PDE – Benasque 2007

Partial differential equations, optimal design and numerics

From Microscopic Topological Asymptotic to Macroscopic Constitutive Behaviour

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Outline

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- Application of the Topological Derivative
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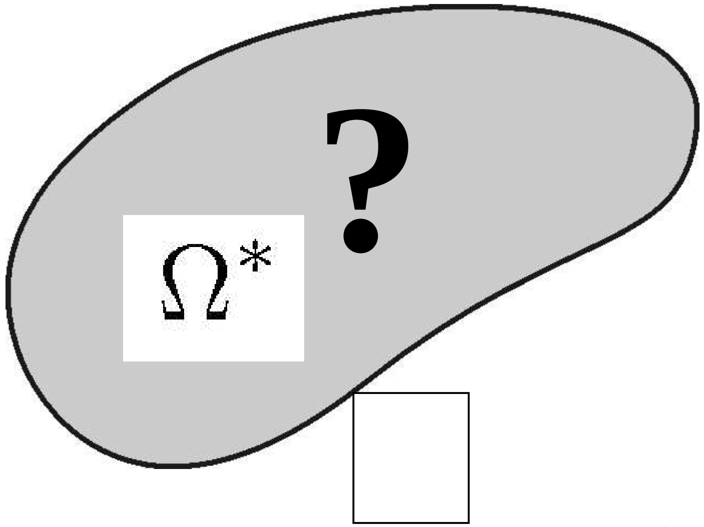
Motivation

$$\begin{cases} \text{find } u \in \mathcal{U}(\Omega), \text{ such that} \\ a(u,\eta) = l(\eta) \quad \forall \eta \in \mathcal{V}(\Omega) \end{cases}$$



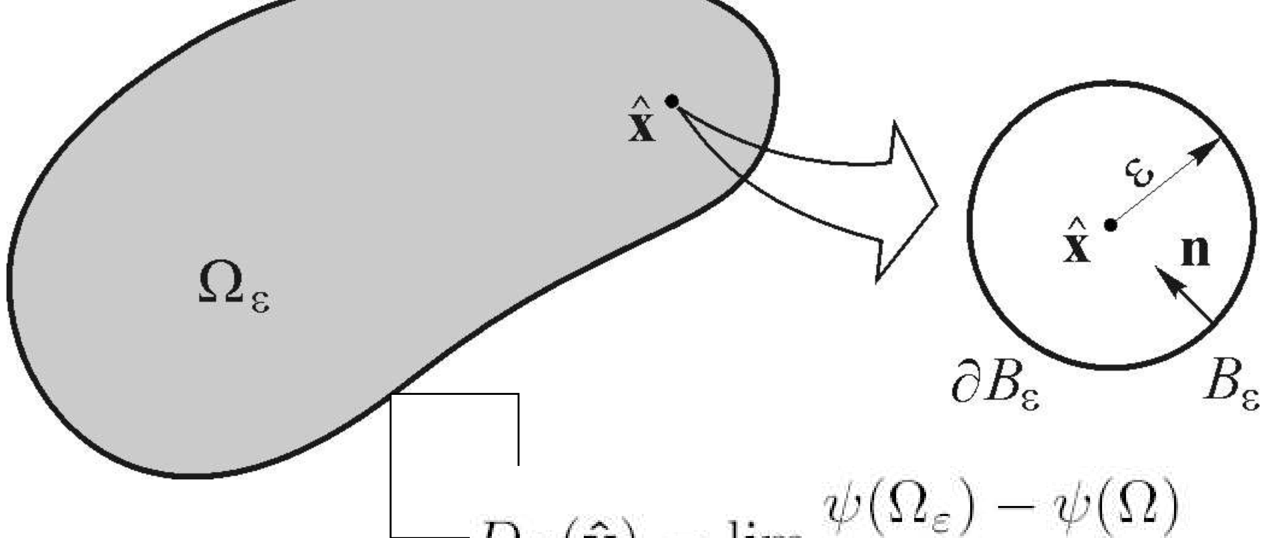
$$\psi(\Omega) = \int_{\varpi} \varphi(u, \nabla u, \nabla\nabla u, ...)$$

$$\varpi = \Omega, \quad \varpi = \partial\Omega \quad \text{or} \quad \varpi \subset \Omega$$

Topological Derivative Concept

Schumacher (1994), Sokolowski (1997), Masmoudi (1998)

$$\Omega_\epsilon = \Omega - \overline{B}_\epsilon$$



$$D_T(\hat{\mathbf{x}}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f(\varepsilon)}$$

$$f(\varepsilon) = |B_\varepsilon|$$

Remark on Second Order Topological Asymptotic

Joint work with J. Rocha de Faria, R.A. Feijóo, E. Tacoco & C. Padra

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f_1(\varepsilon) D_T(\hat{\mathbf{x}}) + f_2(\varepsilon) D_T^2(\hat{\mathbf{x}}) + \mathcal{R}(f_2(\varepsilon))$$

where $f_1(\varepsilon) \to 0$ and $f_2(\varepsilon) \to 0$, when $\varepsilon \to 0^+$, and

$$\lim_{\varepsilon \to 0} \frac{f_2(\varepsilon)}{f_1(\varepsilon)} = 0 \, , \qquad \lim_{\varepsilon \to 0} \frac{\mathcal{R}(f_2(\varepsilon))}{f_2(\varepsilon)} = 0$$

(first order) Topological Derivative

$$D_T(\hat{\mathbf{x}}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f_1(\varepsilon)}$$

Second Order Topological Derivative

$$D_T^2(\hat{\mathbf{x}}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega) - f_1(\varepsilon) D_T(\hat{\mathbf{x}})}{f_2(\varepsilon)}$$

Application for the Laplace Equation

find the temperature field $u \in \mathcal{U}(\Omega)$, such that

$$\int_\Omega \nabla u \cdot \nabla \eta = -\int_{\Gamma_N} q\eta \qquad \forall \eta \in \mathcal{V}(\Omega)$$

$$\mathcal{U}(\Omega) := \{u \in H^n(\Omega) : u|_{\Gamma_D} = \overline{u}\} \qquad \mathcal{V}(\Omega) := \{\eta \in H^n(\Omega) : \eta|_{\Gamma_D} = 0\}$$

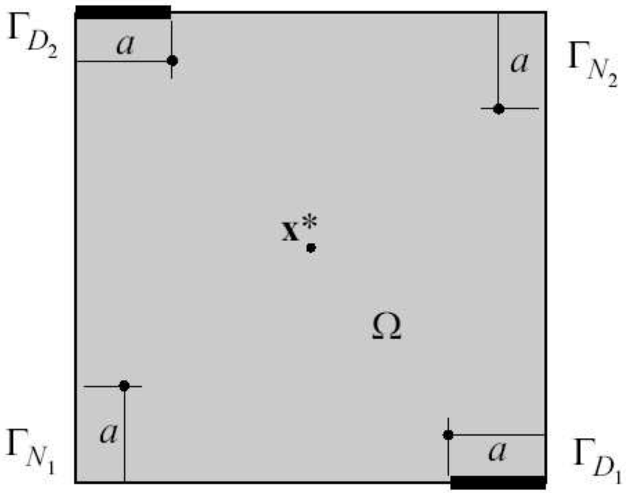
$$\psi(\Omega) = \mathcal{J}_\Omega(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 + \int_{\Gamma_N} qu$$

Neumann boundary condition on the hole

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2 \|\nabla u(\widehat{\mathbf{x}})\|^2 + \pi\varepsilon^4 \left(\frac{1}{2}\det \nabla\nabla u(\widehat{\mathbf{x}}) - \nabla u(\widehat{\mathbf{x}}) \cdot \nabla v(\widehat{\mathbf{x}})\right) + \mathcal{R}(\varepsilon^4)$$

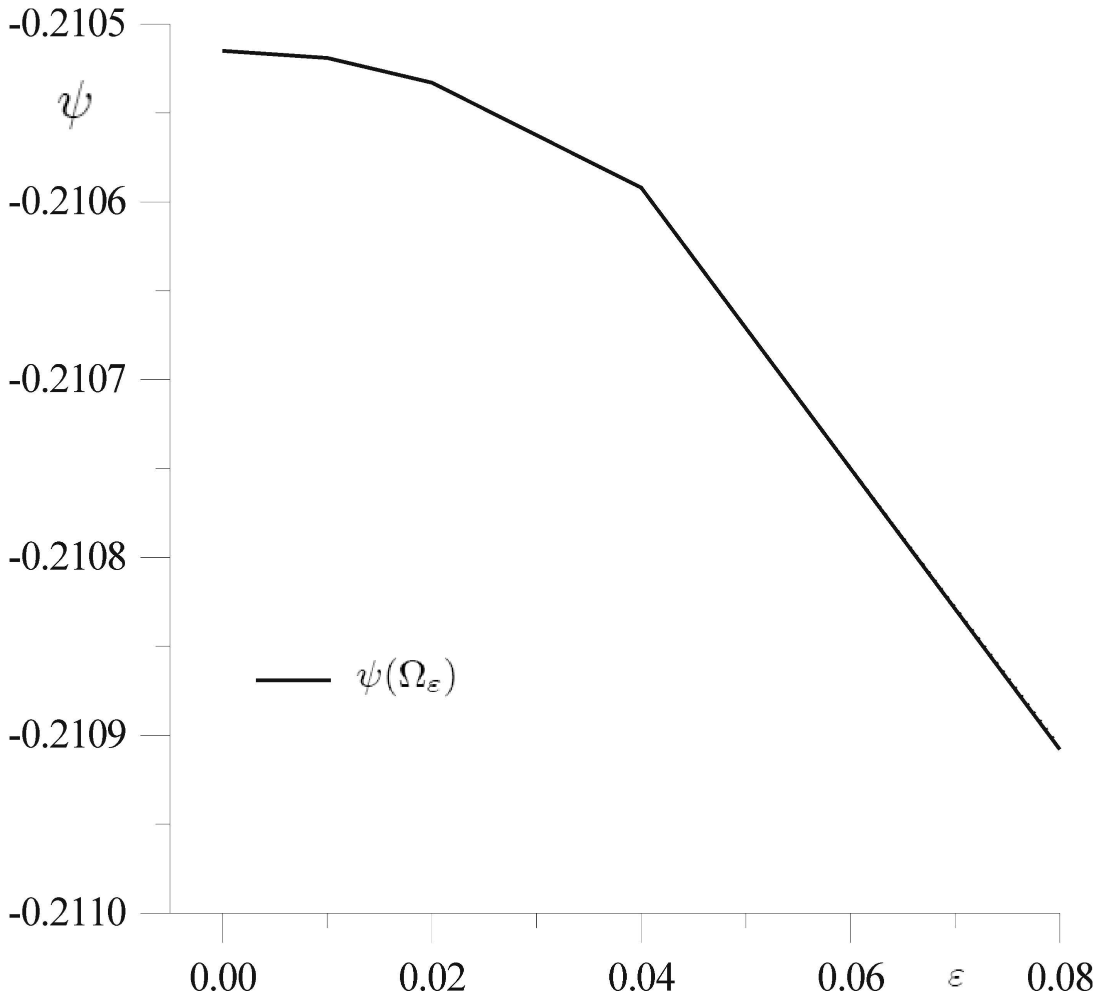
$$\left\{ \begin{array}{cccc} \triangle v & = & 0 & \text{in} \quad \Omega \\ v & = & -g & \text{on} \quad \Gamma_D \\ \frac{\partial v}{\partial n} & = & \frac{\partial g}{\partial n} & \text{on} \quad \Gamma_N \end{array} \right. \qquad g(\mathbf{x}) = \nabla u(\hat{\mathbf{x}}) \cdot \frac{\mathbf{x} - \hat{\mathbf{x}}}{\|\mathbf{x} - \hat{\mathbf{x}}\|^2}$$

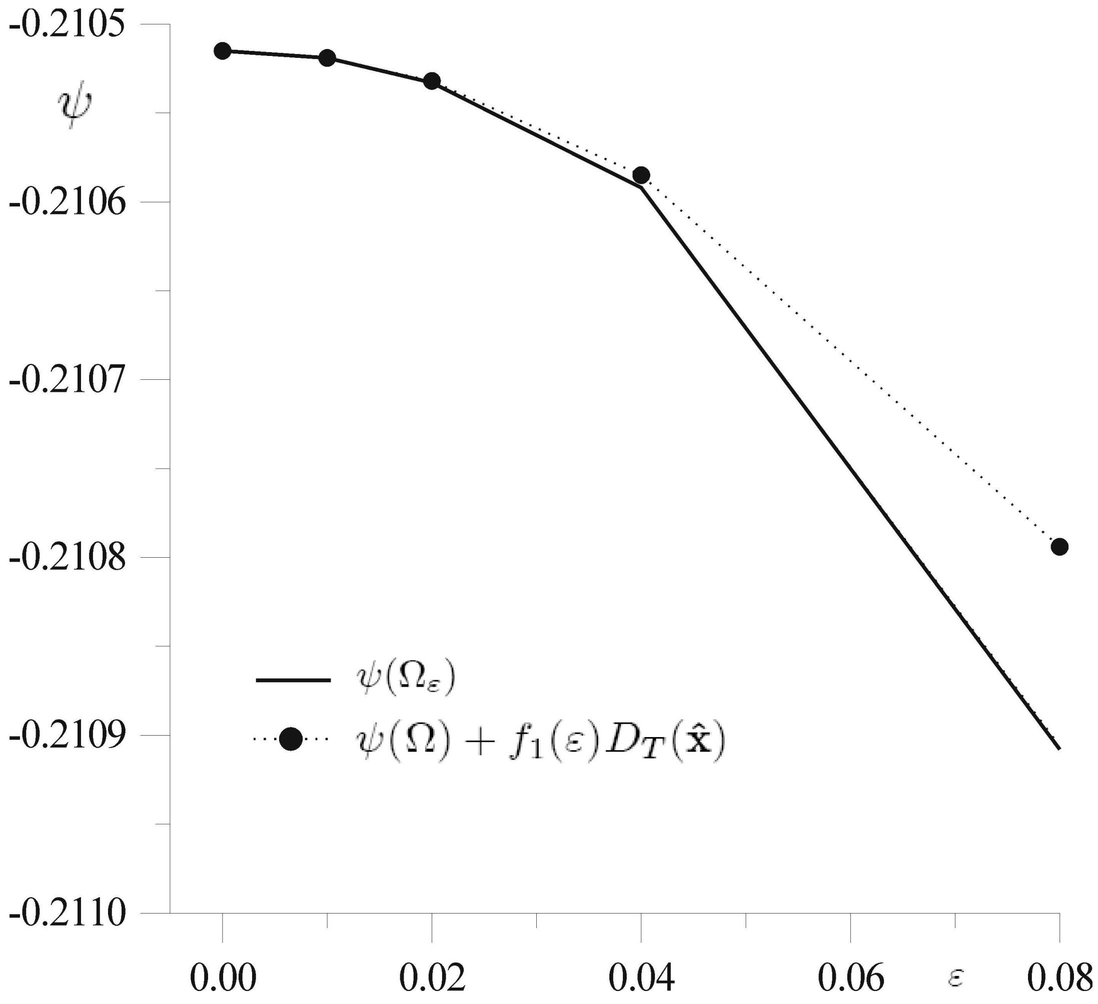
Numerical Experiment

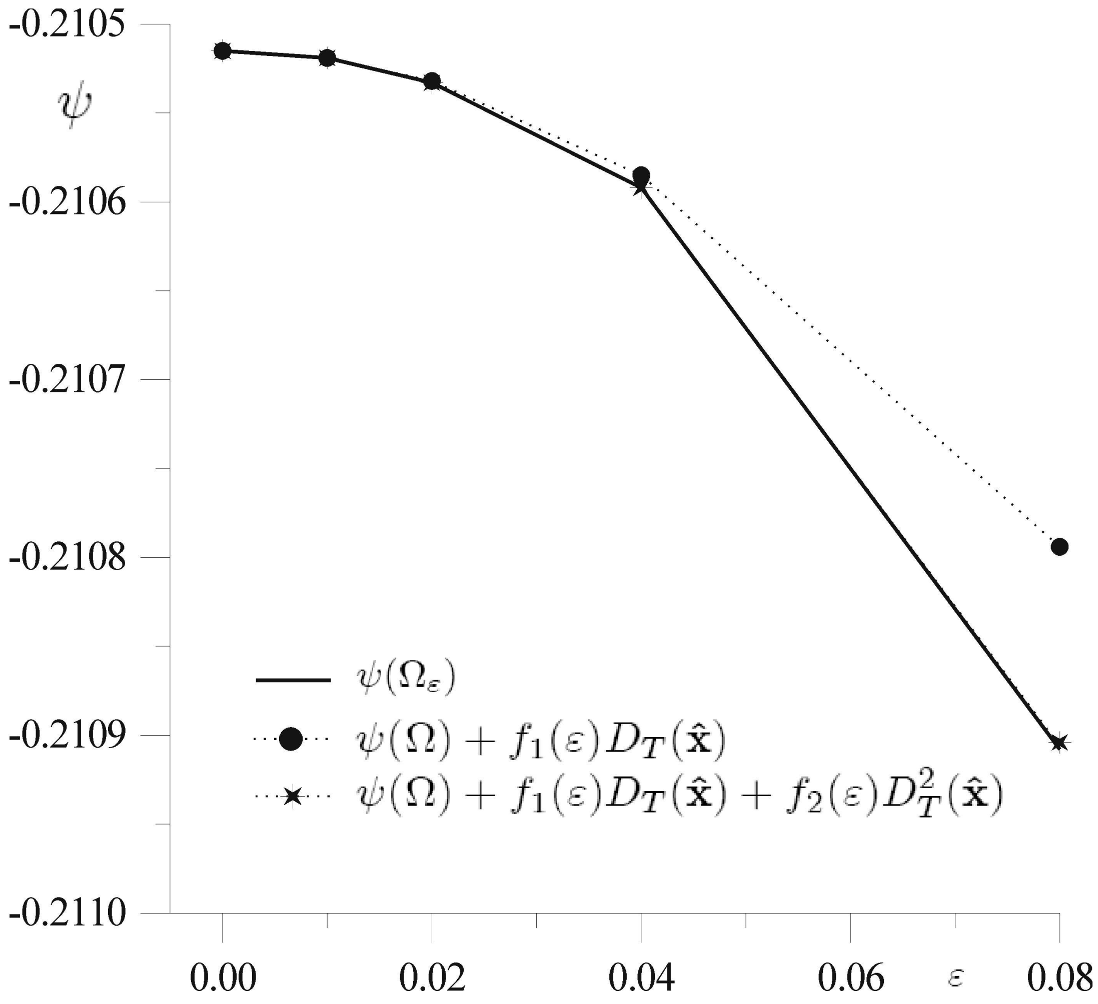


$$
\begin{aligned}
\Omega &= (0,1) \times (0,1) \\
a &= 0.2 \\
u &= 0 \text{ on } \Gamma_{D_1} \text{ and } \Gamma_{D_2} \\
q_1 &= 1 \text{ on } \Gamma_{N_1} \text{ and } q_1 = 2 \text{ on } \Gamma_{N_2}
\end{aligned}
$$

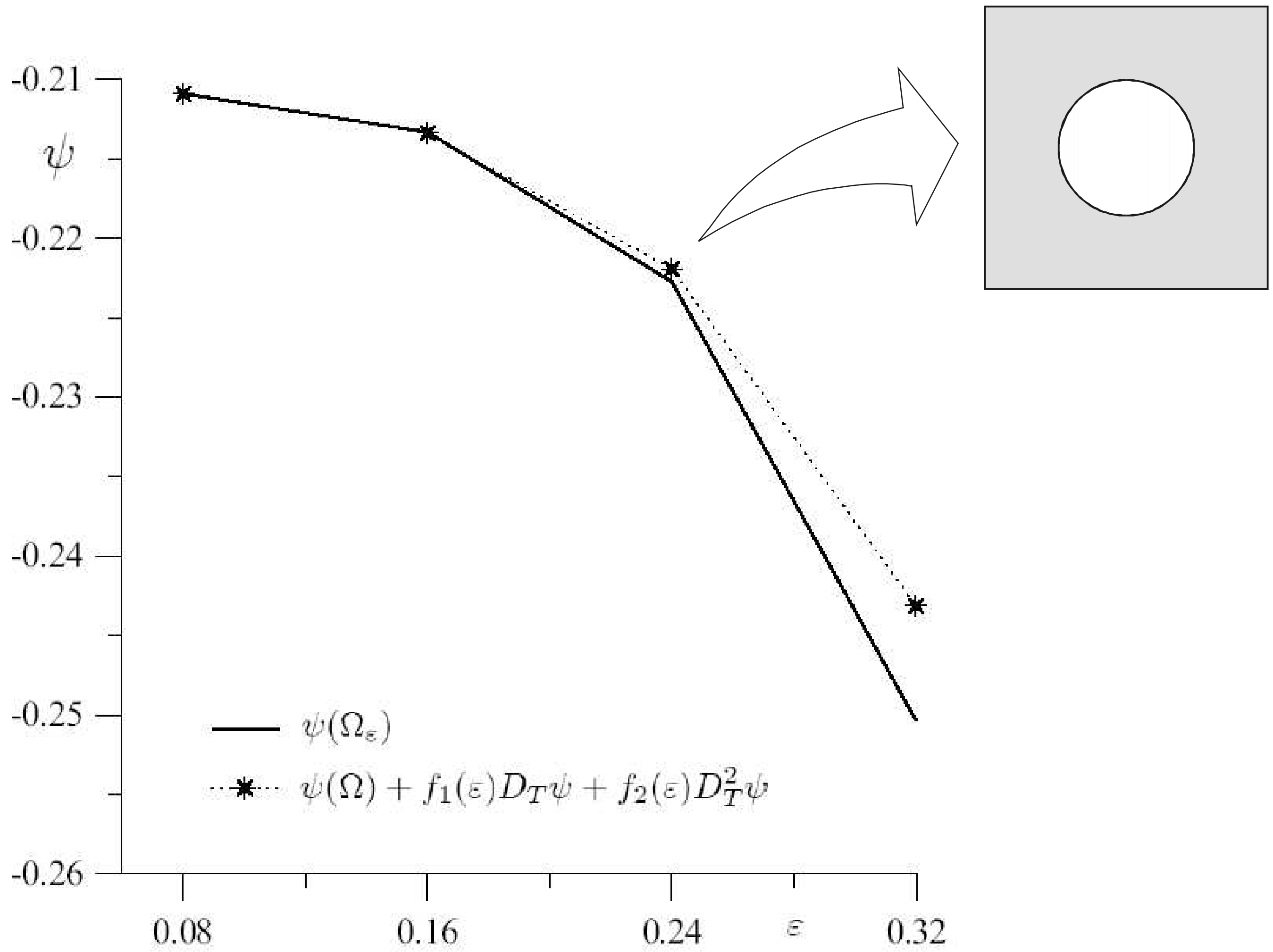
$$
\psi(\Omega_\varepsilon) \approx \psi(\Omega) - \pi\varepsilon^2 \left\|\nabla u\left(\widehat{\mathbf{x}}\right)\right\|^2 + \pi\varepsilon^4 \left(\frac{1}{2} \det \nabla\nabla u\left(\widehat{\mathbf{x}}\right) - \nabla u\left(\widehat{\mathbf{x}}\right) \mathbf{X} \nabla v\left(\widehat{\mathbf{x}}\right)\right)
$$


-0.2105
-0.2106
-0.2107
-0.2108
-0.2109
-0.2110
ψ
$\psi(\Omega_\varepsilon)$
0.00
0.02
0.04
0.06
0.08
ε


-0.2105
-0.2106
-0.2107
-0.2108
-0.2109
-0.2110
ψ
$\psi(\Omega_\varepsilon)$
$\psi(\Omega) + f_1(\varepsilon)D_T(\hat{\mathbf{x}})$
0.00
0.02
0.04
0.06
ε
0.08



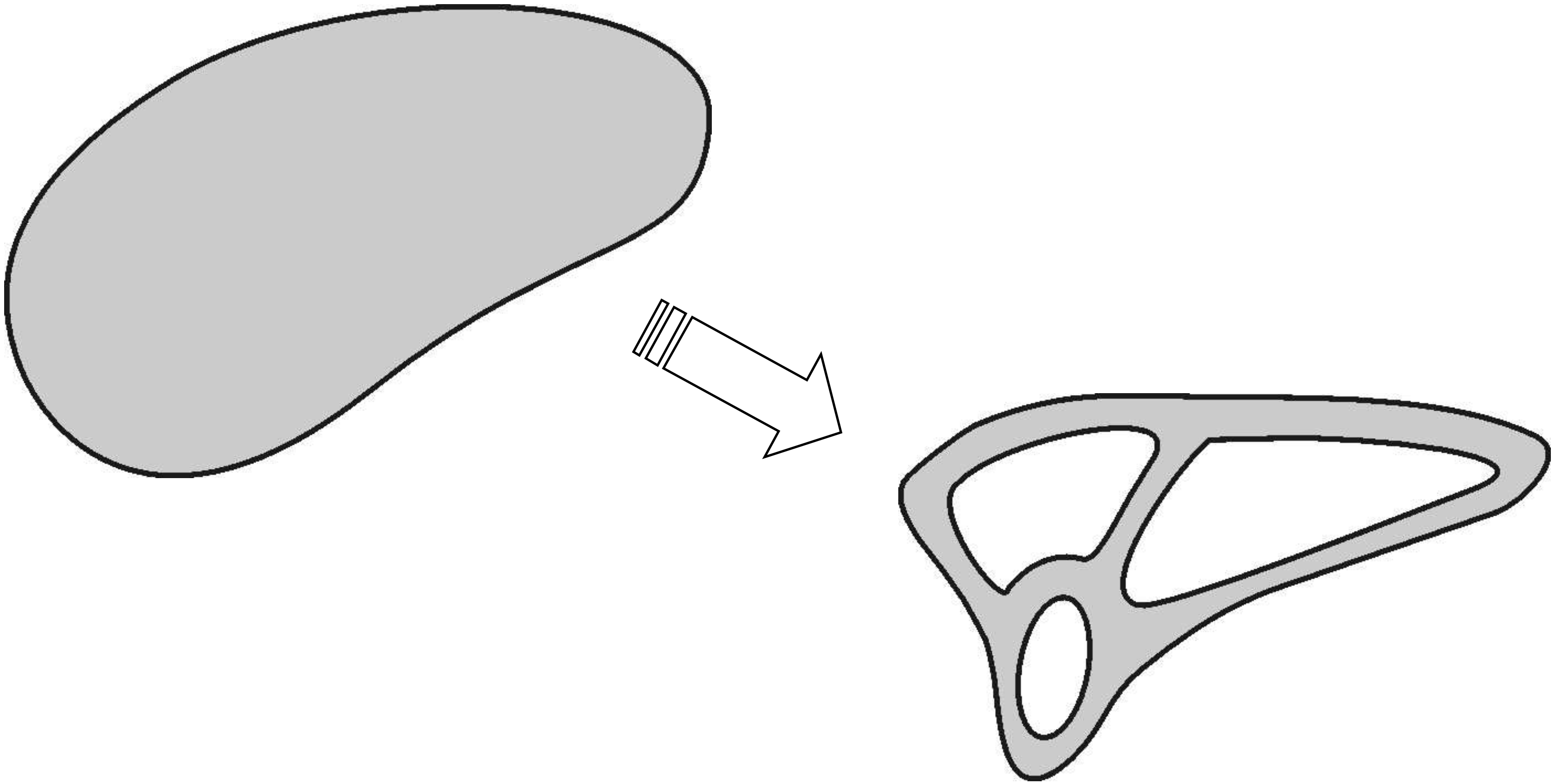
-0.2105
-0.2106
-0.2107
-0.2108
-0.2109
-0.2110
ψ
0.00
0.02
0.04
0.06
0.08
ε
$\psi(\Omega_\varepsilon)$
$\psi(\Omega) + f_1(\varepsilon) D_T(\hat{\mathbf{x}})$
$\psi(\Omega) + f_1(\varepsilon) D_T(\hat{\mathbf{x}}) + f_2(\varepsilon) D_T^2(\hat{\mathbf{x}})$


-0.21
-0.22
-0.23
-0.24
-0.25
-0.26
ψ
0.08
0.16
0.24
ε
0.32
$\psi(\Omega_\varepsilon)$
$\psi(\Omega) + f_1(\varepsilon)D_T\psi + f_2(\varepsilon)D_T^2\psi$

Applications of the Topological Derivative

Topology Optimization

Joint work with R.A. Feijóo, E. Taroco & C. Padra



Linear Elasticity

find the displacement vector field $\mathbf{u} \in \mathcal{U}(\Omega)$, such that

$$\int_{\Omega} \mathbf{T}(\mathbf{u}) \cdot \mathbf{E}(\boldsymbol{\eta}) = \int_{\Gamma_N} \bar{\mathbf{q}} \cdot \boldsymbol{\eta} \qquad \forall \boldsymbol{\eta} \in \mathcal{V}(\Omega)$$

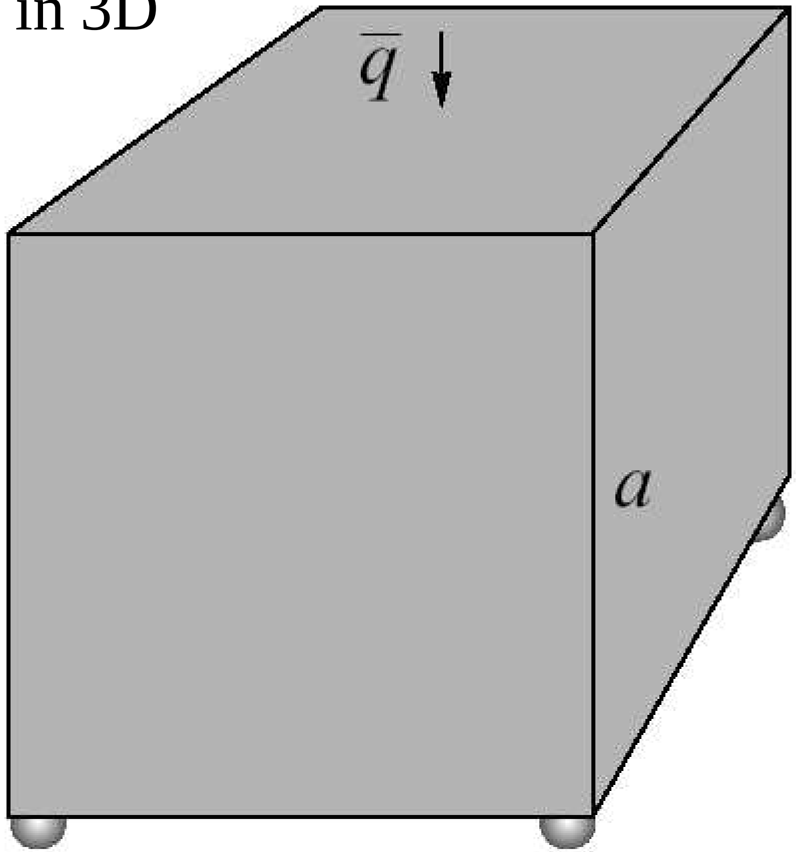
$$\mathbf{E}(\mathbf{u}) = \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right) := \nabla^s \mathbf{u} \qquad \text{and} \qquad \mathbf{T}(\mathbf{u}) = \mathbf{C}\mathbf{E}(\mathbf{u}) = \mathbf{C}\nabla^s \mathbf{u}$$

$$\mathcal{U}(\Omega) = \left\{\mathbf{u} \in H^1(\Omega) : \mathbf{u} = \overline{\mathbf{u}} \text{ on } \Gamma_D\right\}$$

$$\mathcal{V}(\Omega) = \left\{\boldsymbol{\eta} \in H^1(\Omega) : \boldsymbol{\eta} = \mathbf{0} \text{ on } \Gamma_D\right\}$$

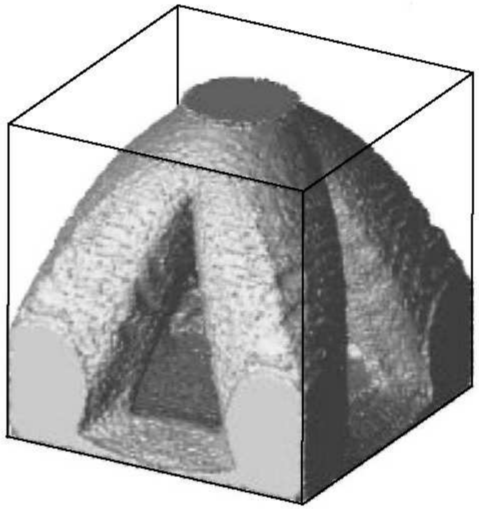
$$\psi(\Omega) := \mathcal{J}(\mathbf{u}) = \frac{1}{2}\int_{\Omega} \mathbf{T}(\mathbf{u}) \cdot \mathbf{E}(\mathbf{u}) - \int_{\Gamma_N} \bar{\mathbf{q}} \cdot \mathbf{u}$$

A *benchmark* example in 3D

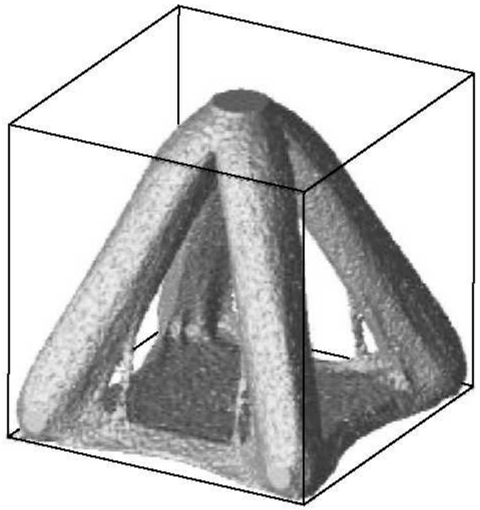


Three-Dimensional

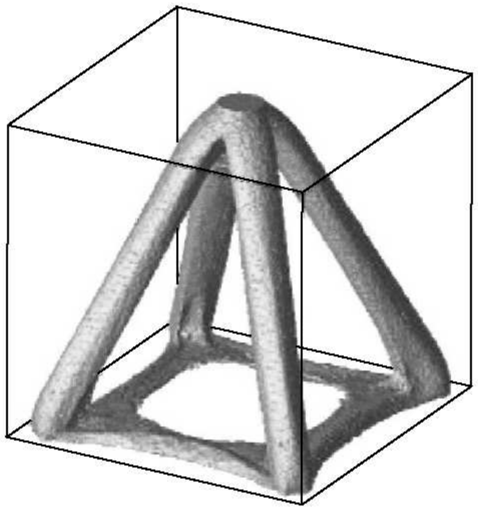
$$D_T(\hat{\mathbf{x}}) = \frac{3}{4}\frac{1-\nu}{7-5\nu}\left[10\mathbf{T}(\mathbf{u})\cdot\mathbf{E}(\mathbf{u}) - \frac{1-5\nu}{1-2\nu}\mathrm{tr}\mathbf{T}(\mathbf{u})\ \mathrm{tr}\mathbf{E}(\mathbf{u})\right]$$



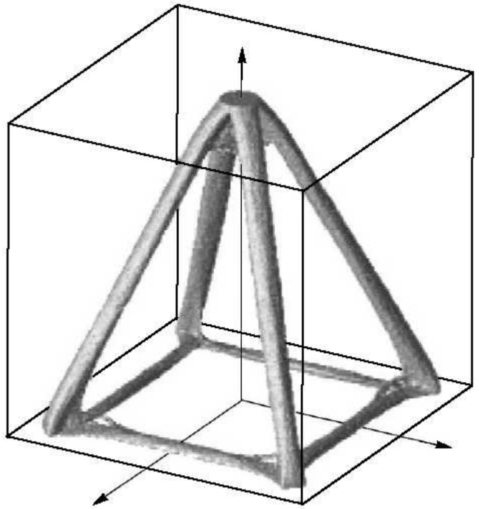
(a) topology at iteration $i = 13$



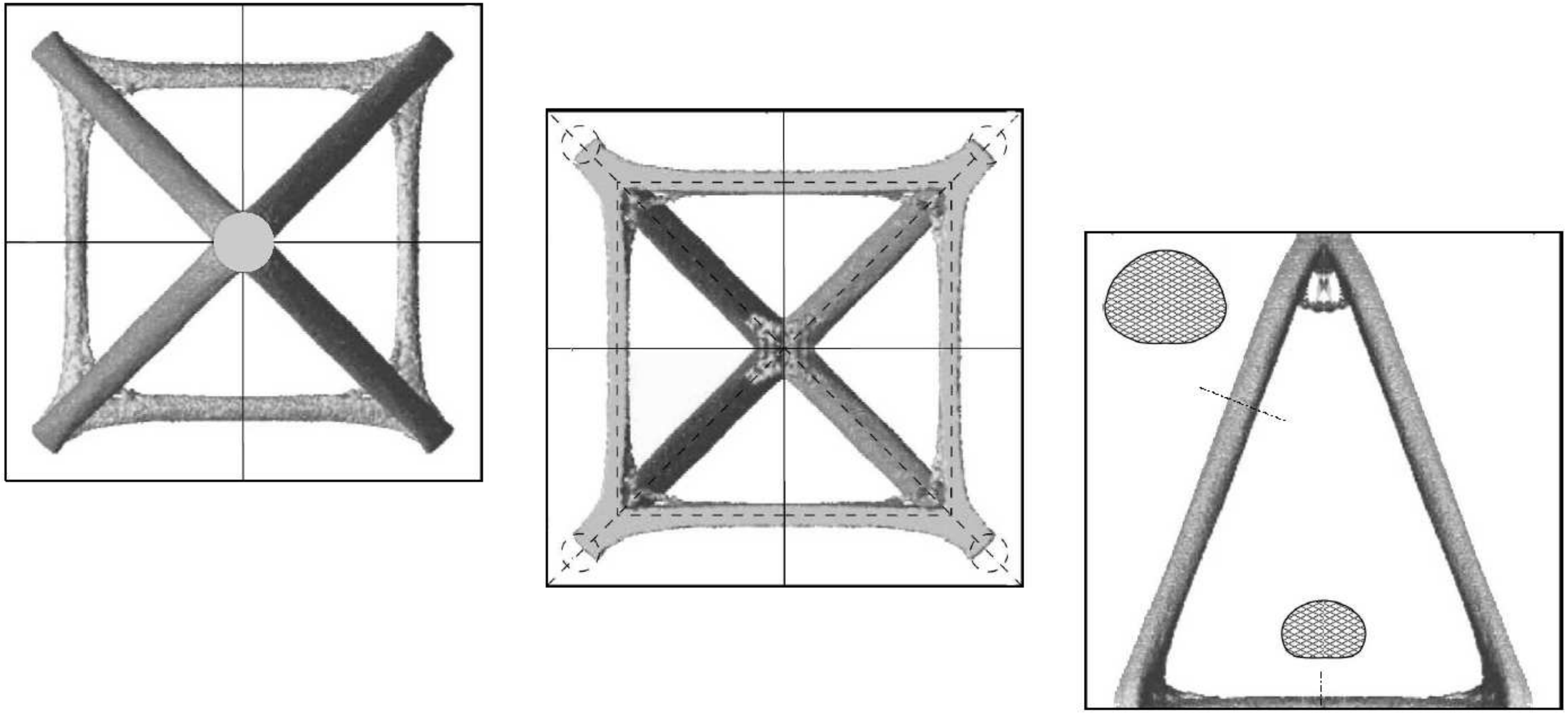
(b) topology at iteration $i = 35$

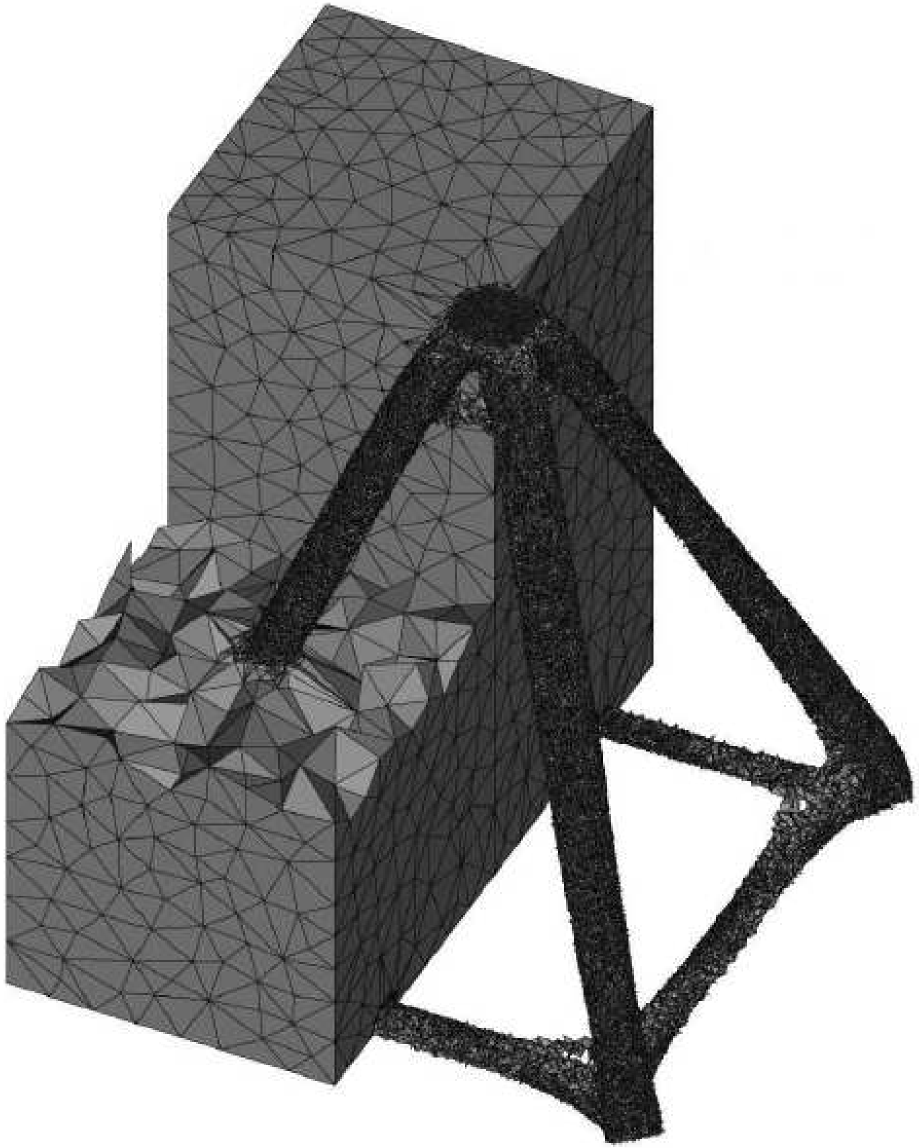


(c) topology at iteration $i = 52$



(d) topology at iteration $i = 76$

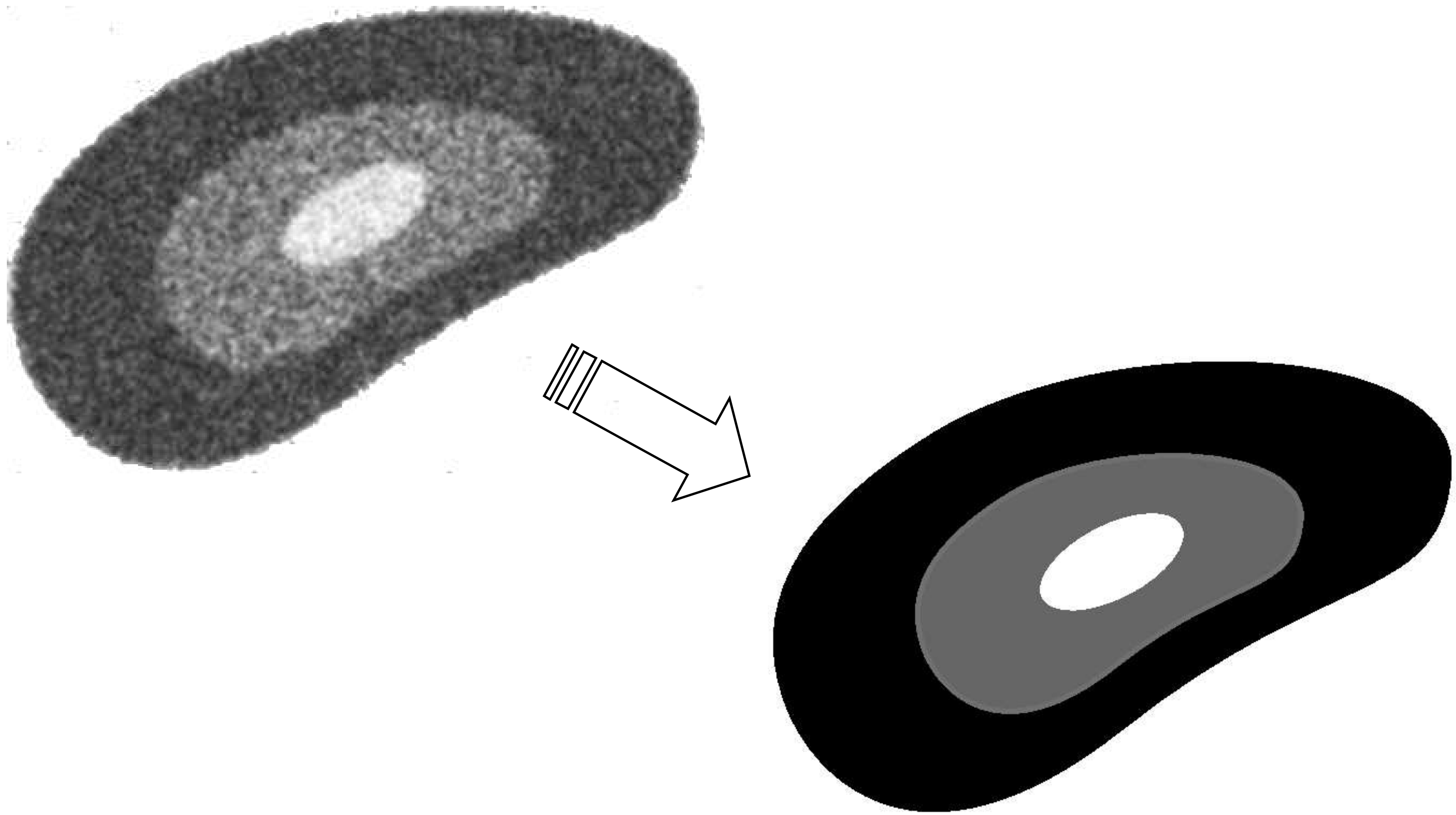




Amstutz & Andrä (2006) and Gournay, Allaire & Jouve (2007)

Image Segmentation

Joint work with R.A. Feijóo & I. Larrabide



$$v \in \mathcal{V} = \{w \in L^2(\Omega) : \ w \text{ constant at pixel/voxel level}\}$$

Find the segmented image $u^* \in \mathcal{U}$ such that minimizes the functional

$$\mathcal{J}(\varphi) = \frac{1}{2}\int_\Omega k\nabla\varphi \cdot \nabla\varphi \, d\Omega \ + \frac{1}{2}\int_\Omega (\varphi - (v-u))^2 \, d\Omega$$

$$\mathcal{U} = \{u \in \mathcal{V} : u(\mathbf{x}) \in \mathcal{C}, \forall \mathbf{x} \in \Omega\}$$

Find $\varphi \in H^1(\Omega)$, such that

$$\mathcal{C} = \{c_1, c_2, \cdots, c_{Nc}\}$$

$$\int_\Omega k\nabla\varphi \cdot \nabla\eta \, d\Omega + \int_\Omega \varphi\eta \, d\Omega = \beta\int_\Omega (v-u)\eta \, d\Omega$$

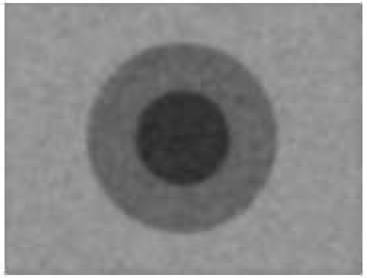
$$u_T : \begin{cases} u_T(\mathbf{x}) = u & \forall \ \mathbf{x} \in \Omega_\varepsilon \\ u_T(\mathbf{x}) = c_i & \forall \ \mathbf{x} \in B_\varepsilon \end{cases} \quad c_i \in \mathcal{C}.$$

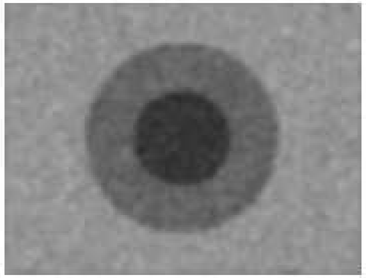
Find $\varphi_\epsilon \in H^1(\Omega)$, such that

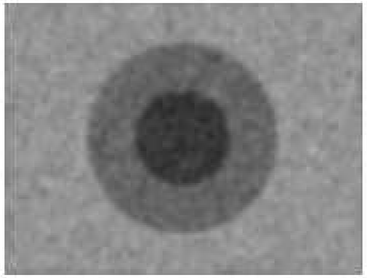
$$\int_\Omega k\nabla\varphi_\epsilon \cdot \nabla\eta \, d\Omega + \int_\Omega \varphi_\epsilon\eta \, d\Omega = \ \beta\int_\Omega (v-u_T)\eta \, d\Omega$$

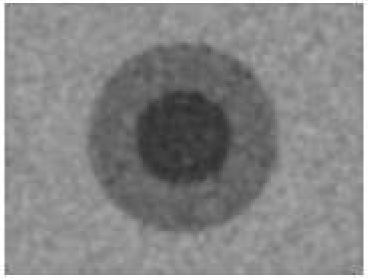
$$D_T(\widehat{\mathbf{x}}) \ = \ \frac{1}{2}(c_i - u)\left[(\varphi(\widehat{\mathbf{x}}) - (v-u)) + (\varphi(\widehat{\mathbf{x}}) - (v-c_i)) + 2(1-\beta)\varphi(\widehat{\mathbf{x}})\right] \quad \forall \widehat{\mathbf{x}} \in \Omega$$

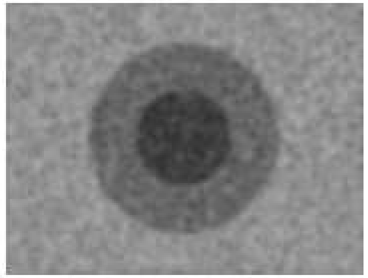
A *benchmark* example: with noise

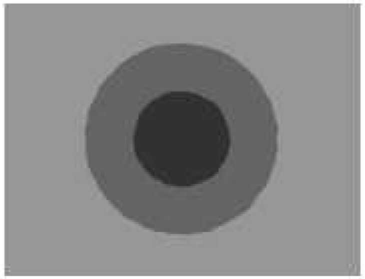

2% WGN

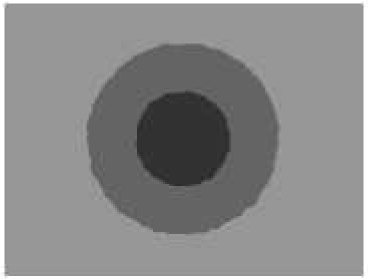

4% WGN

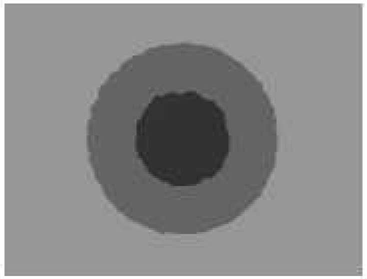

6% WGN

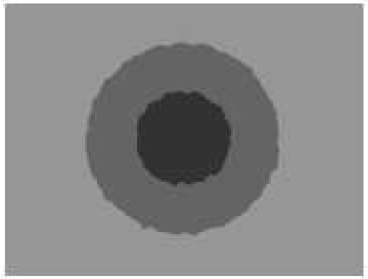

8% WGN

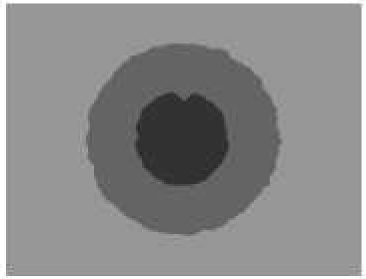

10% WGN



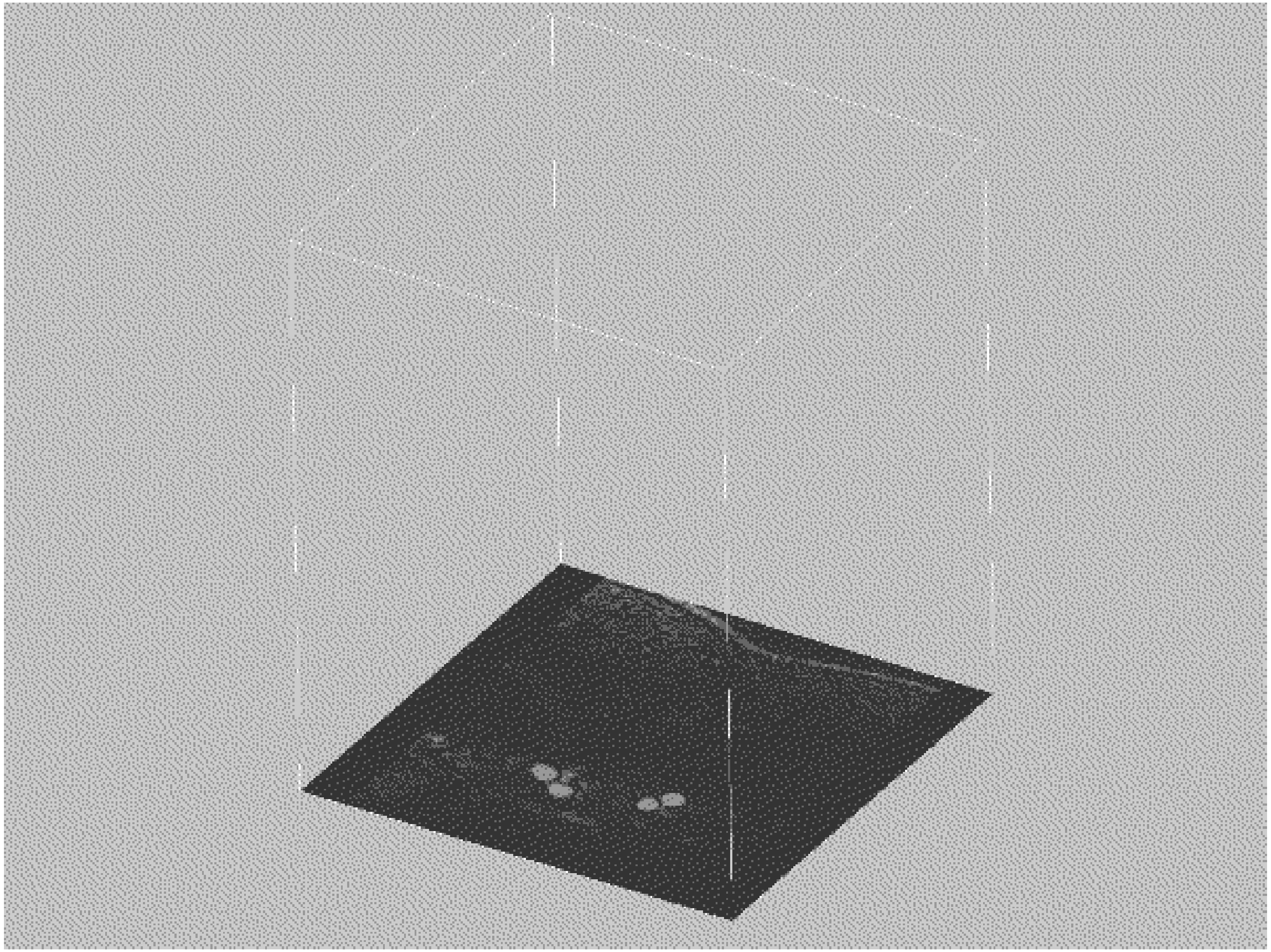


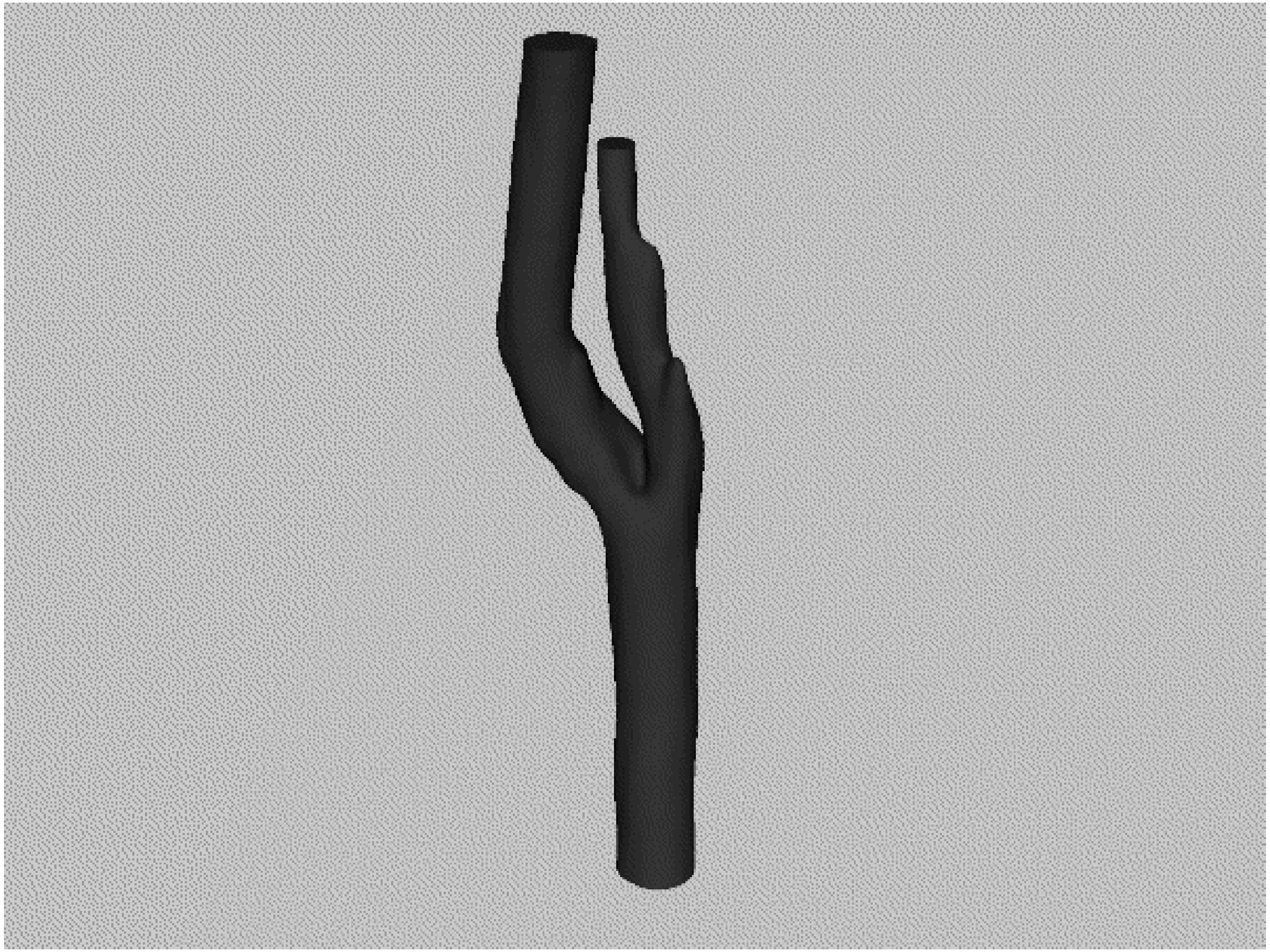






A *real* application: medical image

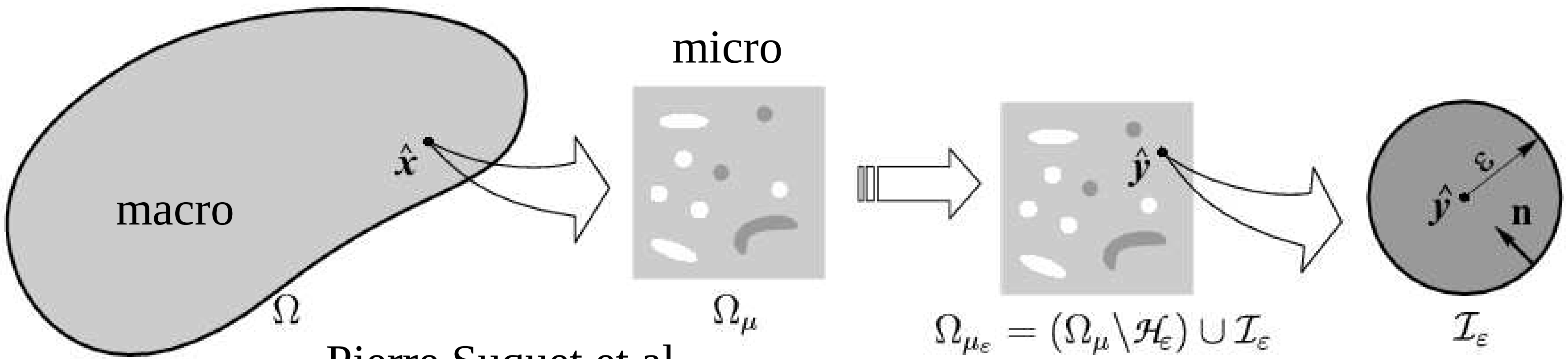




Auroux et al. (2006) and Hintermüller (2007)

Multiscale Modelling

Joint work with E.A. de Souza Neto & S.M. Giusti



Pierre Suquet et al.

Hill-Mandel Principle

$$\boldsymbol{q}(\boldsymbol{x})\cdot\nabla u(\boldsymbol{x}) = \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{q}_\mu(\boldsymbol{y})\cdot\nabla u_\mu(\boldsymbol{y})$$

$$\boldsymbol{q}^\varepsilon(\boldsymbol{x})\cdot\nabla u(\boldsymbol{x}) = \frac{1}{V_\mu}\int_{\Omega_{\mu_\varepsilon}} \boldsymbol{q}_{\mu_\varepsilon}(\boldsymbol{y})\cdot\nabla u_{\mu_\varepsilon}(\boldsymbol{y})$$

$$\boldsymbol{q}^\varepsilon(\hat{\boldsymbol{x}})\cdot\nabla u(\hat{\boldsymbol{x}}) = \boldsymbol{q}(\hat{\boldsymbol{x}})\cdot\nabla u(\hat{\boldsymbol{x}}) + \frac{1}{V_\mu} f(\varepsilon)\, D_T\psi(\hat{\boldsymbol{y}}) + \mathcal{O}(f(\varepsilon))$$

$$u_\mu(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} + \tilde{u}_\mu(\boldsymbol{y})$$

$$\boldsymbol{x} \in \Omega \qquad \boldsymbol{y} \in \Omega_\mu$$

Given $\nabla u(\boldsymbol{x})$: find the temperature fluctuation field $\tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu$, such that

$$\int_{\Omega_\mu} k \nabla \tilde{u}_\mu \cdot \nabla \eta = -\int_{\Omega_\mu} k \nabla u \cdot \nabla \eta \qquad \forall \eta \in \mathcal{V}_\mu \subset \tilde{\mathcal{K}}_\mu$$

$$\tilde{\mathcal{K}}_\mu \equiv \left\{ \tilde{u}_\mu \in \mathcal{W} : \int_{\partial\Omega_\mu} \tilde{u}_\mu \mathbf{n} = \mathbf{0} \right\}$$

(a) Taylor model

$$\mathcal{V}_\mu^T \subset \mathcal{V}_\mu^L \subset \mathcal{V}_\mu^P \subset \mathcal{V}_\mu^U$$

$$\mathcal{V}_\mu^T \equiv \{\mathbf{0}\}\,;$$

(b) Linear RVE boundary temperature model

$$\mathcal{V}_\mu^L \equiv \left\{\tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{u}_\mu(\boldsymbol{y}) = 0,\ \forall \boldsymbol{y} \in \partial\Omega_\mu\right\};$$

(c) Periodic RVE boundary temperature fluctuation model

$$\mathcal{V}_\mu^P \equiv \left\{\tilde{u}_\mu \in \tilde{\mathcal{K}}_\mu : \tilde{u}_\mu\left(\boldsymbol{y}^+\right) = \tilde{u}_\mu\left(\boldsymbol{y}^-\right),\ \forall \text{ par } \left(\boldsymbol{y}^+, \boldsymbol{y}^-\right) \in \partial\Omega_\mu\right\};$$

(d) Uniform RVE boundary flux model

$$\mathcal{V}_\mu^U \equiv \tilde{\mathcal{K}}_\mu = \left\{\tilde{u}_\mu \in \mathcal{W} : \int_{\partial\Omega_\mu} \tilde{u}_\mu \mathbf{n} dA = 0\right\}.$$

$$u_{\mu_\varepsilon}(\boldsymbol{y}) = \nabla u(\boldsymbol{x}) \cdot \boldsymbol{y} + \tilde{u}_{\mu_\varepsilon}(\boldsymbol{y})$$

Given $\nabla u(\boldsymbol{x})$: find the temperature fluctuation field $\tilde{u}_{\mu_\varepsilon} \in \tilde{\mathcal{K}}_{\mu_\varepsilon}$, such that

$$\int_{\Omega_{\mu_\varepsilon}} k^* \nabla \tilde{u}_{\mu_\varepsilon} \cdot \nabla \eta_\varepsilon = -\int_{\Omega_{\mu_\varepsilon}} k^* \nabla u \cdot \nabla \eta_\varepsilon \quad \forall \eta_\varepsilon \in \mathcal{V}_{\mu_\varepsilon}$$

$$\tilde{\mathcal{K}}_{\mu_\varepsilon} \equiv \left\{ \tilde{u}_{\mu_\varepsilon} \in \mathcal{W} : \int_{\partial\Omega_\mu} \tilde{u}_{\mu_\varepsilon} \mathbf{n} = \mathbf{0} \right\}$$

$$k^* = \begin{cases} k & \forall \boldsymbol{y} \in \Omega_\mu \backslash \mathcal{H}_\varepsilon \\ k^i & \forall \boldsymbol{y} \in \mathcal{I}_\varepsilon \end{cases}$$

$$\mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon}) = \int_{\Omega_{\mu_\varepsilon}} \boldsymbol{q}_{\mu_\varepsilon} \cdot \nabla u_{\mu_\varepsilon}$$

$$D_T\psi = \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_{\mu_\varepsilon}}(u_{\mu_\varepsilon})$$

$$\begin{aligned} D_T\psi(\hat{\boldsymbol{y}}) &= 2k^e \frac{k^e - k^i}{k^e + k^i} |\nabla u_\mu(\hat{\boldsymbol{y}})|^2 \\ &= 2k^e \frac{1-\gamma}{1+\gamma} |\nabla u_\mu(\hat{\boldsymbol{y}})|^2 \quad \forall \hat{\boldsymbol{y}} \in \Omega_\mu, \quad k^i = \gamma k^e. \end{aligned}$$

$$\boldsymbol{q}^\varepsilon \cdot \nabla u = \boldsymbol{q} \cdot \nabla u + 2v(\varepsilon) k^e \frac{1-\gamma}{1+\gamma} |\nabla u_\mu|^2 + \mathcal{O}(\varepsilon^2)$$

$$v(\varepsilon) = \pi\varepsilon^2 / V_\mu$$

$$\tilde{u}_\mu = (\nabla u)_i \, \tilde{u}_{\mu_i} \qquad \text{where} \qquad (\nabla u)_i = \nabla u \cdot \mathbf{e}_i$$

Find the temperature fluctuation field $\tilde{u}_{\mu_i} \in \tilde{\mathcal{K}}_\mu$ (for *i*=1,2), such that

$$\int_{\Omega_\mu} \mathbb{K}_\mu \nabla \tilde{u}_{\mu_i} \cdot \nabla \eta = -\int_{\Omega_\mu} \mathbb{K}_\mu \mathbf{e}_i \cdot \nabla \eta \qquad \forall \eta \in \mathcal{V}_\mu \qquad\qquad k(\boldsymbol{y})\,\mathbf{I} = \mathbb{K}_\mu$$

$$D_T \psi = 2k^e \frac{1-\gamma}{1+\gamma} |\nabla u_\mu|^2$$

$$D_T \psi = \mathbb{D}_{T\mu} \nabla u \cdot \nabla u,$$

$$\mathbb{D}_{T\mu} = 2k^e \frac{1-\gamma}{1+\gamma} \left(\nabla u_{\mu i} \cdot \nabla u_{\mu j} \right) \mathbf{e}_i \otimes \mathbf{e}_j .$$

$$\boldsymbol{q}^{\varepsilon} \cdot \nabla u = \boldsymbol{q} \cdot \nabla u + 2v(\varepsilon)k^{e}\frac{1-\gamma}{1+\gamma}\left|\nabla u_{\mu}\right|^{2} + \mathcal{O}(\varepsilon^{2})$$

$$v(\varepsilon) = \pi\varepsilon^{2}/V_{\mu}$$

$\boldsymbol{q} = -\mathbb{K}^{\mathcal{H}}\nabla u$ and $\boldsymbol{q}^{\varepsilon} = -\mathbb{K}_{\varepsilon}^{\mathcal{H}}\nabla u$

$$\delta\mathbb{K}^{\mathcal{H}} = \mathbb{K}_{\varepsilon}^{\mathcal{H}} - \mathbb{K}^{\mathcal{H}}.$$

$$\delta\mathbb{K}^{H} = -v(\varepsilon)\mathbb{D}_{T_{\mu}} + \mathcal{O}(v(\varepsilon))$$

$$\mathbb{D}_{T\mu} = 2k^{e}\frac{1-\gamma}{1+\gamma}\left(\nabla u_{\mu_i} \cdot \nabla u_{\mu_j}\right)\mathbf{e}_i \otimes \mathbf{e}_j.$$

Muchas Gracias!!!