Diffusion in inverse problems and inverse problems in diffusion

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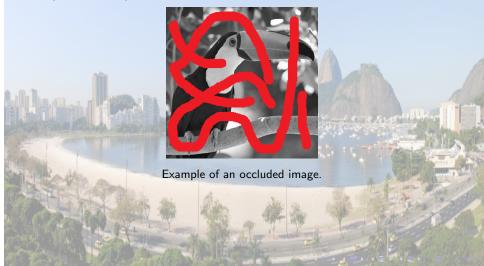
Tentative road map

- The inpainting problem
 - T1, TV and mixed weighted T1-TV inpainting
 - Curvature-driven diffusion inpainting
 - A two step CDD + T1-TV inpainting method
 - Numerical implementation and results
- 2 An inverse heat conduction problem
 - Origins of the problem
 - A brief historical mathematical tracking of the problem
 - Calderón's problem
 - Inverting the conductivity-to-temperature mapping
 - The inverse problem
 - Regularization: finding the right penalizers
 - Examples and numerical experiments
 - Open problems

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Example of an occluded image.

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- $u: \Omega \to [0,1]$ is the light intensity function.

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- $u: \Omega \to [0,1]$ is the light intensity function.
- $v = u \mid_{\Omega \setminus D}$ is the (possibly noisy) known part of u.

The order 1 Tikhonov-Phillips inpainting is obtained by minimizing

$$\mathcal{J}(u) = \|\mathcal{T}u - v\|_{L^2}^2 + \lambda \|\nabla u\|_{L^2}^2, \tag{T11}$$

with respect to u.

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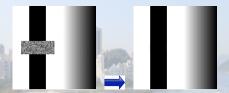


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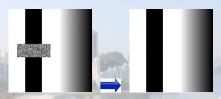
Occluded image and TVI inpainting for a **thin** occlusion.



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Euler-Lagrange equation of (TVI) is the steady state solution of

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where $D = |\nabla u|^{-1}$.

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¹Chan, T.F. and Shen, J. Mathematical models for local nontexture inpaintings, SIAM J. Appl. Math., 2002

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Occluded Image.



Not a CDD steady state.



CDD inpainting.

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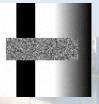
CDD inpainting.

Desired inpainting qualities:

Good performance at smooth regions.

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CDD inpainting.

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Mixed Weighted Regularization Inpainting

$$\mathcal{J}(u) = \|\mathcal{T}u - v\|_{L^{2}}^{2} + \lambda_{T1} \||\sqrt{1 - \theta} A\nabla u|\|_{L^{2}}^{2} + \lambda_{TV} \||\theta A\nabla u|\|_{L^{1}}. \quad (\mathsf{T1A-TVA})$$



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(Mazzieri-Spies-Temperini, "Mixed spatially varying L^2-BV regularization of inverse ill-posed problems", Journal of Inverse and Ill-Posed Problems, 2015: 23(6):571-585.)

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A new two-step inpainting method

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v — L

Low-pass filter

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 $\mathbf{v} \xrightarrow{\text{inpainting}} \mathbf{u_p^*} \xrightarrow{\text{filter}} \mathbf{u_p} = \mathbf{G} * \mathbf{u_p^*} \xrightarrow{\theta} \theta = \theta(\nabla u_p)$

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- $\bullet \ \ U \in \mathbb{R}^{\textit{M} \times \textit{M}}, \ u \in \mathbb{R}^{\textit{M}^2} \ \text{so that} \ u_{\textit{M}(\textit{I}-1)+\textit{m}} = \textit{U}_{\textit{m},\textit{I}} \ \forall \textit{I}, \textit{m}.$



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CDD algorithm

- $\bullet \ \, \mathsf{Set} \,\, u^{(0)} \in \mathbb{R}^{M^2}, \,\, n = 0 \,\, \mathsf{and} \,\, f \doteq \nabla \cdot \left[\frac{|\kappa|}{|\nabla u|} \nabla u \right], \,\, \mathsf{where} \,\, \kappa = \nabla \cdot \left[\frac{\nabla u}{|\nabla u|} \right]$
- Compute a step of the Adams-Bashforth-Moulton predictor-corrector method:

$$\tilde{u}_m^{(n+1)} = u_m^{(n)} + \frac{h}{12} \left[23f(u_m^{(n)}) - 16f(u_m^{(n-1)}) + 5f(u_m^{(n-2)}) \right],$$

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- If the stopping criterion is reached, $u_p^* = u^{(n+1)}$. Else, set n = n+1 and repeat from Step 2.
- **Convolution** $u_p = G * u_p^*$, where G is a low-variance Gaussian kernel.

Anisotropy matrix field A



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- If $\nabla u_p(x,y) = 0$, A(x,y) = I.
- If $\nabla u_p(x,y) \neq 0$, A(x,y) has eigenvalues $\sigma_j(x,y)$ and eigenvectors $v_j(x,y)$, such that

$$v_1(x,y) \perp \nabla u_p(x,y),$$
 $\sigma_1(x,y) = 1$
 $v_2(x,y) \parallel \nabla u_p(x,y),$ $\sigma_2(x,y) = h(|\nabla u_p(x,y)|)$

Anisotropy matrix field A

 $A(x,y) \in \mathbb{R}^{2 \times 2}$ is a symmetric positive definite matrix $\forall (x,y) \in \Omega$, such that:

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(1.1)



• Find
$$u_p^*$$
 by solving $\frac{\partial u}{\partial t} = \nabla \cdot \left[\frac{|\kappa| \chi_D + \chi_{\Omega \setminus D}}{|\nabla u|} \nabla u \right] + \frac{1}{\lambda} (u - v) \chi_{\Omega \setminus D}.$



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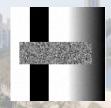


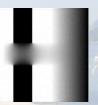
Occluded Image.

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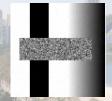


Occluded Image.

T1I inpainting.

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Occluded Image.



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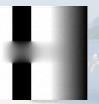
CDD inpainting.

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Occluded Image.

CDD inpainting.

Two-step CDD + T1A-TVA inpainting.

CDD T11. T1A-TVA $PSNR = 20 \log_{10} (M||u_0 - \hat{u}||^{-1}) | 20.140$ 35.496 36.330

Diffusion methods in inpainting

Inpainting as an inverse problem: Total Variation + Curvature Driven Diffusion Method



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Occluded Image.



T1l inpainting.

Ruben D. Spies (IMAL-FIQ, UNL-CONICET)

Inpainting as an inverse problem: Total Variation + Curvature Driven Diffusion Method



Occluded Image.



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CDD inpainting.

Inpainting as an inverse problem: Total Variation + Curvature Driven Diffusion Method



Occluded Image.



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T1A-TVA inpainting.

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Inverse diffusion problems

LACIAM 2023. Rio de Janeiro

Inpainting as an inverse problem: Total Variation + Curvature Driven Diffusion Method



Performance comparisonsGaussian additive noise= 2 %

	T1I	CDD	T1A-TVA
PSNR	20.815	22.292	22.551

Occluded Image.



T1I inpainting.



CDD inpainting.



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Inpainting as an inverse problem: Total Variation + Curvature Driven Diffusion Method



Occluded Image.



T1l inpainting.

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F. Ibarrola, R. Spies, "A two-step mixed inpainting method with curvature-based anisotropy and spatial adaptivity", Inverse Problems and Imaging, Volume 11, No. 2, 2017, pp 247-262, [7]



CDD inpainting.



T1A-TVA inpainting.

Ruben D. Spies (IMAL-FIQ, UNL-CONICET)

Inverse diffusion problems

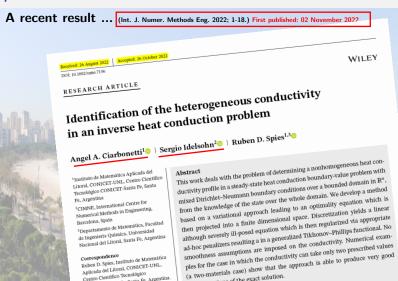
LACIAM 2023, Rio de Janeiro

Identification of the conductivity in a heat conduction problem

A recent result ... (Int. J. Numer. Methods Eng. 2022; 1-18.) First published: 02 November 2022



Identification of the conductivity in a heat conduction problem



Centro Científico Tecnológico

Origin of the problem

Flux manipulation - design of thermal materials or metamaterials



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International Journal of Thermal Sciences 128 (2018)



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journal homepage; www.elsevier.com/locate/jits



Optimization-based design of easy-to-make devices for heat flux manipulation



Víctor D. Fachinotti^{a,*}, Ángel A. Ciarbonetti^a, Ignacio Peralta^a, Ignacio Rintoul^b

**Centro de Investigación de Médicolo Computacionades (CIMEC), Universidad Nacional del Liberal (UNL)/ Consejo Nacional del Investigaciones Cimifficas y Técnicas (CONCIET) Predio DOSIGET Pre Albero Lossamos "Colectron Runa E. 168 Nn. O, Paroli Je Bano, O Pasolo Sana E. A Agrantina "Instituto del Desarrollo Tecnologico para la Industria Quintes (INTES), Universidad Nacional del Liberal (UNL)/ Consejo Nacional del Investigaciones Cimifficas y Tecnicas (CONCIET), Predio CONCIET Pr. Adero Cossumo", Colectron Runa Nue. 168 Nn. O Pareja E Preso, O 2000, Sanas E, Agrantina

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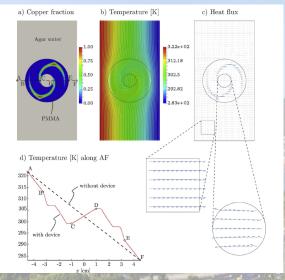
Keywords: Heat flux manipulation Optimization-based design Easy-to-make device Heat flux inversion Metamaterial

ABSTRACT

Numerical results ...



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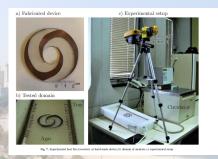
Experimental set-up and validation ...



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3.00e+02
2.55e+102
2.56e+102
2.56e+102
3.01e+62
2.56e+102
3.01e+62

1 Experimental set-up

2 Experimental results

Comparison...



Comparison...

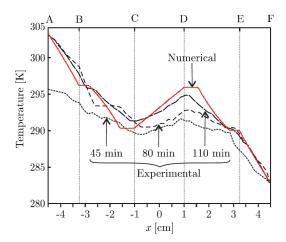


Fig. 9. Temperature along the line AF: experimental vs. numerical.

A brief historical mathematical tracking of the problem

Problem: of determining the elliptic coefficient profile function in an elliptic boundary value problem.



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Applications: electrical conductivity problems, oil resevoir and ground water flow problems ([3], [4], [8], [11], [17])

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A. P. Calderón's problem ([6], 1980, ATAS of SBM, Rio de Janeiro 1980):

 $\Omega \subset \mathbb{R}^n$, $n \geq 2$ bounded, $\partial \Omega$ Lipschitz, $u_{\varphi} \in H^1(\Omega)$ solution of the Dirichlet BVP

$$\begin{cases} \nabla \cdot (k\nabla u) = 0, & x \in \Omega, \\ u = \varphi, & x \in \partial\Omega, \end{cases}$$

and

$$Q_k(\varphi) = \int_{\Omega} k(x) \left(\nabla u_{\varphi}(x) \right)^2 dx = \int_{\partial \Omega} \varphi(x) k(x) \frac{\partial u_{\varphi}}{\partial \nu} ds,$$

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- $M: k \to Q_k$ is bounded and analytic in $L^{\infty}_{>0}(\Omega)$;
- For the linearized problem the answer is affirmative: dM|_{k=const.} is an injective mapping;
- If $k \approx const.$ then k is "nearly" determined by Q_k .

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- ✓ Sylvester and Uhlmann, 1987 ([16]): \underline{k} sufficiently smooth $\Rightarrow Q_k$ uniquely determines k. More precisely, they showed that the mapping M is injective over $C^{\infty}(\overline{\Omega}) \cap L^{\infty}_{>0}(\Omega)$.

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Problem of recovering k from information about u:

- all works assume some degree of smoothness on k (at least differentiability);
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Although the mathematical theory of elliptic equations with discontinuous principal coefficients is well known ([14], [12]), there is not much done on the inverse problem of recovering k in these cases.

A regularized variational approach

Setting: Let $\Omega \subset \mathbb{R}^n$ $(n \geq 2)$ a bounded open set with smooth boundary $\Gamma = \partial \Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, with $\Gamma_D \cap \Gamma_N = \emptyset$, $c, k, f, g, h \in L^2(\Omega)$ with $0 < \gamma_1 \leq k(x) \leq \gamma_2$ and $c \geq 0$.

Problem:

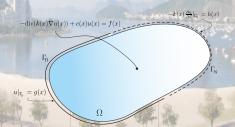
$$\mathcal{P} = \mathcal{P}(k, c, f, g, h) : \begin{cases} -\operatorname{div}(k(x)\nabla u(x)) + c(x)u(x) = f(x), & x \in \Omega, \\ u(x) = g(x), & x \in \Gamma_D, \\ k(x)\nabla u(x) \cdot \vec{n} = h(x), & x \in \Gamma_N. \end{cases}$$
 (a)

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Schematic representation of problem P(k, c, f, g, h)

Assume $g \in C(\Gamma_D)$ and define $H^1_{\Gamma_D,g}(\Omega) \doteq \left\{ v \in H^1(\Omega) : v|_{\Gamma_D} = g \right\}$. Multiplying (a) by $v \in H^1_{\Gamma_D,0}(\Omega)$ and integrating we obtain:



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$$0=\int_{\Omega}\left(\langle k
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abla v
angle+cuv
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$$\begin{split} 0 &= \int_{\Omega} \left(\langle k \nabla u, \nabla v \rangle + c u v \right) \ dx - \int_{\Omega} f v \ dx - \int_{\Gamma_N} h v \ ds \\ &\doteq F(u, v). \end{split}$$

Variation formulation of \mathcal{P} :

 $VF(\mathcal{P})$: Find u in $H^1_{\Gamma_0,\mathfrak{g}}(\Omega)$ such that F(u,v)=0 for all $v\in H^1_{\Gamma_0,0}(\Omega)$, i.e.

$$\int_{\Omega} (\langle k \nabla u, \nabla v \rangle + cuv) \ dx = \int_{\Omega} fv \ dx + \int_{\Gamma_{U}} hv \ ds, \quad \text{for all } v \in H^{1}_{\Gamma_{D},0}(\Omega).$$

An inverse heat conduction problem

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$$\int_{\Omega} (\langle k \nabla u, \nabla v \rangle + cuv) \ dx = \int_{\Omega} fv \ dx + \int_{\Gamma_N} hv \ ds, \quad \text{for all } v \in H^1_{\Gamma_D,0}(\Omega).$$

Define $B_{k,c}: H^1(\Omega) \times H^1(\Omega) \to \mathbb{R}$ by

$$B_{k,c}(u,v) \doteq \int_{\Omega} (\langle k\nabla u, \nabla v \rangle + cuv) dx.$$

Then $B_{k,c}$ defines an inner product on $H^1(\Omega)$ with associated norm

$$\|u\|_{B_{k,c}}^2 \doteq \int_{\Omega} (k\|\nabla u\|^2 + c|u|^2) dx.$$

Define also the energy functional $J: H^1_{\Gamma_D,g}(\Omega) o \mathbb{R}$ by

$$\begin{split} J(v) \; &\doteq \; \frac{1}{2} B_{k,c}(v,v) - \int_{\Omega} f v \; dx - \int_{\Gamma_N} h v \; ds \\ &= \frac{1}{2} \int_{\Omega} \left(\langle k \nabla v, \nabla v \rangle + c \; v^2 \right) \; dx - \int_{\Omega} f v \; dx - \int_{\Gamma_N} h v \; ds. \end{split}$$



Define also the energy functional $J:H^1_{\Gamma_D,g}(\Omega) o\mathbb{R}$ by

$$J(v) \doteq \frac{1}{2}B_{k,c}(v,v) - \int_{\Omega} fv \ dx - \int_{\Gamma_N} hv \ ds$$
$$= \frac{1}{2}\int_{\Omega} \left(\langle k\nabla v, \nabla v \rangle + c \ v^2 \right) \ dx - \int_{\Omega} fv \ dx - \int_{\Gamma_N} hv \ ds.$$

Then

Lemma

For any $u\in H^1_{\Gamma_D,g}(\Omega)$ and any $v\in H^1_{\Gamma_D,0}(\Omega)$ there holds

$$\frac{d}{dt}J(u+tv)|_{t=0} = F(u,v),$$



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and finally

Theorem

Problem $VF(\mathcal{P})$ does have a unique solution $u^* \in H^1_{\Gamma_D,g}(\Omega)$, characterized by the unique minimizer of the energy functional J, i.e.

$$u^* = \operatorname{argmin}_{u \in H^1_{\Gamma_{\Omega},g}(\Omega)} J(u).$$

The inverse problem

Given Ω , Γ_D , Γ_N , c, f, g and h, and a prescribed temperature distribution $\hat{u} \in H^1_{\Gamma_D,g}(\Omega)$ find the corresponding distributed conductivity field $k(\cdot)$ such that $u^* = \hat{u}$. That is, "invert" problem $\mathcal{P} = \mathcal{P}(k,c,f,g,h)$ with respect to k.



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For simplicity n=2, and $f=h\equiv 0$. Thus given $\hat{u}(x,y)\in H^1_{\Gamma_D,g}(\Omega)$ we want to find k=k(x,y) such that \hat{u} be the unique solution of problem $\mathcal{P}(k,c,f,g,h)$. Then k(x,y) must satisfy:

$$0 = \frac{d}{dt} J(\hat{u} + tv)|_{t=0}$$

= $\int_{\Omega} (\langle k \nabla \hat{u}, \nabla v \rangle + c \hat{u} v) dx dy, \quad \forall v \in H^{1}_{\Gamma_{D},0}(\Omega).$

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The optimality equation

Let Ω_i , $1 \le i \le L$, be a partition of Ω by open sets. For each i let $(x_i, y_i) \in \Omega_i$ and for any function q(x, y) defined on Ω let us denote with q_i the value of q at the point (x_i, y_i) , i.e. $q_i \doteq q(x_i, y_i)$. The optimality equation reads:

$$0 = \sum_{i=1}^{L} \left[k_i \left(\hat{u}_{x,i} v_{x,i} + \hat{u}_{y,i} v_{y,i} \right) + c_i \hat{u}_i v_i \right] m(\Omega_i), \quad \forall v \in H^1_{\Gamma_D,0}(\Omega),$$

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or, assuming a regular partition so that $m(\Omega_i)$ is constant

$$\sum_{i=1}^L k_i \left(\hat{u}_{x,i} v_{x,i} + \hat{u}_{y,i} v_{y,i} \right) = -\sum_{i=1}^L c_i \hat{u}_i v_i, \qquad \forall v \in H^1_{\Gamma_D,0}(\Omega).$$

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Consider now a finite, arbitrary set of functions

$$v^r \in H^1_{\Gamma_D,0}(\Omega), \qquad 1 \leq r \leq R.$$

Then we must have

$$\sum_{i=1}^{L} k_{i} \left(\hat{u}_{x,i} v_{x,i}^{r} + \hat{u}_{y,i} v_{y,i}^{r} \right) = -\sum_{i=1}^{L} c_{i} \hat{u}_{i} v_{i}^{r}, \qquad \forall \, 1 \leq r \leq R.$$

By defining

$$a_{r\ell} \doteq \hat{u}_{x,\ell} v_{x,\ell}^r + \hat{u}_{y,\ell} v_{y,\ell}^r \text{ and } f_r \doteq -\sum_{i=1}^L c_i \, \hat{u}_i \, v_i^r, \, 1 \leq \ell \leq L, \, 1 \leq r \leq R,$$

we end up with

$$\sum_{\ell=1}^{L} a_{r\ell} k_{\ell} = f_r, \qquad \forall \, 1 \leq r \leq R,$$

or simply

$$\mathbf{A}\,\mathsf{K}=\mathsf{F},\qquad (**)$$

where $\mathbf{A} \in \mathbb{R}^{R \times L}$, $K \in \mathbb{R}^L$ and $F \in \mathbb{R}^R$.

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Still need to impose the condition that all components of the vector K be bounded between the values γ_1 and γ_2 .

Idea: solve (**) in the least squares sense, weakly imposing this restriction through a penalizer



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$$J_{\alpha,W}(K) \doteq \|\mathbf{A}K - F\|^2 + \alpha W(K),$$

where $\alpha > 0$, and W(K) must be designed so as to deter non-admissible values as well as any undesired property of the conductivity profile k(x, y).

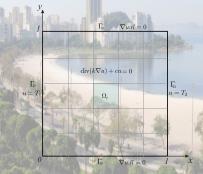


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Assumptions and numerical implementation:

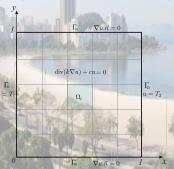


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Assumptions and numerical implementation:



 $T_1 > T_2$ and assume k(x,y) can take only two possible values, say k_L and k_U , with $0 < k_L < k_U < \infty$ (only two different materials are present in Ω).

At each point $(x, y) \in \Omega$, k(x, y) can only take one of the values k_L or k_U . Then W(K) must be designed so that it deters each and every component of the vector K to take any but one of those two values.



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Option 1: Let $p: \mathbb{R} \to \mathbb{R}$, $p(z) \doteq (z - k_L)(z - k_U) = z^2 - (k_L + k_U)z + k_L k_U$ and define $W_1: \mathbb{R}^L \to \mathbb{R}_0^+$ as

$$W_1(K) \doteq ||p(K)||_{\mathbb{R}^L}^2$$

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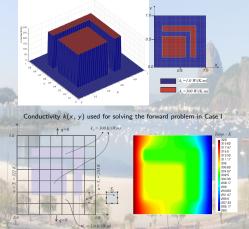
$$W_1(K) \doteq \|p(K)\|_{\mathbb{R}^L}^2.$$

Option 2: Add data-driven information about where to take one or the other value. Let $b \in \mathbb{R}^L$ binary, $b_i = 1$ iif $\|\nabla \hat{u}(x_i, y_i)\| > \gamma$, γ is a given threshold value,

$$W_2(K) \doteq ||b_U \odot (K - k_L \mathbf{1})||^2.$$

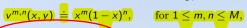
Examples and numerical experiments

Case I: We first solved \mathcal{P} with $T_1 = 322 [K]$, $T_2 = 283 [K]$, c(x,y) = 1 = const., and k(x,y) as shown (used a standard discretization by FEM, with biquadratic interpolation elements S2 with 8-nodes for computing $\hat{u}(x,y)$, $\hat{u}_x(x,y)$ and $\hat{u}_y(x,y)$)



a) Sketch of the distretized domain used to solve the forward problem, for case I. The finite element mesh S2 used is regular with elements size h = 1/200. b) Temperature distribution $\hat{u}(x, y)$

Setting 1: Picked $\alpha=0$ (non-penalized case) and $v^r\in H^1_{\Gamma_D,0}(\Omega),\ 1\leq r\leq R$ given by



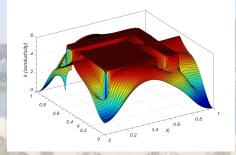
Severe ill-posedness: $Cond(A) \approx 2.5 \times 10^{18}$.



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 $v^{m,n}(x,y) \doteq x^m(1-x)^n, \quad \text{for } 1 \leq m,n \leq M,$

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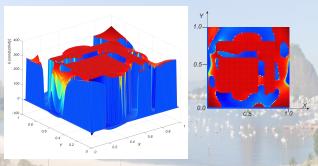


Reconstruction of k(x, y) obtained using a non-penalized least squares approach.

Setting 2: Take $\alpha > 0$ and $W(K) = W_1(K)$



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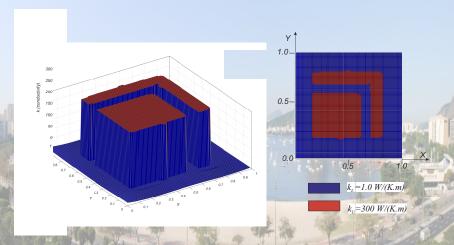


Reconstruction of k(x, y) obtained using $W(K) = W_1(K)$

Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$

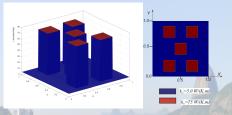


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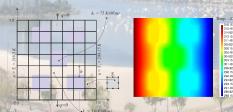


Reconstruction of k(x, y) obtained using $W(K) = W_2(K)$, Case I.

Conductivity profile shown below; $T_1=318,15$ [K], $T_2=288,15$ [K], c(x,y)=1=constant.



Distributed values of the conductivity k(x, y) used for solving the forward problem in Case II

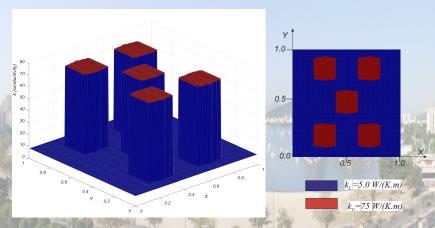


a) Sketch of the distretized domain used to solve the forward problem for Case II. The finite element mesh S2 used is regular with elements size h=1/200. b) Temperature distribution $\hat{u}(x,y)$ for k(x,y) for Case II.

Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$



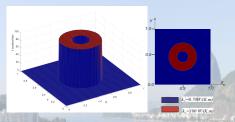
Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$



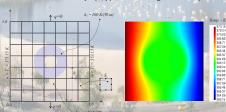
Reconstruction of k(x, y) obtained using $W(K) = W_2(K)$, Case II

Case III

Conductivity profile shown below; $T_1 = 373,15$ [K], $T_2 = 353,15$ [K], c(x,y) = 1,0 = constant, $k_U = 100$ and $k_L = 0,7$.



Distributed values of the conductivity k(x, y) used for solving the forward problem in Case III



a) Sketch of the distretized domain used to solve the forward problem for Case III. The finite element mesh S2 used is regular with elements size

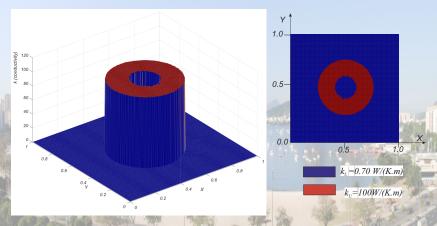
Case III

Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$



Case III

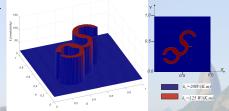
Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$



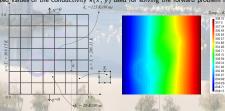
Reconstruction of k(x, y) obtained using $W(K) = W_2(K)$, Case III

Conductivity profile shown below; $T_1 = 308,15$ [K], $T_2 = 298,15$ [K], c(x,y) = 1,0 = constant,

$$k_U = 125$$
 and $k_L = 20$.



Distributed values of the conductivity k(x, y) used for solving the forward problem in Case IV

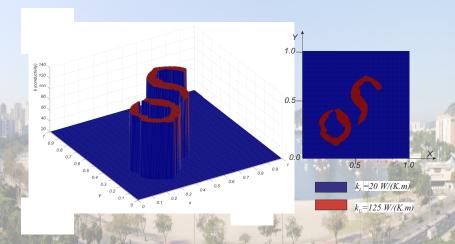


a) Sketch of the distretized domain used to solve the forward problem for Case IV. The finite element mesh S2 used is regular with elements size h = 1/200. b) Temperature distribution $\hat{u}(x, y)$ for k(x, y) for Case IV.

Setting 3: Take $\alpha > 0$ and $W(K) = W_2(K)$



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Reconstruction of k(x, y) obtained using $W(K) = W_2(K)$, Case IV



There are many open problems:

• The case of *n* materials



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 This is the basis of the EIT
- Many more...

...and that's all...



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thanks for your attention!

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