Phase–field method and optimal design

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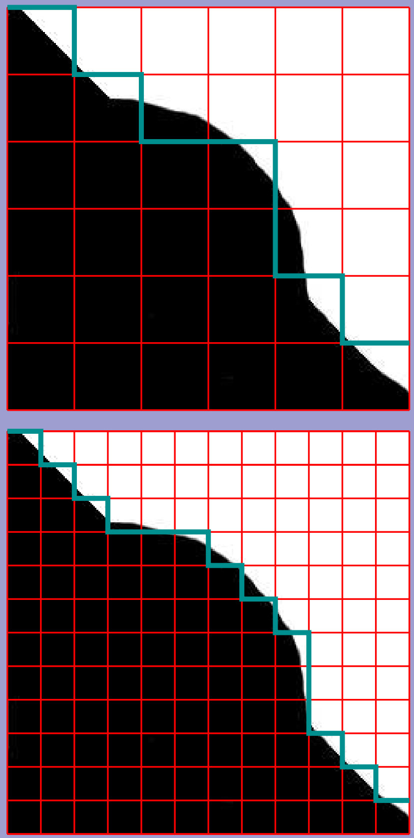
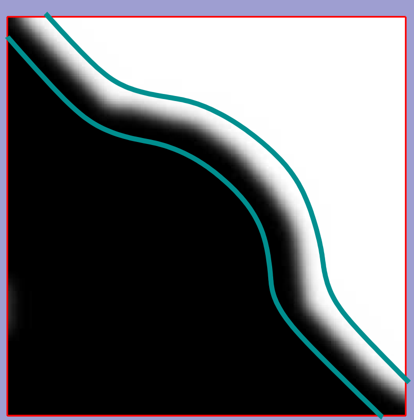
Fundamental idea



Problem involving a set D and its interface $F(D, \partial D)$:

- Represent $D \longleftrightarrow \chi$
  approximate its volume/area
  $$|D| \longleftrightarrow \int_\Omega \chi \, dx \longleftrightarrow \int_\Omega \chi_h \, dx$$
- Represent $\partial D \longleftrightarrow J_\chi$
  approximate its area/length
  $$\mathcal{H}^{N-1}(\partial D) \longleftrightarrow \mathcal{H}^{N-1}(J_\chi) \longleftrightarrow ?$$



- Introduce a characteristic length ε.
- **Diffuse** the interface

Phase field method

- Minimization problem
- Free Discontinuity Problems

$$\min_{D \text{ admissible}} F(D, \partial D) \text{ or } \min_{u \text{ admissible}} F(u, J_u).$$

  - Mumford-Shah:
    $E(u, J_u) = \int_\Omega |\nabla u|^2 \, dx + \int_\Omega (u - g)^2 \, dx + \mathcal{H}^{N-1}(J_u)$
  - Minimum interface problem: $F(D, \partial D) = \mathcal{H}^{N-1}(\partial D)$.
  - Regularization of inverse problems.
  - Regularization of optimal design problems.
- Variational approximation of functionals:
  $F_\varepsilon(u) \stackrel{?}{\longrightarrow} F(u, J_u)$, Γ–convergence.

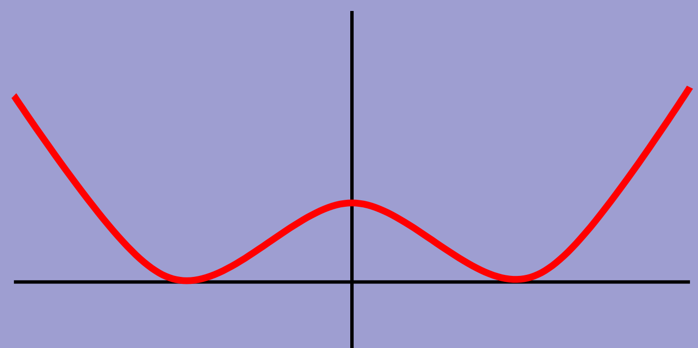
A first example

$$P(\chi, J_\chi) = \mathcal{H}^{N-1}(J_\chi \cap \Omega)$$

$$P_\varepsilon(\varphi) = \int_\Omega \varepsilon |\nabla \varphi|^2 + \frac{1}{\varepsilon} W(\varphi)\, dx.$$

$$P_\varepsilon \stackrel{\Gamma}{\rightharpoonup} P$$

- $\forall \varphi_\varepsilon \longrightarrow \chi, \underline{\lim} P_\varepsilon(\varphi_\varepsilon) \geq P(\chi, J_\chi)$
  $\exists \varphi_\varepsilon \longrightarrow \chi, \overline{\lim} P_\varepsilon(\varphi_\varepsilon) \leq P(\chi, J_\chi)$
- The minimizers of P_ε converge to that of P



Building up

Γ–convergence stable wrt continuous perturbation

- F continuous , then $F + P_\varepsilon \stackrel{\Gamma}{\rightharpoonup} F + P$, ex. regularization for inverse problems
- Implement constraints by means of Lagrange multiplicators Volume constraints
- Surface terms: $\nabla\varphi_\varepsilon \rightharpoonup \mathcal{H}^{N-1} \llcorner J_\varphi . \nu_\varphi$

Also a numerical method

- Fix ε relatively to the discretization, and minimize
- Only continuous functions
- Only one dimensionality
- Not tied to a specific numerical method

Simple restoration problem

Joint work with M. Burger

Problem: $F(\chi) = \int_\Omega |u_\chi - f|^2 \, dx$, where u_χ is the solution of $\Delta u_\chi = \chi$, $u_\chi = 0$ on $\partial\Gamma$.

- "Perimeter penalization": $\min\limits_{\chi} F(\chi) + \lambda \mathcal{H}^{N-1}(J_\chi)$, λ small.
- Phase field approximation: $\min\limits_{\varphi} \int_\Omega |u_\varphi - f|^2 \, dx + \lambda P_\varepsilon(\varphi)$, where $\Delta u_\varphi = \varphi$.
- Finite element discretization.
- Gradient descent.
  $$\varphi_{n+1} = \varphi_n + r_n \delta^{-1} \left(\delta^{-1} \varphi_n - f\right) + \lambda \int_\Omega \frac{1}{\varepsilon} W'(\varphi_n) - 2\varepsilon \Delta \varphi_n \, dx$$

Phase–field and optimal design

- Admissible designs:
  Partitions $D_1, \ldots, D_p$ of a ground domain Ω.
  Fixed volume fractions: $|D_i| = \theta_i |\Omega|$, $\sum \theta_i = 1$.
- Objective function:

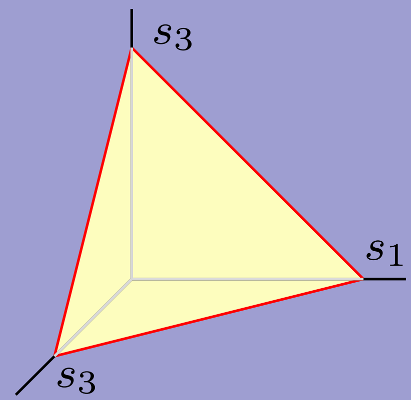
$$F(D_1, \ldots, D_p) \text{ or } F\left(D_1, \ldots, D_p, (\partial D_i \cap \partial D_j)_{i,j}\right)$$

$$\inf_{D_1,\ldots,D_p \text{ admissible}} F$$

- Ill-posed in general
  Non-compactness of admissible designs, existence of solutions is not granted, without knowledge of the properties of F.

$$\inf_{D_1,\ldots D_p} F(D_1, \ldots, D_p) + \sum \lambda_{i,j} \mathcal{H}^{N-1}(\partial D_i \cap \partial D_j)$$

Phase–field approximation

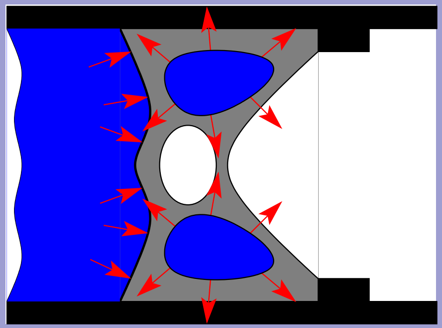


- s_i: vertices of p–dimensional simplex
- *Phase–field*:
  $\rho \in H^1(\Omega\,;\,\mathbb{R}^p)$
- p–wells potential:
  $W(x) > 0$ if $x \notin \{s_1, \ldots, s_p\}$, $W(s_i) = 0$
  $$\lambda_{i,j} = \sqrt{2}\int_{s_i}^{s_j} W^{1/2}(s)\,ds$$
- Variational approximation of the perimeters

$$\int_\Omega \varepsilon|D\rho|^2 + \frac{1}{\varepsilon}W(\rho)\,dx \xrightarrow{\Gamma} \sum \lambda_{i,j}\mathcal{H}^{N-1}(\partial D_i \cap \partial D_j).$$

- Independent on material interpolation scheme
- Any dimension, any number of materials, multi-physics...

Application: pressurized structures



- *Three* “phases” S, L, V
- *Design-dependent* pressure force p (surface load)
- *Given* volume fractions θ_S, θ_L, θ_V

Objective function: compliance of the structure

$$\mathcal{C}(S,L,V) := \int_{\partial S\cap\partial L} p(x)\, u^* \cdot \nu_{L,S}\, d\mathcal{H}^{N-1}(x),$$

where

$$\int_S Ee(u^*) : e(v)\, dx = \int_{\partial S\cap\partial L} p(x)\, v\cdot \nu_{L,S}\, d\mathcal{H}^{N-1}(x), \forall v$$

Minimum compliance problem:

$$\inf_{S,L,V} \mathcal{C}(S,L,V) + \lambda\mathcal{H}^1(\partial S)$$

Phases are “ordered”, scalar phase–field

Implementation

- Objective function depends implicitly on the design
  - Explicit expression for $D_\rho C$.
  - Gradient–based descent scheme (semi-explicit in ρ.)
- Volume fractions through Lagrange multipliers
- Good approximation of $\mathcal{P}_\varepsilon$ requires fine discretization
  - But we don't need very accurate approximation of $\mathcal{P}_\varepsilon$
  - Isotropy important: linear finite elements, unstructured triangulations
- Each iteration requires solving an elasticity problem (PDE constrained optimization)
- Non convex problem: local minimizers, stability
  - Continuation method
  - Prediction/correction descent step

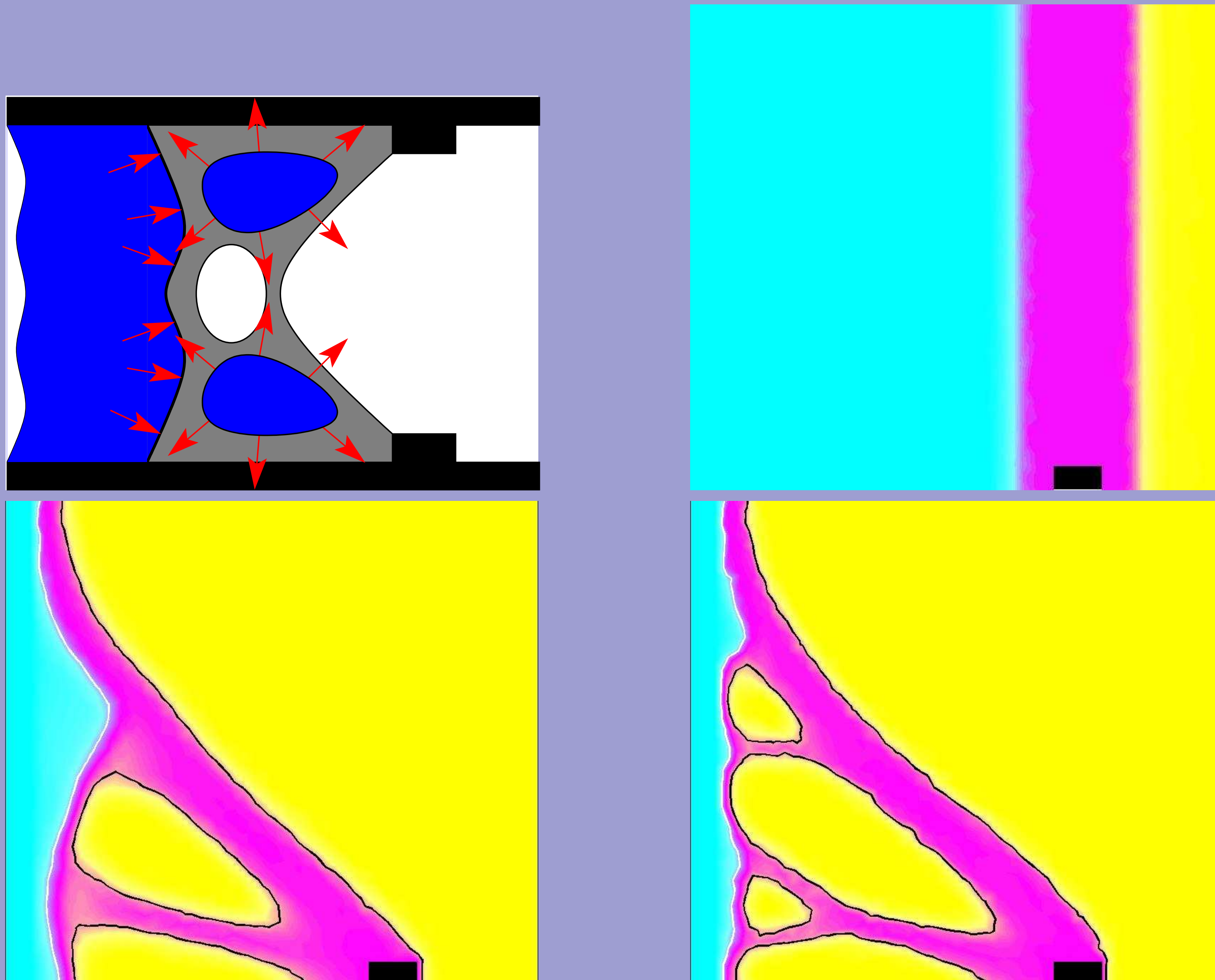
Implementation -2-

- Semi implicit scheme
  - Explicit step:
    $\rho^{n+1} = \rho^n - r\left(\frac{\lambda}{\varepsilon} W'(\rho^n) - 2\,\lambda\varepsilon\Delta\rho^n + D_\rho C(\rho^n)\right)$
  - take k such that $W(x) + k\frac{x^2}{2}$ is convex in $[-1, 1]$

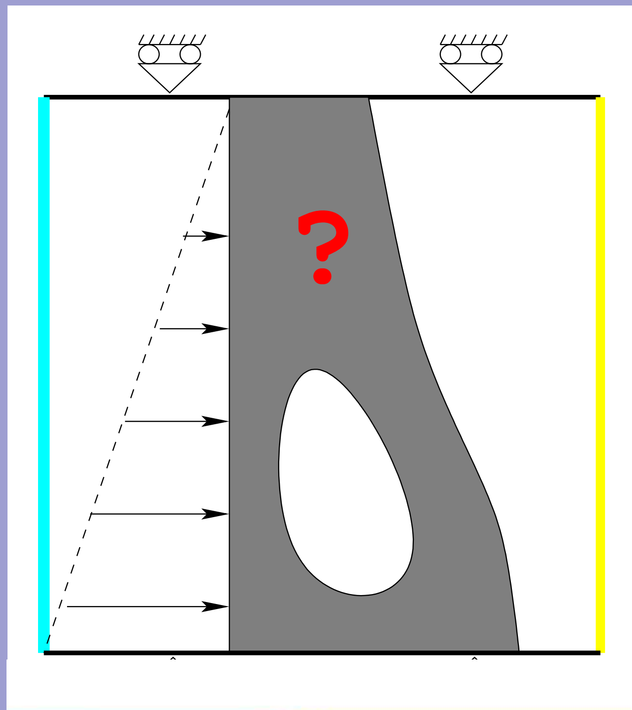
$$(1 - k\lambda\frac{r}{\varepsilon} - 2r\lambda\varepsilon\Delta)\rho^{n+1} = \rho^n - \lambda\frac{r}{\varepsilon}(W' + k)(\rho^n) - rD_\rho C(\rho^n)$$

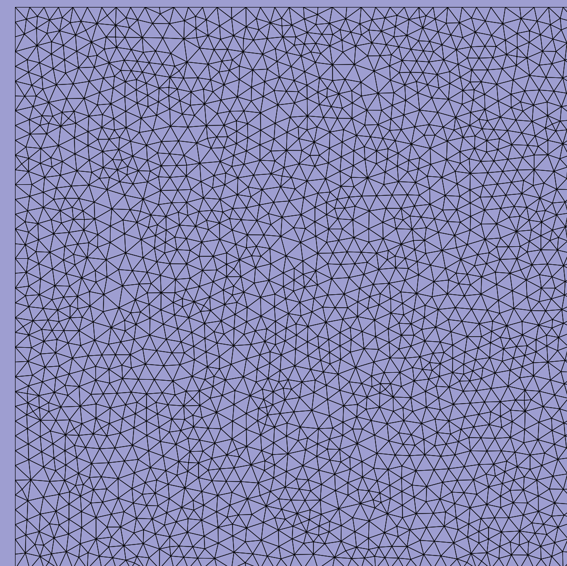
- Continuation
  - "Intuitively": gradually increase λ.
  - "Front propagation speed" depends on ε.
  - Gradually *increase* r, *decrease* ε.
    (Graduate non-convexity)
- Prediction / correction
  - Gradually increase the step r.
  - If the objective function increases, reduce r, roll back a few iterations

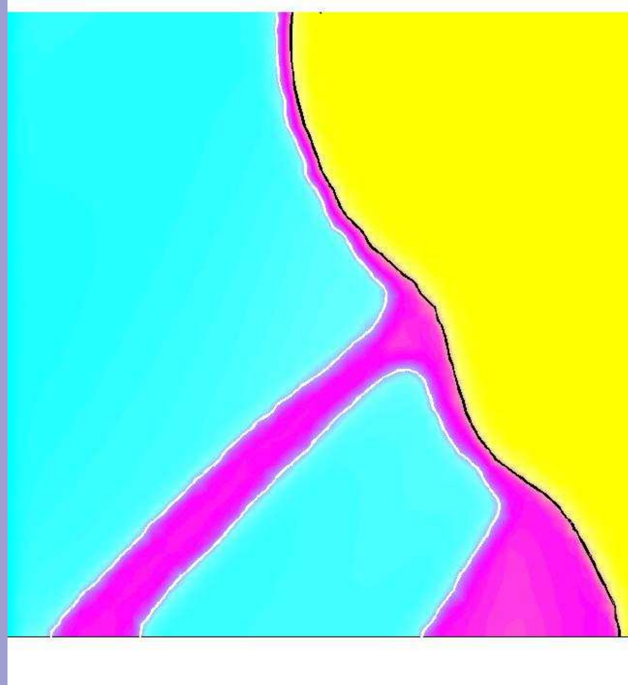
Design of a cork

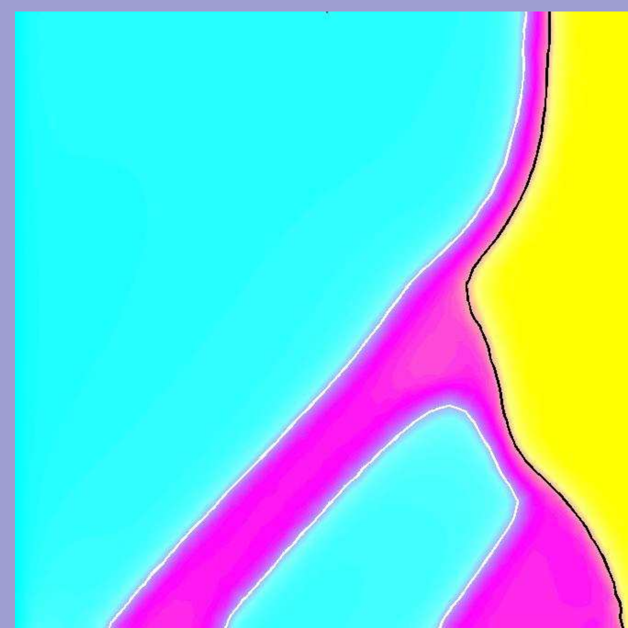


Design of a dam



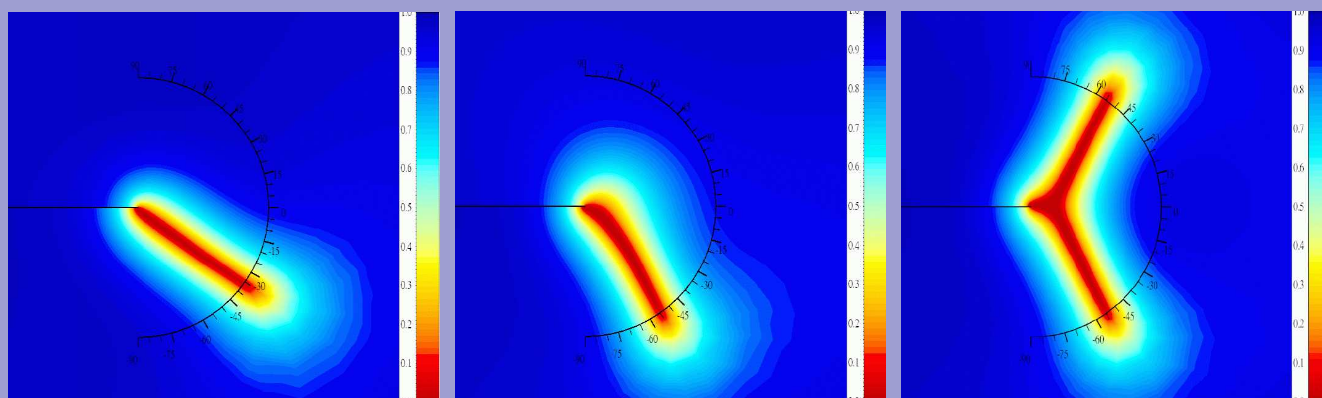






What else...

- Not restricted to closed curves, or perimeter.
  - Image segmentation: Mumford Shah problem
  - Fracture mechanics



- Only for minimization problems.
  Γ–convergence doesn't implies convergence of gradient flows, for instance.
- Deals easily with multiple phases.
  Ordered, or non-ordered.