1D Griffith fracture with $u_0 = 0$ and as forcing term the boundary condition $u(0) = 0$, $u(1) = t$
quasistatic: fracture at a critical t_c ($t_c = 1$ for our parameters)
minimizing movement: no fracture, evolution following the heat equation

Minimizing movements along a sequence F_ε

For a family of energies F_ε (*Hilbert-space setting*)
(1) (**time-discrete scheme**) fix $\tau > 0$, $\varepsilon > 0$, and initial datum u_0 (or u_0^ε) define $u_{k+1}^{\tau,\varepsilon}$ recursively as a minimizer of

$$\min\Big\{F_\varepsilon(u) + \frac{1}{2\tau}\|u - u_k^{\tau,\varepsilon}\|^2\Big\}$$

(2) (**passage to the limit**) define $u^{\tau,\varepsilon}(t) = u^{\tau,\varepsilon}_{\lfloor t/\tau \rfloor}$ and pass to the limit as $\tau \to 0$ and $\varepsilon \to 0$ (up to subsequences).

Each such limit is called a **minimizing movement along F_ε** from u_0

Note: the limit depends on how $\tau \to 0$ and $\varepsilon \to 0$ (simultaneously)

(In)compatibility with Γ-convergence

Theorem (extreme asymptotic behaviours)
(a) if $\tau << \varepsilon$ *fast enough* then the MM along F_ε from u_0 is a limit of the MM for F_ε from u_0 (at ε fixed) as $\varepsilon \to 0$ ("the MM is the limit of the Gradient Flows")
(b) if $\varepsilon << \tau$ *fast enough* and $F_\varepsilon \xrightarrow{\Gamma} F_0$ then the MM along F_ε from u_0 is a MM for F_0 from u_0 ("the MM is the Gradient Flow of the limit")

Proof: use of the property of convergence of minimum problems.

Theorem (stability for convex energies)
If F_ε are convex and $F_\varepsilon \xrightarrow{\Gamma} F_0$ then all MM are equal (to the unique MM for F_0)

Proof: use of the theory of Gradient Flows by Ambrosio-Gigli-Savaré in the case $\tau << \varepsilon$

General picture

• if $\tau << \varepsilon$ *fast enough* then we may have "pinning" at local minimizers of F_ε

• if $\varepsilon << \tau$ *fast enough* then we have the MM of the limit

• at a **critical regime** we have an "interpolation" of the extreme cases.

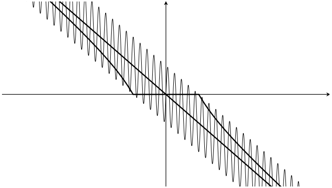
A simple example

In $\mathbb{R}$ consider $F_\varepsilon(x) = -\varepsilon \sin\left(\frac{x}{\varepsilon}\right) + \frac{1}{2}x^2$

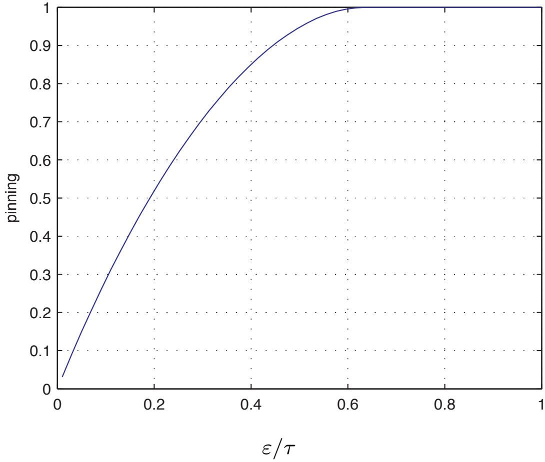
- critical regime: $\varepsilon \approx \tau$
- for $\varepsilon << \tau$ the limit satisfies $x' = -x$ (corresp., $F_0(x) = \frac{1}{2}x^2$)
- for $\tau << \varepsilon$ we compute the limit of the gradient flows

$$x'_\varepsilon = \cos\left(\frac{x_\varepsilon}{\varepsilon}\right) - x_\varepsilon$$

which converge to $x' = -\operatorname{sign} x \sqrt{(x^2-1)^+}$



- for $\tau \approx \varepsilon$ the pinning threshold moves from 0 to 1



Example of a Geometric Evolution

(B-Gelli-Novaga ARMA 2010) F_ε = inhomogeneous perimeter converging to F_0 = α times the crystalline perimeter.

critical regime: $\tau \approx \varepsilon$

• if $\tau << \varepsilon$ all initial data are pinned (by density of loc. min.)

• if $\varepsilon << \tau$ the MM of the limit F_0 is motion by crystalline curvature (Almgren Taylor) with law for the velocity $v = 2\alpha k$, where κ is the suitably defined crystalline curvature.

• (**effective homogenized motion**) if $\frac{\tau}{\varepsilon} \to \gamma$ then the law is

$$v = \frac{1}{\gamma} \lfloor 2\alpha\gamma\kappa \rfloor$$

Note: the case $\gamma = 1$ gives every MM

Note: the "interpolation" between the cases $\tau << \varepsilon$ and $\varepsilon << \tau$ depends on the details of F_ε: in this example we may have

$$\widetilde{F}_\varepsilon(A) = \int_{\partial A} \widetilde{a}\Big(\frac{x}{\varepsilon}\Big) d\mathcal{H}^1$$

with the same Γ-limit and with the same total pinning for $\tau << \varepsilon$ but with a different law for the velocity: we may have a **homogenized** effective motion

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

with $f_{\rm hom}$ highlighting a "microscopic" homogenization of the velocity. In particular we have an effective pinning threshold depending on the "geometry" of $\widetilde{a}$
(B-Scilla 2012, Scilla 2013)

Time scaling

We may introduce (time-)scale λ and consider the iterations $u^{\tau,\varepsilon}_{\lambda,k+1}$ by minimization of

$$\min\Big\{\frac{1}{\lambda}F_\varepsilon(u) + \frac{1}{2\tau}\|u - u^{\tau,\varepsilon}_{\lambda,k}\|^2\Big\}.$$

- this corresponds to considering *time-scaled trajectories*

$$u^{\tau,\varepsilon}_\lambda(t) = u^{\tau,\varepsilon}(\lambda t)$$

for the MM along F_ε.
If $\lambda \to 0$ then we look for long-time behavior of $u^{\tau,\varepsilon}$

- this procedure is meaningful also if $F_\varepsilon = F$.

Example. For the 1D scalar Ginzburg-Landau equation we obtain motion with λ_ε exponential (Kohn-Bronsard). Note that all u are locally minimizing for F_0 (usual time scale gives pinning)

Example (long-time behaviour for Lennard-Jones systems).

• in this case we have *stability*, even though F_ε are not convex, and we always converge to the MM of the Griffith/Mumford-Shah functional (B-Defranceschi-Vitali)

• piecewise-constant initial data u_0 are local minima for F_0; hence, for such u_0 we have pinning for the limit;

• if $\lambda_\varepsilon = \varepsilon^6$ the MM along $F_\varepsilon/\lambda_\varepsilon$ from u_0 piecewise-constant is non trivial.

• (long-time "validation" of the Cohesive Fracture model) if we take the Barenblatt cohesive-fracture energies with

$$g(w) \approx 1 - \frac{1}{w^6} + o\Big(\frac{1}{w^6}\Big)$$

then we have the same long-time behavior.

Other issues:

• use of MM for suitable F_ε to define a motion for ill-posed problems (e.g., backward motions, gradient flow for non-convex energies, etc.)

• asymptotics of stable points (few results by Sandier-Serfaty, Jerrard-Sternberg, B-Larsen)

• connection with *quasistatic motion* (formally obtained by time-scaling $\lambda = 0$)

• etc.

Lecture notes: B. Local minimization, variational evolution and Γ-convergence (downloadable from my web page)

Thank you for your attention!