Level Set Methods for Optimal Design of Two-Phase Composite Materials for Wave Propagation

Alex Kelly, Gregoire Allaire
Supported by Chaire MMSN
Ecole Polytechnique

Formulation of the Problem

$$\rho_\chi \frac{\partial^2 u_\chi}{\partial t^2} - div\left(A_\chi \nabla u_\chi\right) = f$$

Model Problem in Conductivity

$$u_\chi = u_D \text{ on } \Gamma_D$$

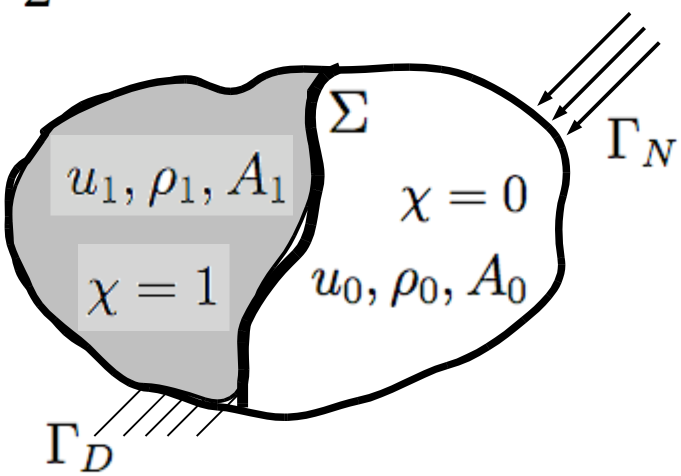
$$A_\chi \nabla u_\chi \cdot \hat{n} = g \text{ on } \Gamma_N$$

$$\rho_\chi \frac{\partial^2 u_\chi}{\partial t^2} - div\left(A_\chi e_\chi\right) = f$$

Model Problem in Elasticity

$$A_\chi e_\chi \hat{n} = g \text{ on } \Gamma_N$$

$$e\left(u\right) = \frac{1}{2}\left(\nabla u + \nabla u^T\right)$$



$$\rho_\chi = \chi\rho_1 + \left(1-\chi\right)\rho_0$$

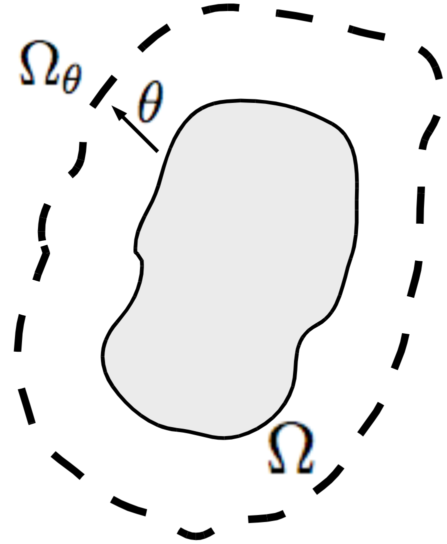
$$A_\chi = \chi A_1 + \left(1-\chi\right) A_0$$

$$u_\chi = \chi u_1 + \left(1-\chi\right) u_0$$

Find the microstructure which minimizes some objective function:

$$J\left(\chi\right) = \int_0^T \int_\Omega j\left(x, u_\chi\left(x\right)\right) dxdt + \int_0^T \int_\Gamma l\left(x, u_\chi\left(x\right)\right) dxdt$$

Hadamard's Method



Desire determination of the *Shape Derivative* →
Define mapping of one shape to a nearby one:

$$\Omega_\theta = (Id + \theta)\,\Omega$$

Definition of directional derivative for $F(\Omega) = \int_\Omega \varphi(x)\,dx$

$$\langle \frac{\partial F}{\partial \Omega}, \theta \rangle = \int_\Omega div\,(\theta(x)\,\varphi(x))\,dx = \int_{\partial\Omega} \theta(x) \cdot \hat{n}(x)\,\varphi(x)\,dx$$

$$F(\Omega) = \int_{\partial\Omega} \phi(x)\,ds$$

$$\langle \frac{\partial F}{\partial \Omega}, \theta \rangle = \int_{\partial\Omega} \theta(x) \cdot \hat{n}(x) \left(\frac{\partial \phi}{\partial n} + H\phi \right) ds \qquad H = div\,(\hat{n})$$

Want to use gradient method to optimize → Exploit the form of the directional derivative:

$$\langle \frac{\partial F}{\partial \Omega}, \theta \rangle = \int_{\partial\Omega} v(x)\,(\theta(x) \cdot \hat{n}(x))\,ds$$

To insure we move in a descent direction select:

$$\theta(x) = -v(x)\,\hat{n}(x)$$

Shape Derivative

To optimize J define the *Lagrangian*:

$$L(\Omega, v, q) = \int_{\Omega}\int_0^T j(x, v(x))\, dtdx + \int_{\partial\Omega}\int_0^T l(x, v(x))\, dtdx - \int_{\Omega}\int_0^T \rho q(x) \cdot \frac{\partial^2 v(x)}{\partial t^2} dtdx$$
$$- \int_{\Omega}\int_0^T Ae(v(x)) \cdot e(q(x))\, dtdx - \int_{\Omega}\int_0^T q(x) \cdot f dtds$$
$$- \int_{\Gamma_N}\int_0^T q(x) \cdot g dtdx \int_{\Gamma_D}\int_0^T (q(x) \cdot Ae(v(x))\, \hat{n} + v(x) \cdot Ae(q(x)))\, dtds$$

Boundary Velocity-chosen to insure directional derivative of the Lagrangian < 0:

$$\langle \frac{\partial L}{\partial \Omega}(\Omega, u, p), \theta \rangle = \int_{\partial\Omega}\int_0^T \theta \cdot \hat{n} \left(j(u(x)) - \rho p(x) \frac{\partial^2 u(x)}{\partial t^2} - Ae(u(x)) \cdot e(p(x)) - p(x) \cdot f \right) dtds$$
$$+ \int_{\partial\Omega}\int_0^T \theta \cdot \hat{n} \left(\frac{\partial l(u(x))}{\partial n} + Hl(u(x)) \right) dtds$$
$$- \int_{\Gamma_N}\int_0^T \theta \cdot \hat{n} \left(\frac{\partial (g \cdot (x))}{\partial n} + Hg \cdot p(x) \right) dtds$$

Two-Phase Complication

Reformulate two separate field equations:

$$\rho_0 \frac{\partial^2 u_0}{\partial t^2} - div\left(A_0 \nabla u_0\right) = f \text{ for } \psi \leq 0 \qquad \rho_1 \frac{\partial^2 u_1}{\partial t^2} - div\left(A_1 \nabla u_1\right) = f \text{ for } \psi \geq 0$$

Shape-Derivative of the associated Lagrangian:

$$\begin{aligned}\langle \frac{\partial L}{\partial \chi}\left(v_0, v_1, q_0, q_1\right), \theta \rangle = \int_{\partial \Omega_0} \int_0^T & \theta \cdot \hat{n}_0 \{ j\left(x, u_0(x)\right) - \rho_0 \frac{\partial^2 u_0(x)}{\partial t^2} \cdot p_0(x) \\ & - \nabla p_0(x) \cdot A_0 \nabla u_0(x) - f_0 \cdot p_0(x) \} dtds \\ + \int_{\partial \Omega_0} \int_0^T & \theta \cdot \hat{n}_1 \{ j\left(x, u_1(x)\right) - \rho_1 \frac{\partial^2 u_1(x)}{\partial t^2} \cdot p_1(x) \\ & - \nabla p_1(x) \cdot A_1 \nabla u_1(x) - f_1 \cdot p_1(x) \} dtds + \ \ldots\end{aligned}$$

Boundary velocity determined by *jump across interface*:

$$v = \int_0^T \left[\!\left[\rho \frac{\partial^2 u(x)}{\partial t^2} \cdot p(x) + \nabla p(x) \cdot A \nabla u(x) - f \cdot p(x) \right]\!\right] dt \text{ on } \Sigma$$

In the case of conductivity*

$$v = \int_0^T \left[\!\left[\rho \frac{\partial^2 u(x)}{\partial t^2} \cdot p(x) \right]\!\right] dt + [\![A]\!] \int_0^T \frac{\partial u(x)}{\partial \tau} \cdot \frac{\partial p(x)}{\partial \tau} dt + [\![A^{-1}]\!] \int_0^T A \frac{\partial u(x)}{\partial n} \cdot A \frac{\partial p(x)}{\partial n} dt - \int_0^T [\![f \cdot p(x)]\!] \, dt$$

*O. Pantz CRAS Paris (2005)

Level Set Method

Phase distribution is represented by a level set function, ψ :

$$\psi \leq 0 \Longrightarrow \chi = 0$$

$$\psi \geq 0 \Longrightarrow \chi = 1$$

Zero level set represents the interface between the two phases.

The evolution of the boundary is represented by the advection of the level set function:

$$\psi\left(\tilde{t}, x\left(\tilde{t}\right)\right) = 0 \text{ for any } x\left(\tilde{t}\right) \in \Sigma$$

From Hamilton-Jacobi equation:

$$\frac{\partial \psi}{\partial \tilde{t}} + v\hat{n} \cdot \nabla\psi = 0 \qquad \hat{n} = \frac{\nabla\psi}{|\nabla\psi|}$$

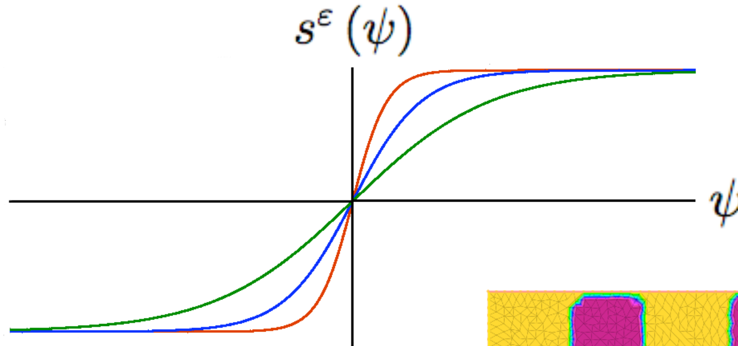
$$\frac{\partial \psi}{\partial \tilde{t}} + v|\nabla\psi| = 0$$

Desire an application of this equation to the entire domain.

Boundary Detection

Advection velocity cannot be assigned immediately to the whole field.
Jump conditions can only be evaluated on the interface.

Approximate sign function:

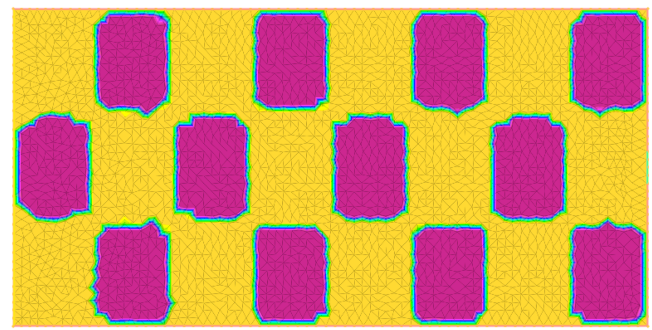


$$s^{\varepsilon}(x) = tanh(\varepsilon\psi)$$

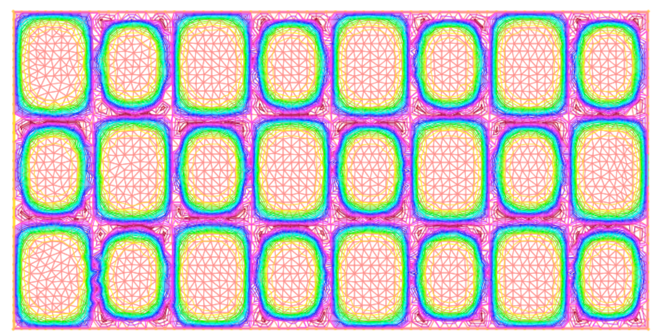
"Dirac mass" on the boundary

$$\int_{\Sigma} f(x)\, ds = \int_{\Omega} f(x)\, \delta_{\Sigma} dx$$

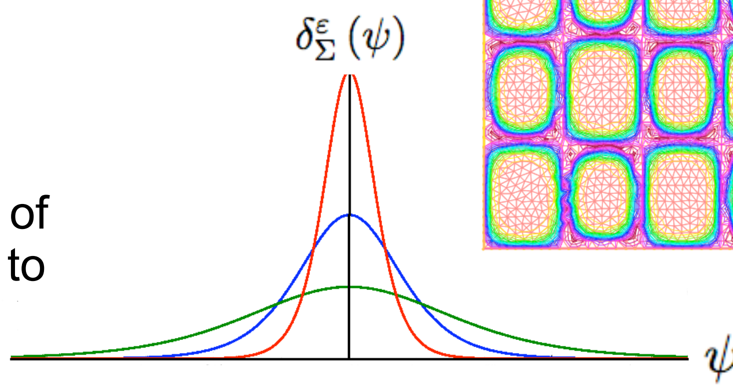
can be recovered from the sign function:



$$\nabla s^{\varepsilon}(x) = \varepsilon sech^2(\varepsilon\psi)$$



$$\delta_{\Sigma}^{\varepsilon} = \frac{1}{2}|\nabla s^{\varepsilon}|$$

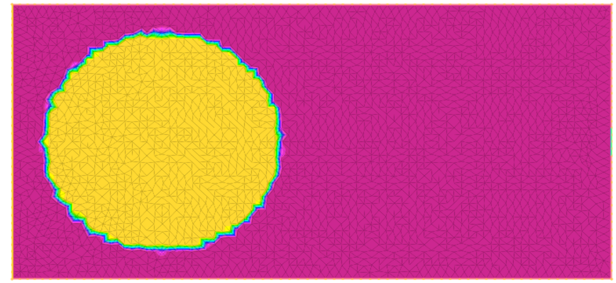


Here ε is chosen to select the width of the boundary (usually about 5 cells to either side)

Jump Conditions → Advection Velocity

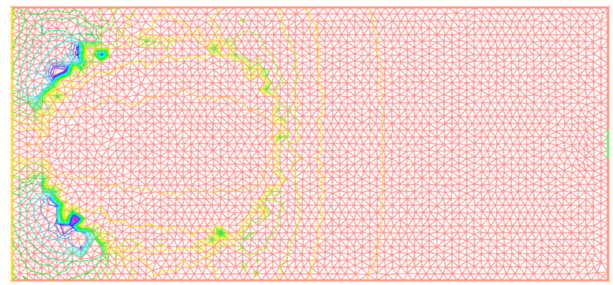
Combine the actual sign function with the approximate Dirac mass to integrate the jump conditions at the interface:

$$\int_{\Sigma} [f]\, ds \approx \frac{1}{2} \int_{\Omega} sgn\left(\psi\right) f \delta_{\Sigma}^{\varepsilon} \left(\psi\right) dx$$



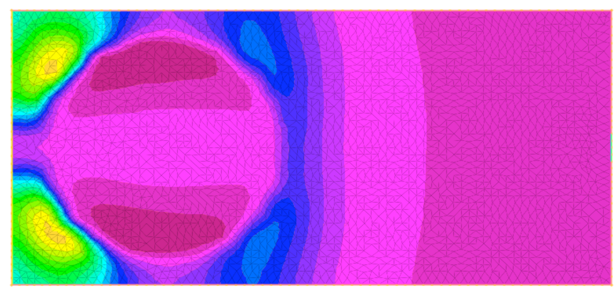
In practice want to smooth this away from the interface:

$$\begin{aligned} -\Delta v + v &= [f]\, \delta_{\Sigma}^{\varepsilon} \text{ in } \Omega \\ v &= 0 \text{ on } \partial\Omega \end{aligned}$$



Yields a simple variational form that can be implemented in FreeFEM++:

$$\int_{\Omega} \left(\nabla v \cdot \nabla \gamma + v\gamma\right) dx = \int_{\Omega} sgn\left(\psi\right) \delta_{\Sigma}^{\varepsilon} f \gamma dx$$



Implementation in FreeFEM++

Level sets tracked by characteristic Galerkin method → FreeFEM++ `convect` operator.

$$\psi^{n+1} = \quad \texttt{convect} \quad \left(\left[v\hat{n}_x, v\hat{n}_y\right], \Delta\tilde{t}, \psi^n\right)$$

Problems with `convect` operator and Finite Elements of type `P2`, implementation with elements of type `P1`

Level set function is periodically reinitialized by iteration of the scheme:

$$\frac{\partial\psi}{\partial\check{t}} + sgn\left(\psi_0\right)\left(|\nabla\psi| - 1\right) = 0$$
$$\psi\left(\check{t} = 0, x\right) = \psi_0\left(x\right)$$

To prevent formation of extraneous structures at the interface possible to penalize the total length of the interface:

$$L_{\text{new}}\left(u_0, u_1, p_0, p1\right) = L\left(u_0, u1, p_0, p_1\right) + \alpha|\Sigma| \qquad \langle\frac{\partial L_{\text{new}}}{\partial\Omega}, \theta\rangle = \langle\frac{\partial L}{\partial\Omega}, \theta\rangle + \alpha\int_\Sigma H\theta\cdot\hat{n}ds$$

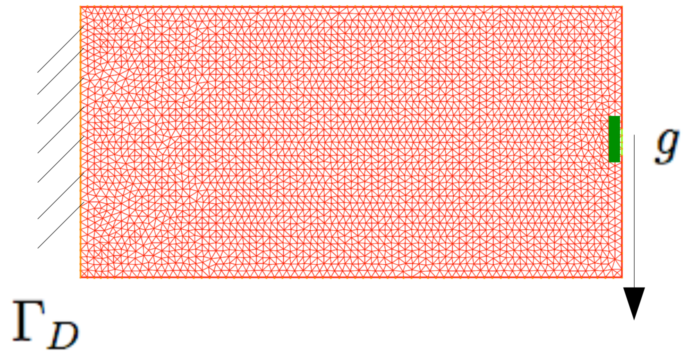
Which leads to new convection scheme:

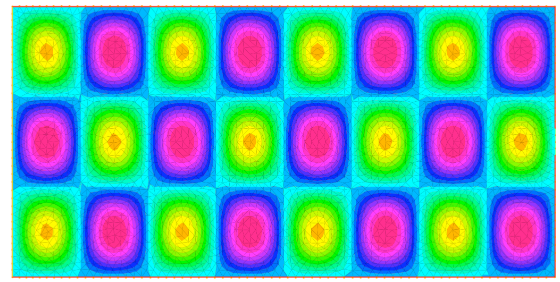
$$\partial_{\tilde{t}}\psi - \left(v + \alpha H\right)|\nabla\psi| = 0$$
$$H = div\left(\frac{\nabla\psi}{|\nabla\psi|}\right)$$

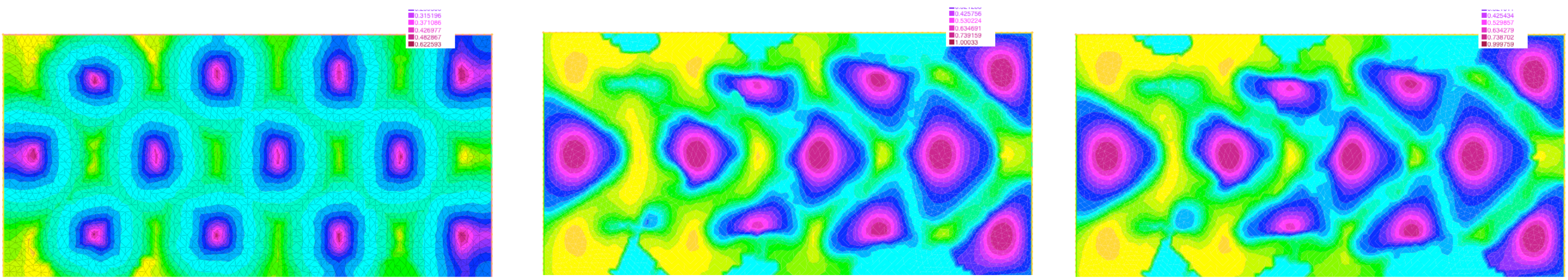
$$\partial_{\tilde{t}}\psi - v|\nabla\psi| - \alpha\left(Id - \frac{\nabla\psi\otimes\nabla\psi}{|\nabla\psi|^2}\right)\cdot\nabla\nabla\psi = 0$$

A Toy Example

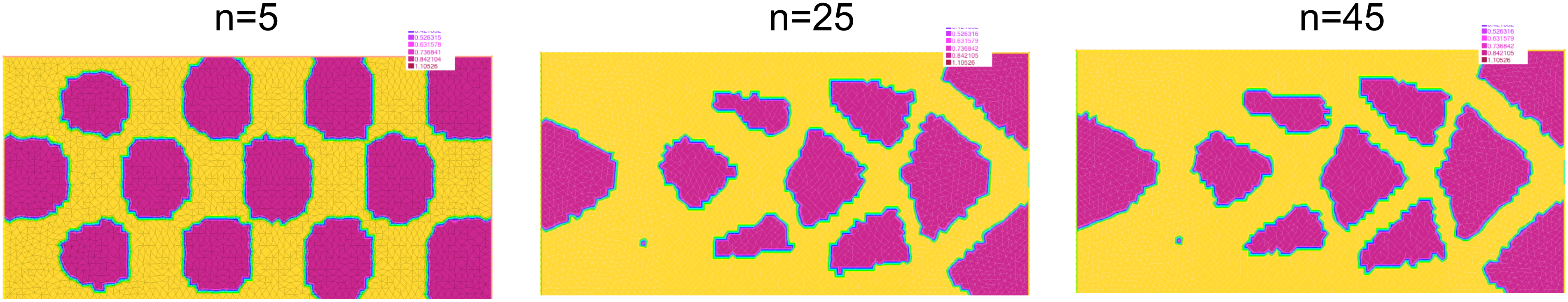
$$J(\chi) = \int_{\Gamma_N} \int_0^T g \cdot u dt dx$$







n=5 n=25 n=45



Conclusions

The evolution of the geometry in the two-phase problem is governed by jumps in the driving force at interfaces between the phases.

This complication is addressed by the using information contained in the level set function to approximate the jumps at each interface. This is used as a source term in a variational form for a velocity equation easily implemented in `FreeFEM++`.

Evolution of the level set function is accomplished by the characteristic Galerkin method that is the standard `convect` operator.

Level set method's relative robustness with regards to 2D → 3D should make 3D implementation in `FreeFEM++` relatively straightforward.