Shape optimization for interface identification in nonlocal models

Volker Schulz

and

Christian Vollmann

ALGORITHMIC OPTIMIZATION

www.alop.uni-trier.de

Universität Trier

Why nonlocal operators?

Because of a wealth of application fields:

- fractional diffusion (Brockmann et al. 2008, D'Elia and Gunzburger 2013, Harbir 2015,...)
- peridynamics (Silling 2000, Du and Zhou 2010/11, D'Elia et al. 2016,...)
- image processing (Gilboa and Osher 2009, Lou et al. 2010, Peyre et al. 2008,...)
- cardiology (Cusimano et al. 2015,...)
- machine learning (Rosasco et al. 2010,...)
- finance (Lvendoskii et al. 2004,...)
- growth models in economics (Augeraud-Veron et al. 2019 [survey], Frerick/Müller-Fürstenberger/Sachs/Somorowsky 2019,...)

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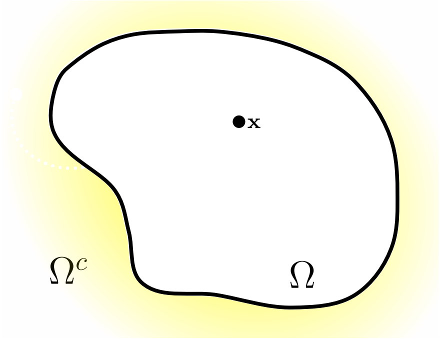
Because of interesting structures:

- full matrices lacking sparsity
- nevertheless, on structured grids, tensor based methods exist for fractional Laplacians limiting the overall effort to $\mathcal{O}(n \log n)$ – also in the optimal control case (Heidel/Khoromskaia/Khoromskij/Schulz 2018)
- general nonlocal operators on structured grids provide Toeplitz structures leading to high efficiency (Vollmann/Schulz 2019)

$\rightarrow$ numerical solution of nonlocal shape optimization problems is a new challenge and has to be done on unstructured meshes



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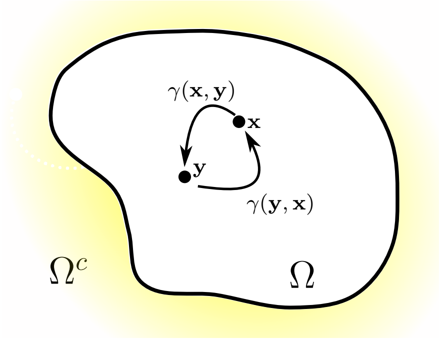

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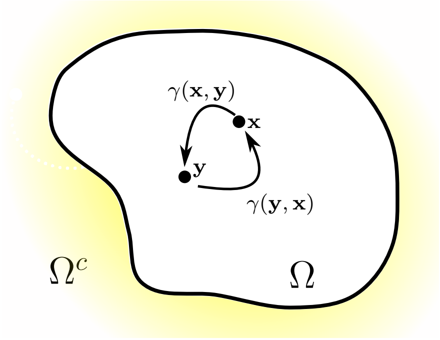

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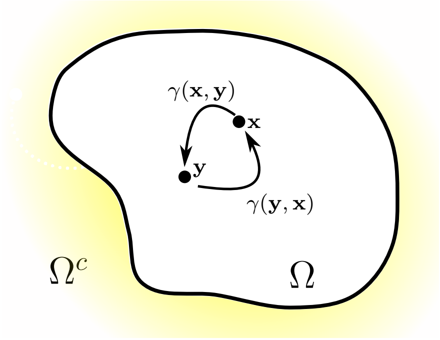

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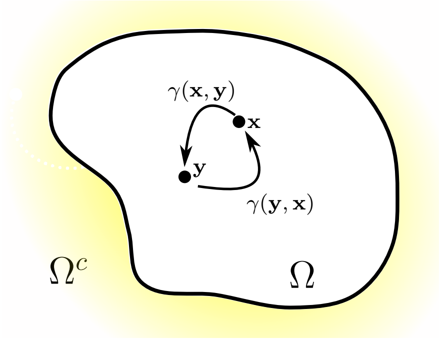

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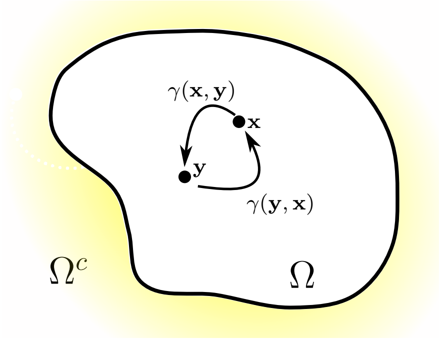

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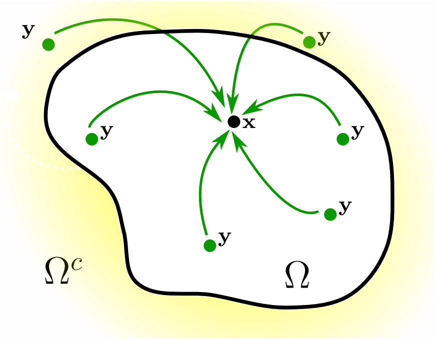

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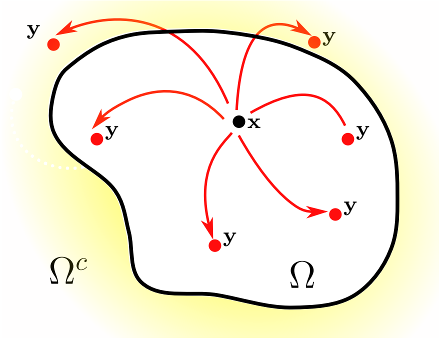

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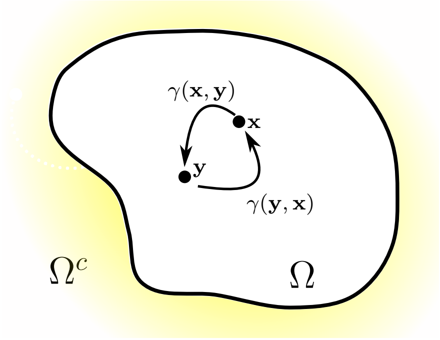

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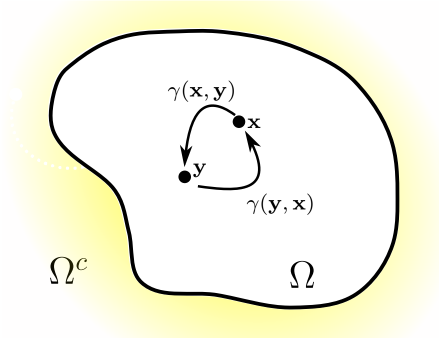

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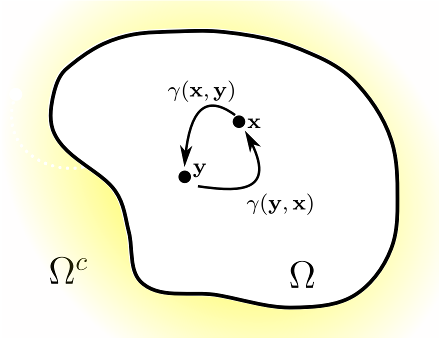

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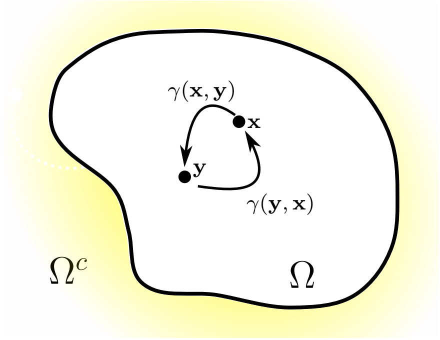

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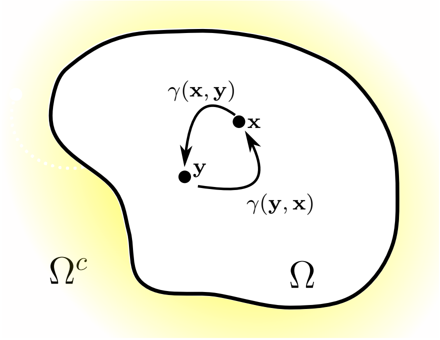

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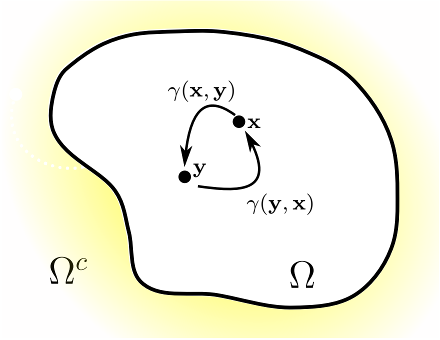

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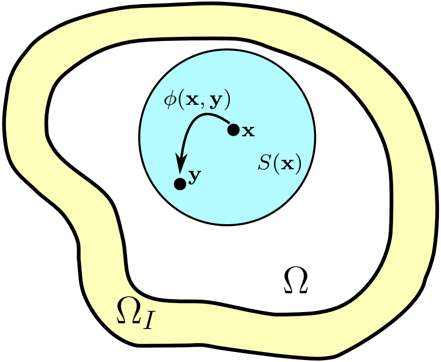

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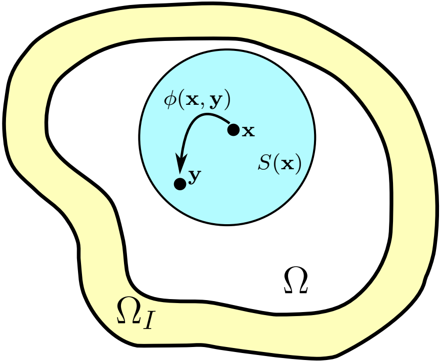

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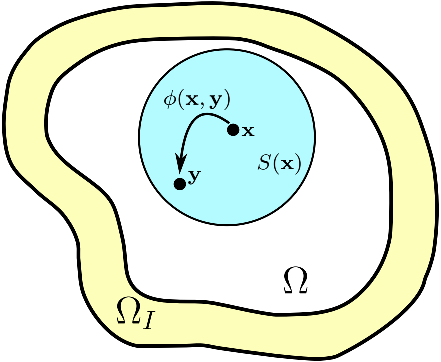

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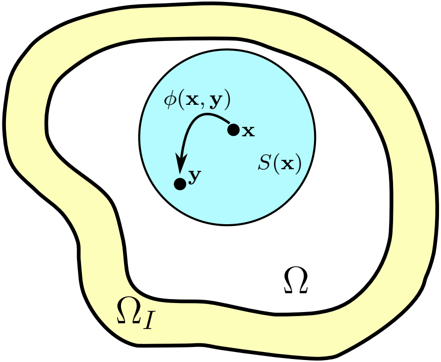

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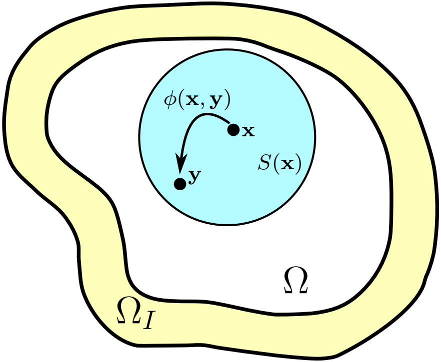

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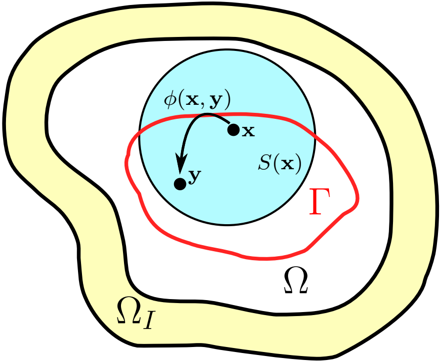
Steady-state nonlocal Dirichlet problem

$$\begin{cases} -\mathcal{L}u = f & \text{on } \Omega \\ u = g & \text{on } \Omega_I \end{cases}$$



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Overview

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1 The optimization problem

2 Shape derivatives

3 Numerical results

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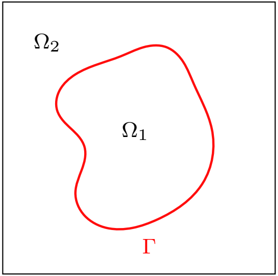
$$\min_{(u,\Gamma)} \ \frac{1}{2}\,\|u-\bar{u}\|^2_{L^2(\Omega)} + \ \mathcal{R}(\Gamma)$$

$$\text{s.t.} \quad \mathcal{L}_\Gamma u = f_\Gamma$$



$\Omega = (0,1)^2 = \Omega_1 \,\dot\cup\, \Gamma \,\dot\cup\, \Omega_2$

1. Problem formulation

ALGORITHMIC OPTIMIZATION

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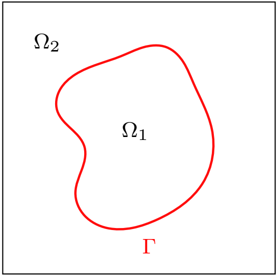
s.t. $\mathcal{L}_\Gamma u = f_\Gamma$



$\Omega = (0,1)^2 = \Omega_1 \,\dot\cup\, \Gamma \,\dot\cup\, \Omega_2$

Well studied example *(e.g. Schulz, Siebenborn, Welker; SIOPT 2016)*:

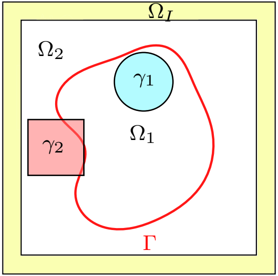
$$\mathcal{L}_\Gamma u(\mathbf{x}) = -\operatorname{div} k_\Gamma \nabla u(\mathbf{x})$$

$$k_\Gamma(\mathbf{x}) = \begin{cases} k_1(\mathbf{x}) & : \mathbf{x} \in \Omega_1 \\ k_2(\mathbf{x}) & : \mathbf{x} \in \Omega_2 \end{cases} \qquad f_\Gamma(\mathbf{x}) = \begin{cases} f_1(\mathbf{x}) & : \mathbf{x} \in \Omega_1 \\ f_2(\mathbf{x}) & : \mathbf{x} \in \Omega_2 \end{cases}$$

- shape derivative used as force for elastic mesh deformation
- in line with shape Hessian estimation on the boundary (Eppler/Harbrecht/Schneider 2007)

$$\min_{(u,\Gamma)} \; \frac{1}{2}\,\|u-\bar{u}\|^2_{L^2(\Omega)} + \; \mathcal{R}(\Gamma)$$

$$\text{s.t.} \qquad \mathcal{L}_\Gamma u = f_\Gamma$$



$$\Omega = (0,1)^2 = \Omega_1 \,\dot\cup\, \Gamma \,\dot\cup\, \Omega_2$$

Here:

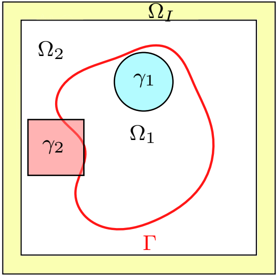
$$\mathcal{L}_\Gamma u(\mathbf{x}) := \int_{\Omega\cup\Omega_I} \left(u(\mathbf{x})\gamma_\Gamma(\mathbf{x},\mathbf{y}) - u(\mathbf{y})\gamma_\Gamma(\mathbf{y},\mathbf{x})\right) d\mathbf{y}$$

$$\gamma_\Gamma(\mathbf{x},\mathbf{y}) = \begin{cases} \gamma_1(\mathbf{x},\mathbf{y}) & : \mathbf{x}\in\Omega_1 \\ \gamma_2(\mathbf{x},\mathbf{y}) & : \mathbf{x}\in\Omega_2\cup\Omega_I \end{cases} \qquad f_\Gamma(\mathbf{x}) = \begin{cases} f_1(\mathbf{x}) & : \mathbf{x}\in\Omega_1 \\ f_2(\mathbf{x}) & : \mathbf{x}\in\Omega_2 \end{cases}$$

1. Problem formulation

$$\min_{(u,\Gamma)} \ \frac{1}{2}\|u-\bar{u}\|^2_{L^2(\Omega)} + \mathcal{R}(\Gamma)$$

$$\text{s.t.} \quad \mathcal{L}_\Gamma u - \mu\Delta u = f_\Gamma$$



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$\mu > 0$ small perturbation parameter to guarantee regularity

$$\min_{(u,\Gamma)} \quad \frac{1}{2}\|u-\bar{u}\|^2_{L^2(\Omega)} + \mathcal{R}(\Gamma)$$

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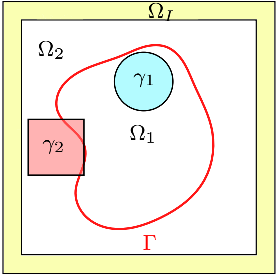

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- **Shape definition**
  $\rightarrow$ *Here:* Simple closed, smooth curve $\Gamma \subset \Omega$.

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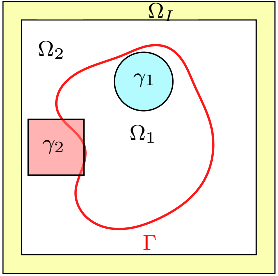

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- **Derivative concept**

  $\rightarrow$ *Here:* Eulerian derivative

  For a smooth vector field $\mathbf{V}\colon \Omega \to \mathbb{R}^2$ let $F_t := \mathbf{Id} + t\mathbf{V}$ (*perturbation of identity*), then we define

$$DJ(\Gamma)[\mathbf{V}] := \lim_{t \searrow 0} \frac{1}{t}\big(J(F_t(\Gamma)) - J(\Gamma)\big).$$

Optimal control for nonlocal operators

- M. D'Elia and M. Gunzburger: *Optimal distributed control of nonlocal steady diffusion problems.* SICON (2014).
- M. D'Elia and M. Gunzburger: *Identification of the diffusion parameter in nonlocal steady diffusion problems.* Appl. Math. Optim. (2016)
- M. D'Elia, C. Glusa, and E. Otárola: *A priori error estimates for the optimal control of the integral fractional Laplacian.* SICON (2019)
- E. Otárola and A.J. Salgado: *Sparse optimal control for fractional diffusion.* CMAM (2018)
- . . .

$\rightarrow$ Control variable is typically modeled to be an element of a suitable function space.

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Shape optimization for nonlocal operators

- J.F. Bonder and J.F. Spedaletti: *Some nonlocal optimal design problems.* Jour. of Math. Anal. and Appl. (2018)
- E. Parini and A. Salort: *Compactness and dichotomy in nonlocal shape optimization.* arXiv:1806.01165 (2018)
- Y. Sire, J.L. Vázquez, and B. Volzone: *Symmetrization for fractional elliptic and parabolic equations and an isoperimetric application.* Chin. Ann. of Math., Ser. B (2017).
- J. Fernández Bonder, A. Ritorto, and A. Salort: *A class of shape optimization problems for some nonlocal operators.* Advances in Calculus of Variations (2017).
- A.-L. Dalibard and D. Gérard-Varet: *On shape optimization problems involving the fractional Laplacian.* ESAIM: COCV (2013).
- A. Burchard, R. Choksi, and I. Topaloglu: *Nonlocal shape optimization via interactions of attractive and repulsive potentials.* arXiv:1512.07282 (2018).
- . . . ?

→ All of them are of theoretical nature and do not involve numerics.

Overview

ALGORITHMIC OPTIMIZATION

1 The optimization problem

2 Shape derivatives

3 Numerical results

- **Optimization approach**
  → *Here:* Formal Lagrangian analogous to (Laurain/Sturm 2016)

$$\min_{(u,\Gamma)} \; J(u,\Gamma) \quad \text{s.t.} \quad c(u,\Gamma)=0$$

where

$$J(u,\Gamma) := \tfrac{1}{2}\,\|u-\bar{u}\|^2_{L^2(\Omega)}$$
$$c(u,\Gamma) := A_\Gamma(u,\cdot) + \mu(\nabla u, \nabla \cdot)_{L^2} - \ell_\Gamma(\cdot)$$

- **Optimization approach**
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Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

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Then $DJ^{red}(\Gamma) = J_u u'_\Gamma + J_\Gamma$, but u'_Γ is hard to determine.

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Therefore we consider the **Lagrange functional**

$$L(u,\Gamma,v) := \tfrac{1}{2}\, \|u - \bar{u}\|^2_{L^2(\Omega)} + A_\Gamma(u,v) + \mu(\nabla u, \nabla v)_{L^2(\Omega)} - \ell_\Gamma(v).$$

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2. Shape Derivatives

- **Optimization approach**
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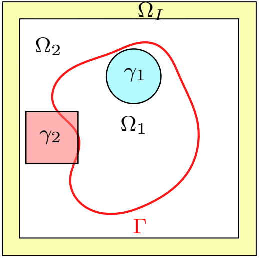
$\rightarrow$ **Crucial here:** Shape derivatives of $A_\Gamma(u,v)$ and $\ell_\Gamma(v)$.



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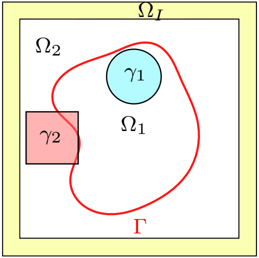
$$DJ^{red}(\Gamma)[\mathbf{V}] = D_\Gamma L(u, \Gamma, v)[\mathbf{V}] = D_\Gamma A_\Gamma(u, v)[\mathbf{V}] - D_\Gamma \ell_\Gamma(v)[\mathbf{V}]$$



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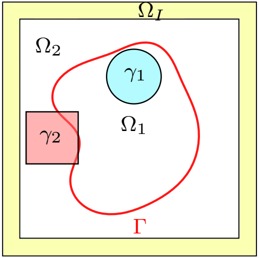

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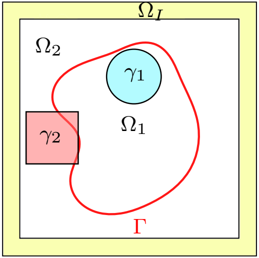

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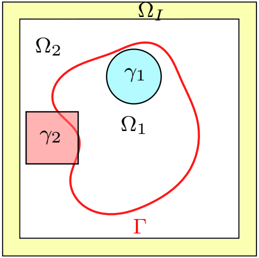
$$A_\Gamma(u,v) = (\mathcal{L}_\Gamma u, v)_{L^2(\Omega)}$$

ALGORITHMIC OPTIMIZATION



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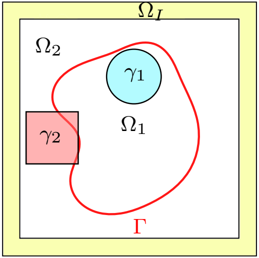

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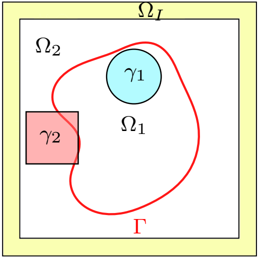

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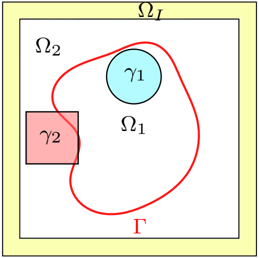
\end{aligned}$$



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&= \sum_{i=1,2} \sum_{j=1,2} \int_{\Omega_i} \int_{\Omega_j} v(\mathbf{x})(u(\mathbf{x})\gamma_i(\mathbf{x},\mathbf{y}) - u(\mathbf{y})\gamma_j(\mathbf{y},\mathbf{x})) d\mathbf{y} d\mathbf{x} \\
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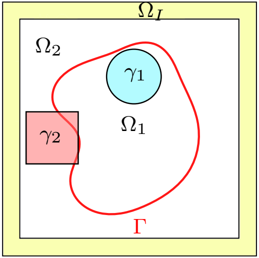
$$= \int_{\Omega_j} \int_{\Omega_i} v(\mathbf{y})u(\mathbf{x})\gamma_j(\mathbf{x},\mathbf{y}) d\mathbf{y} d\mathbf{x}$$



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$$DJ^{red}(\Gamma)[\mathbf{V}] = D_\Gamma L(u,\Gamma,v)[\mathbf{V}] = \underbrace{D_\Gamma A_\Gamma(u,v)[\mathbf{V}]}_{\uparrow} - \underbrace{D_\Gamma \ell_\Gamma(v)[\mathbf{V}]}_{\checkmark}$$

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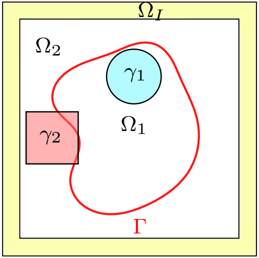
ALGORITHMIC OPTIMIZATION



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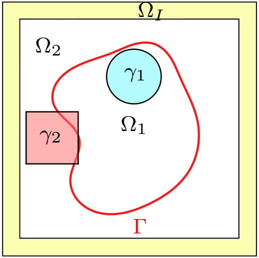

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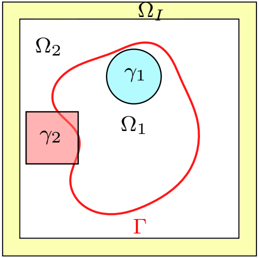

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&= \sum_{i=1,2}\sum_{j=1,2}\int_{\Omega_i}\int_{\Omega_j} u(\mathbf{x})(v(\mathbf{x}) - v(\mathbf{y}))\underbrace{\gamma_i(\mathbf{x},\mathbf{y})}_{=\phi_i(\mathbf{x},\mathbf{y})\chi_{S_i(\mathbf{x})}(\mathbf{y})} d\mathbf{y}d\mathbf{x}
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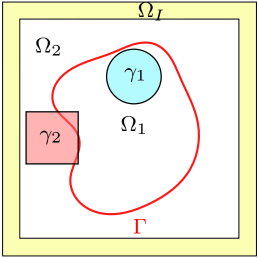

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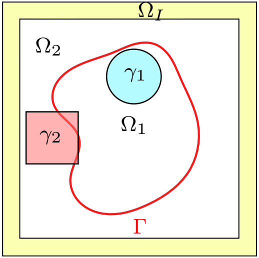
\end{aligned}$$



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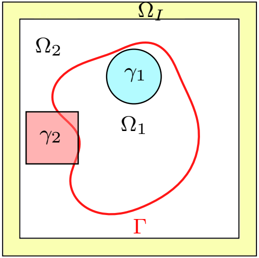

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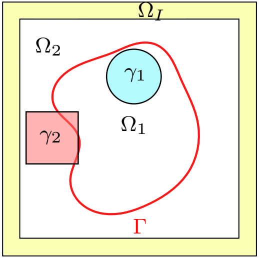

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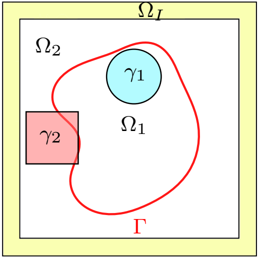

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$$\vdots$$

$$= \sum_{i=1,2} \int_{\Omega_i} \int_{S_i(\mathbf{x})} \left(\nabla_{\mathbf{x}}\psi_i(\mathbf{x},\mathbf{y}) + \nabla_{\mathbf{y}}\psi_i(\mathbf{x},\mathbf{y})\right)^T \mathbf{V} + \psi_i(\mathbf{x},\mathbf{y}) \operatorname{div} \mathbf{V} \; d\mathbf{y} d\mathbf{x}$$

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Theorem (Vollmann/Schulz 2019)

Let the partial kernel functions ϕ_1, ϕ_2 be differentiable and let the interaction sets be translation invariant, so that $S_i(\mathbf{x}) = \mathbf{x} + S_i(\mathbf{0})$. Further, let $u = u(\Gamma)$ and $v = v(\Gamma)$ solve the state and adjoint equation, respectively, then we find

$$\begin{aligned} DJ^{red}(\Gamma)[\mathbf{V}] = & -\int_{\Omega} \nabla f_{\Gamma}^T \mathbf{V}\ v\ d\mathbf{x} - \int_{\Omega} f_{\Gamma} v\ \operatorname{div} \mathbf{V}\ d\mathbf{x} - \left(u - \overline{u}, \nabla u^T \mathbf{V}\right)_{L^2(\Omega)} \\ & + \mu \left(\int_{\Omega} \nabla u^T \nabla v\ \operatorname{div} \mathbf{V} d\mathbf{x} - \int_{\Omega} \nabla u^T \left(\nabla \mathbf{V} + \nabla \mathbf{V}^T \right) \nabla v d\mathbf{x} \right) \\ & + \sum_{i=1,2} \int_{\Omega_i} \int_{S_i(\mathbf{x})} u(\mathbf{x}) \left(v(\mathbf{x}) - v(\mathbf{y}) \right) \phi_i(\mathbf{x}, \mathbf{y})\ \operatorname{div} \mathbf{V}(\mathbf{x})\ d\mathbf{y} d\mathbf{x} \\ & + \sum_{i=1,2} \int_{\Omega_i} \int_{S_i(\mathbf{x})} u(\mathbf{x})(v(\mathbf{x}) - v(\mathbf{y})) \left(\nabla_{\mathbf{x}} \phi_i(\mathbf{x}, \mathbf{y}) + \nabla_{\mathbf{y}} \phi_i(\mathbf{x}, \mathbf{y}) \right)^T \mathbf{V}(\mathbf{x})\ d\mathbf{y} d\mathbf{x}. \end{aligned}$$

Overview

ALGORITHMIC OPTIMIZATION

1 The optimization problem

2 Shape derivatives

3 Numerical results

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$

while $\|DJ^{red}(\Gamma_k)\| >$ *tol* **do**

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$

while $\|DJ^{red}(\Gamma_k)\| > \textit{tol}$ **do**

(1) Assemble stiffness matrices and solve **state** and **adjoint** equation
$\rightarrow u(\Gamma_k)$, $v(\Gamma_k)$

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$

while $\|DJ^{red}(\Gamma_k)\| > tol$ **do**

> **(1)** Assemble stiffness matrices and solve **state** and **adjoint** equation
>
> $\rightarrow u(\Gamma_k),\ v(\Gamma_k)$
>
> **(2)** Compute the mesh deformation ("gradient")
>
> Assemble shape derivative $DJ^{red}(\Gamma_k)[\mathbf{V}]$
>
> Assemble linear elasticity a_{Γ_k} and solve the deformation equation
>
> $$a_{\Gamma_k}(\mathbf{U}_k, \mathbf{V}) = DJ^{red}(\Gamma_k)[\mathbf{V}] \quad \text{for all} \quad \mathbf{V}$$
>
> $\rightarrow \mathbf{U}_k$

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$

while $\|DJ^{red}(\Gamma_k)\| > $ *tol* **do**

 (1) Assemble stiffness matrices and solve **state** and **adjoint** equation

  $\rightarrow u(\Gamma_k)$, $v(\Gamma_k)$

 (2) Compute the mesh deformation (“gradient”)

  Assemble shape derivative $DJ^{red}(\Gamma_k)[\mathbf{V}]$

  Assemble linear elasticity a_{Γ_k} and solve the deformation equation

$$a_{\Gamma_k}(\mathbf{U}_k, \mathbf{V}) = DJ^{red}(\Gamma_k)[\mathbf{V}] \quad \text{for all} \quad \mathbf{V}$$

  $\rightarrow \mathbf{U}_k$

 (3) Backtracking line search (with parameters $\alpha = 1, \tau, c \in (0,1)$)

  while $J^{red}(\Gamma_k - \alpha \mathbf{U}_k) \geq c J^{red}(\Gamma_k)$ **do**

   $\alpha = \tau\alpha$

  end

  $\rightarrow \alpha_k$

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$
while $\|DJ^{red}(\Gamma_k)\| > tol$ **do**
  (1) Assemble stiffness matrices and solve **state** and **adjoint** equation
    $\to u(\Gamma_k)$, $v(\Gamma_k)$
  (2) Compute the mesh deformation ("gradient")
    Assemble shape derivative $DJ^{red}(\Gamma_k)[\mathbf{V}]$
    Assemble linear elasticity a_{Γ_k} and solve the deformation equation
      $a_{\Gamma_k}(\mathbf{U}_k, \mathbf{V}) = DJ^{red}(\Gamma_k)[\mathbf{V}]$ for all $\mathbf{V}$
    $\to \mathbf{U}_k$
  (3) Backtracking line search (with parameters $\alpha = 1, \tau, c \in (0,1)$)
    while $J^{red}(\Gamma_k - \alpha \mathbf{U}_k) \geq c J^{red}(\Gamma_k)$ **do**
      $\alpha = \tau\alpha$
    end
    $\to \alpha_k$
  (4) Update mesh
    $\Omega_{k+1} = \Omega_k - \alpha_k \mathbf{U}_k(\Omega_k) = \{\mathbf{x} - \alpha_k \mathbf{U}_k(\mathbf{x}) \colon \mathbf{x} \in \Omega_k\}$
end

Reduced problem:

$$\min_{\Gamma} J^{red}(\Gamma) := J(u(\Gamma), \Gamma)$$

Shape optimization algorithm:

Initialize: $\bar{u}, \gamma_\Gamma, f_\Gamma, \Gamma_0$

while $\|DJ^{red}(\Gamma_k)\| > tol$ **do**

  (1) Assemble stiffness matrices and solve **state** and **adjoint** equation

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    Assemble linear elasticity a_{Γ_k} and solve the deformation equation

$$a_{\Gamma_k}(\mathbf{U}_k, \mathbf{V}) = DJ^{red}(\Gamma_k)[\mathbf{V}] \quad \text{for all} \quad \mathbf{V}$$

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end

for

$$\gamma_\Gamma(x,y) := (\phi_1(x,y)\chi_{\Omega_1}(x) + \phi_2(x,y)\chi_{\Omega_2}(x))\chi_{B_{\delta,\infty}}(y)$$

where

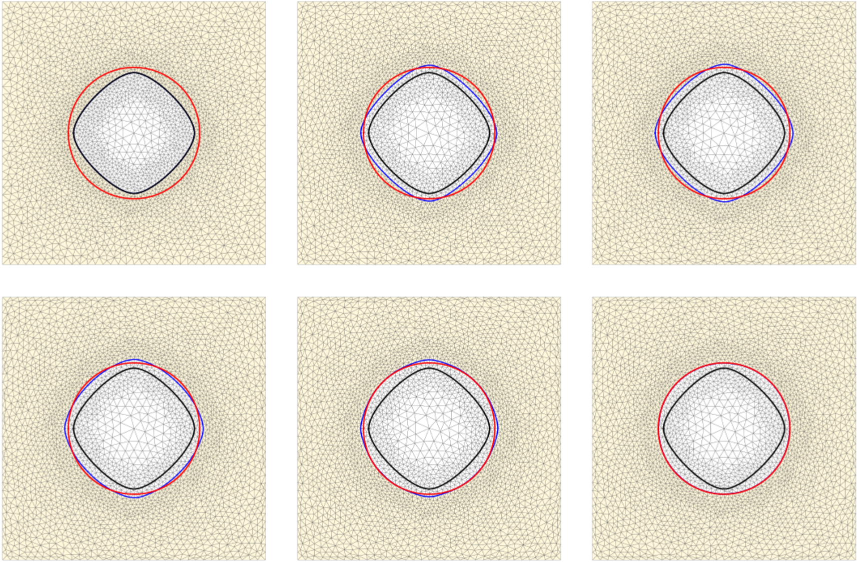
$$\phi_1(x,y) = \frac{1}{1000}c_\delta$$

$$\phi_2(x,y) = 100c_\delta\left(1 - \frac{\|y-x\|_\infty}{\delta}\right)^2$$

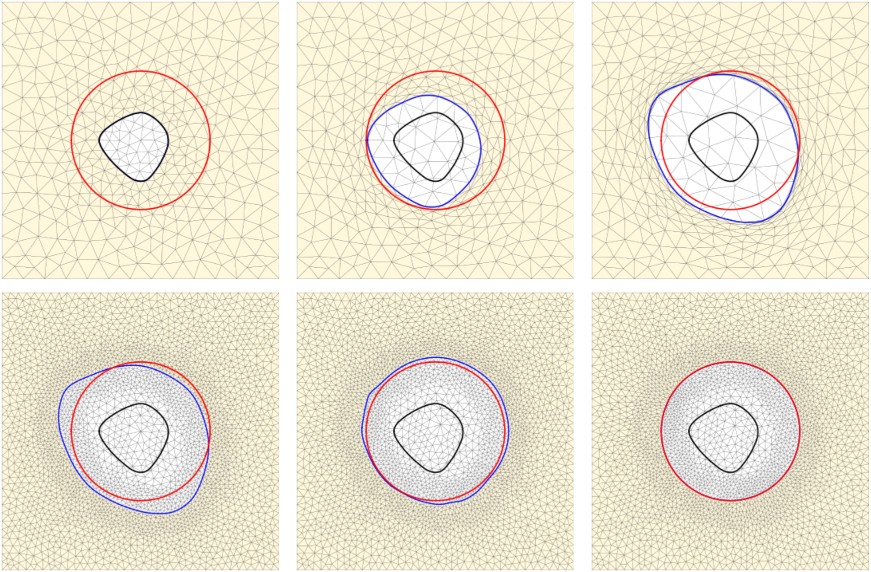
and

$$f_\Gamma(x) := 100\chi_{\Omega_1}(x) + \chi_{\Omega\setminus\Omega_1}(x)$$

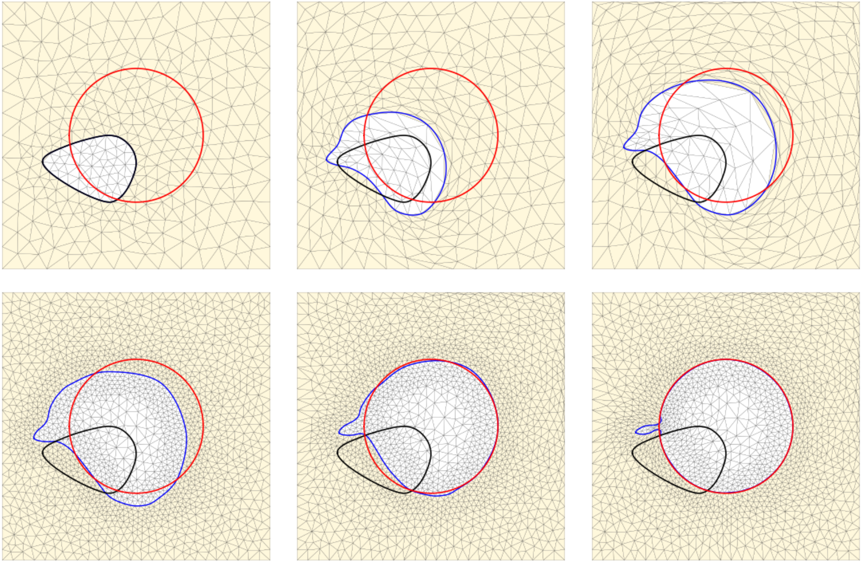
3. Numerical results I



3. Numerical results II



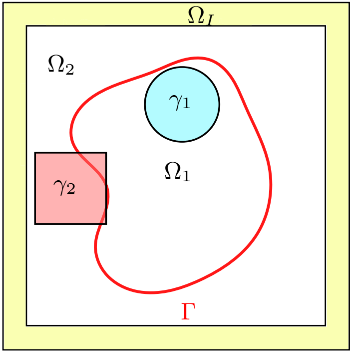
3. Numerical results III



Summary *(arXiv:1909.08884)*

$$\min_{(u,\Gamma)} \ \frac{1}{2}\|u-\bar{u}\|^2_{L^2(\Omega)} + \mathcal{R}(\Gamma)$$

$$\text{s.t.} \quad \mathcal{L}_\Gamma u - \mu\Delta u = f_\Gamma$$



Done:

- Definition of an interface-dependent **nonlocal coupled system**.
- **Shape derivative** of the corresponding nonlocal bilinear form.
- Implementation of a shape optimization **algorithm**.

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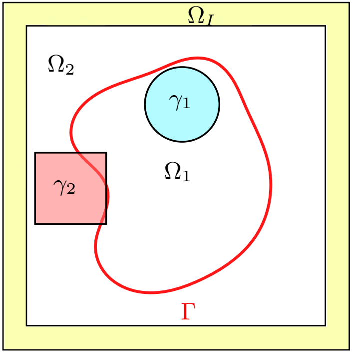

Done:

- Definition of an interface-dependent **nonlocal coupled system**.
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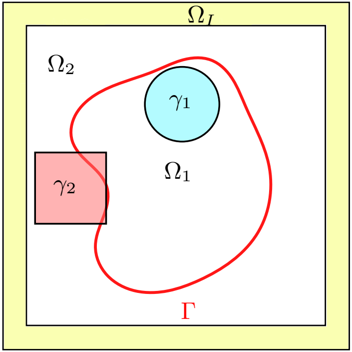
To do:

- More analytic investigations for shape derivative.
- Local limit: Do we recover corresponding local shape derivatives?
- Analyze different inner products for determining the gradient.

Summary *(arXiv:1909.08884)*



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$$\text{s.t.} \quad \mathcal{L}_\Gamma u - \mu \Delta u = f_\Gamma$$

Done:

- Definition of an interface-dependent **nonlocal coupled system**.
- **Shape derivative** of the corresponding nonlocal bilinear form.
- Implementation of a shape optimization **algorithm**.

Thank you for your attention!

Volker Schulz (volker.schulz@uni-trier.de)
Christian Vollmann (vollmann@uni-trier.de)