Spatial regression models over two-dimensional Riemannian manifolds

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Joint Work with Simona Perotto and Laura Sangalli

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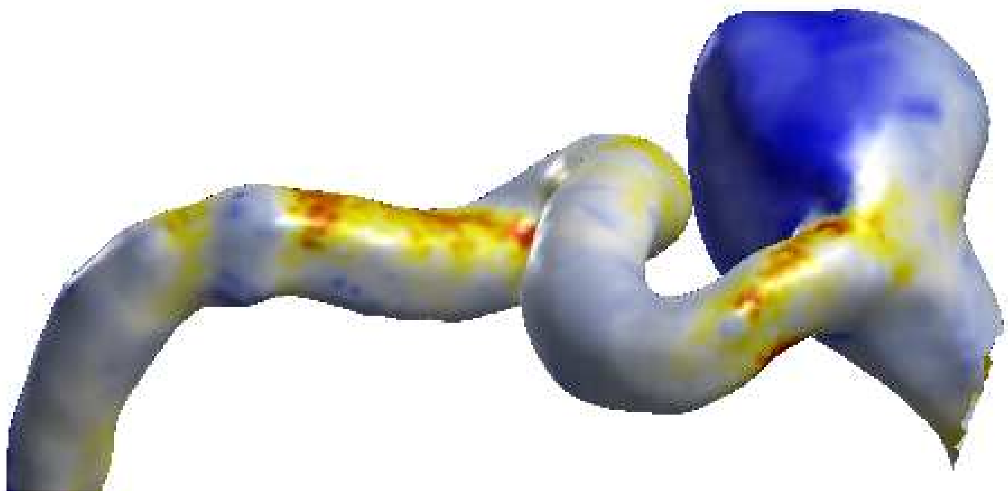
MOX MODELLISTICA E CALCOLO SCIENTIFICO
MODELING AND SCIENTIFIC COMPUTING

Modeling wall shear stress



- Wall shear stress modulus at the systolic peak on real inner carotid artery geometry affected by aneurysm
- data obtained by CFD, courtesy of the AneuRisk project
  - Passerini, 2009, PhD Thesis, Politecnico di Milano
  - http://mox.polimi.it/it/progetti/aneurisk/

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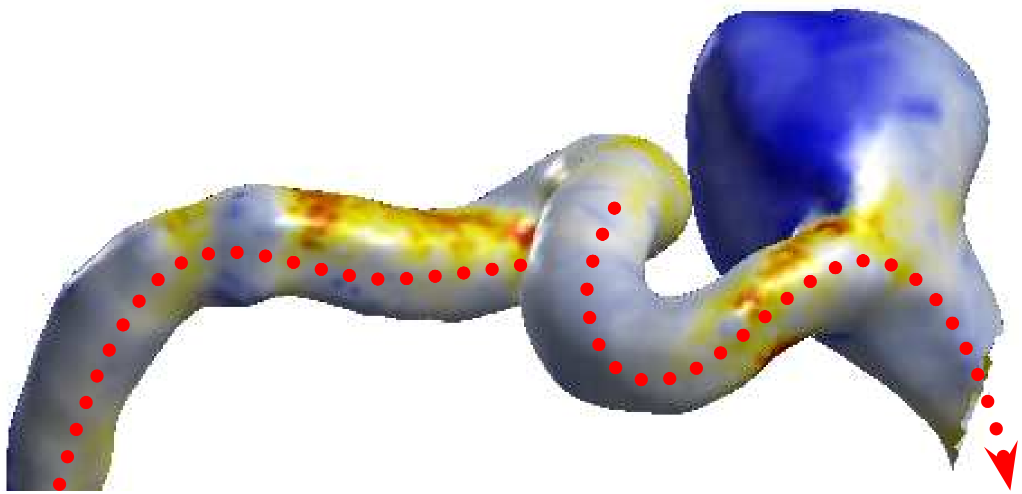
Angular flattening map

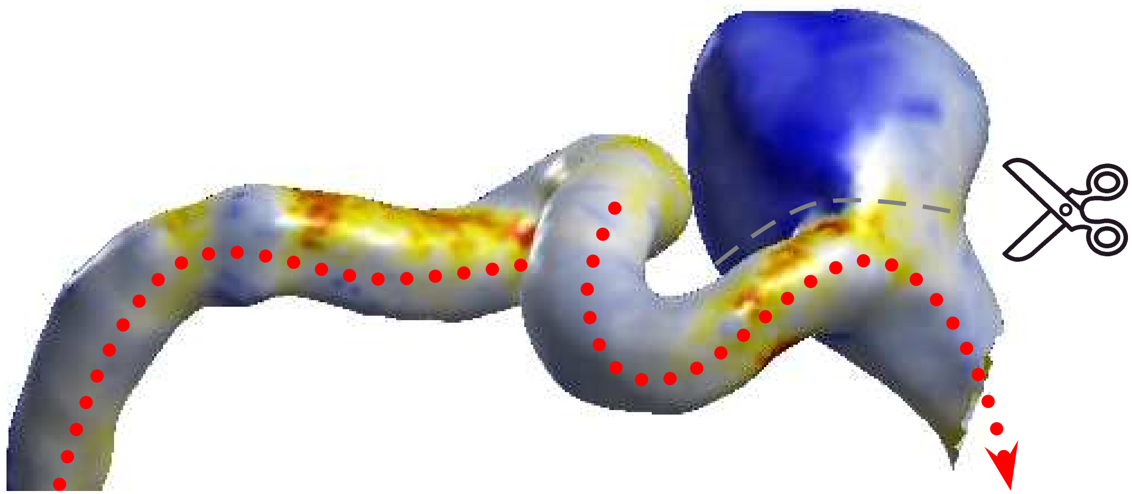


A new coordinate system is defined by (s, r, θ)

- s is the curvilinear abscissa along the artery centerline
- θ the angle of the surface point with respect to the artery centerline.
- r the artery radius

The domain is then reduced to the plane $(s, \theta * \bar{r})$

Angular flattening map issues



1. important factors of the parent vasculature are ignored
    - the curvature
    - the radius

2. the aneurysm must be removed

Current smoothing methods for surface domains

1. Nearest Neighbor Averaging (Hagler et al., 2006)

   simple

2. Heat Kernel Smoothing (Chung et al., 2005)

   inference

Spatial Spline Regression model for non-planar domains

- Data locations:

  $\{\mathbf{x}_i = (x_{1i}, x_{2i}, x_{3i});\ i = 1, \ldots, n\}$ on a surface $\Sigma \subset \mathbb{R}^3$

- The model: $z_i = f(\mathbf{x}_i) + \epsilon_i$

  ϵ_i are i.i.d. errors with $E[\epsilon_i] = 0$ and $Var(\epsilon_i) = \sigma^2$

  f is a twice continuously differentiable real-valued function

- The estimate:

$$J_\lambda(f(\mathbf{x})) = \sum_{i=1}^{n} (z_i - f(\mathbf{x}_i))^2 + \lambda \int_\Sigma (\Delta_\Sigma f(\mathbf{x}))^2 \ d\Sigma$$

  Δ_Σ - Laplace-Beltrami operator for functions on the surface Σ

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- The model: $z_i = f(\mathbf{x}_i) + \epsilon_i$ or $z_i = \mathbf{w}_i' \beta + f(\mathbf{x}_i) + \epsilon_i$

  ϵ_i are i.i.d. errors with $E[\epsilon_i] = 0$ and $Var(\epsilon_i) = \sigma^2$

  f is a twice continuously differentiable real-valued function

  $\beta \in \mathbb{R}^q$ is the vector of regression coefficients

  $\mathbf{w}_i = (w_{i1}, \ldots, w_{iq})$ is a q-vector of covariates

- The estimate:

$$J_\lambda(f(\mathbf{x})) = \sum_{i=1}^{n} \left(z_i - \mathbf{w}_i' \beta - f(\mathbf{x}_i)\right)^2 + \lambda \int_\Sigma \left(\Delta_\Sigma f(\mathbf{x})\right)^2 \, d\Sigma$$

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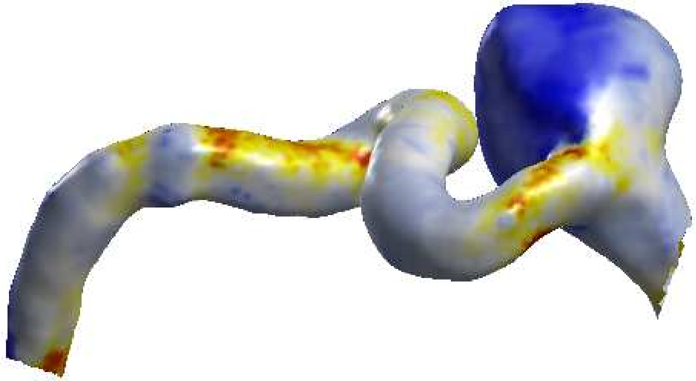
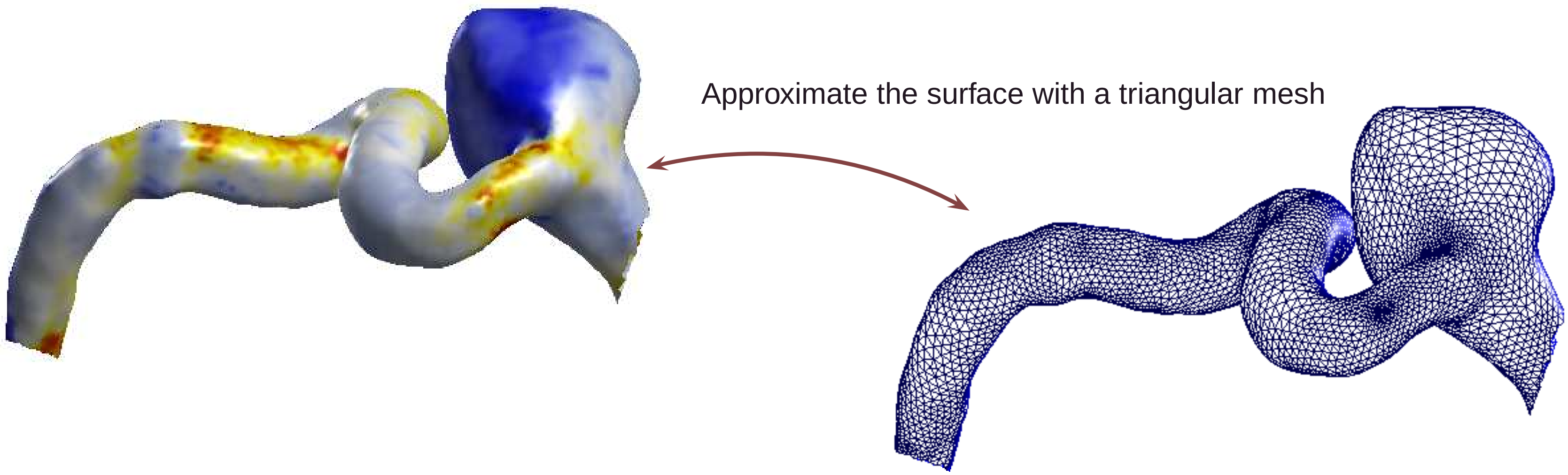
The plan



The plan



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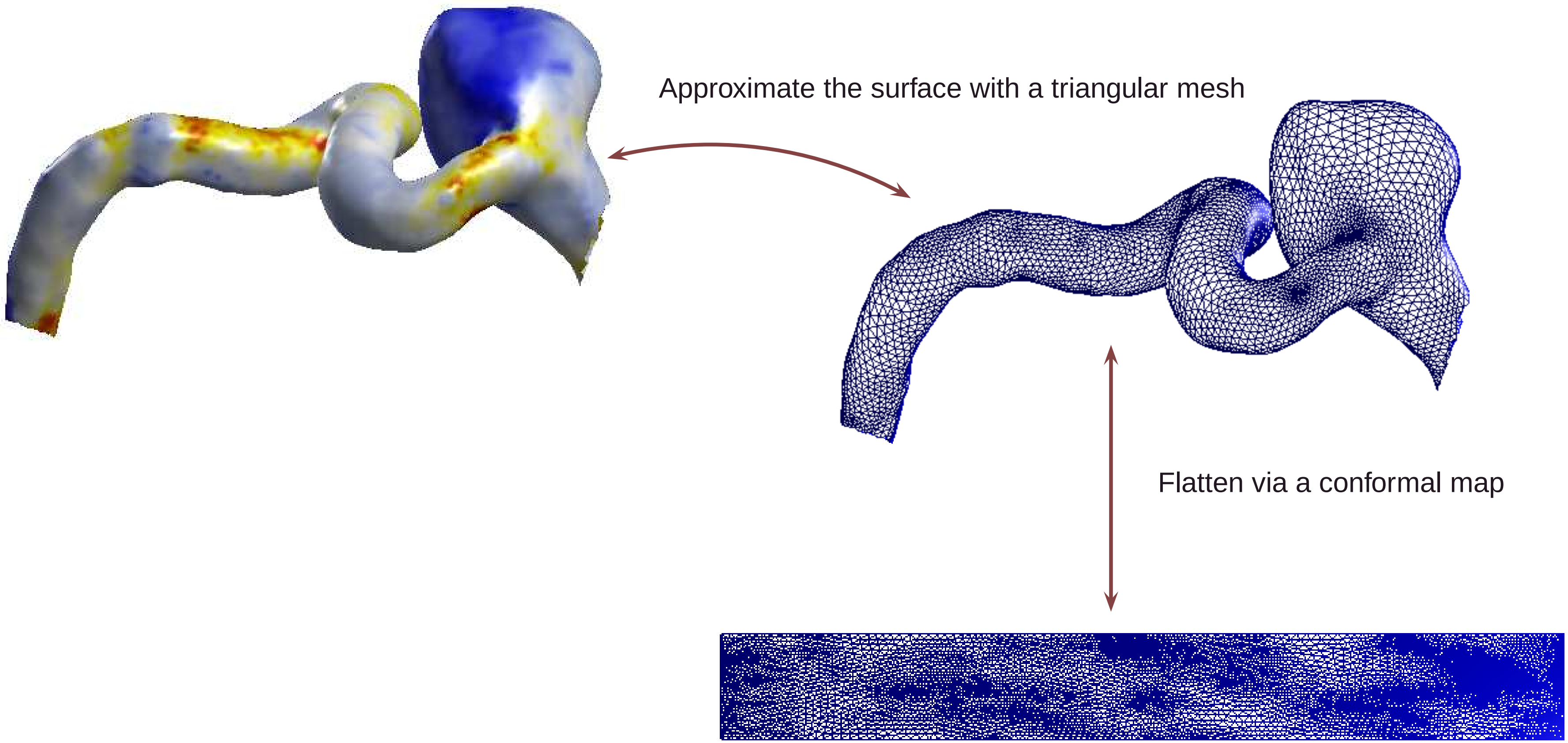
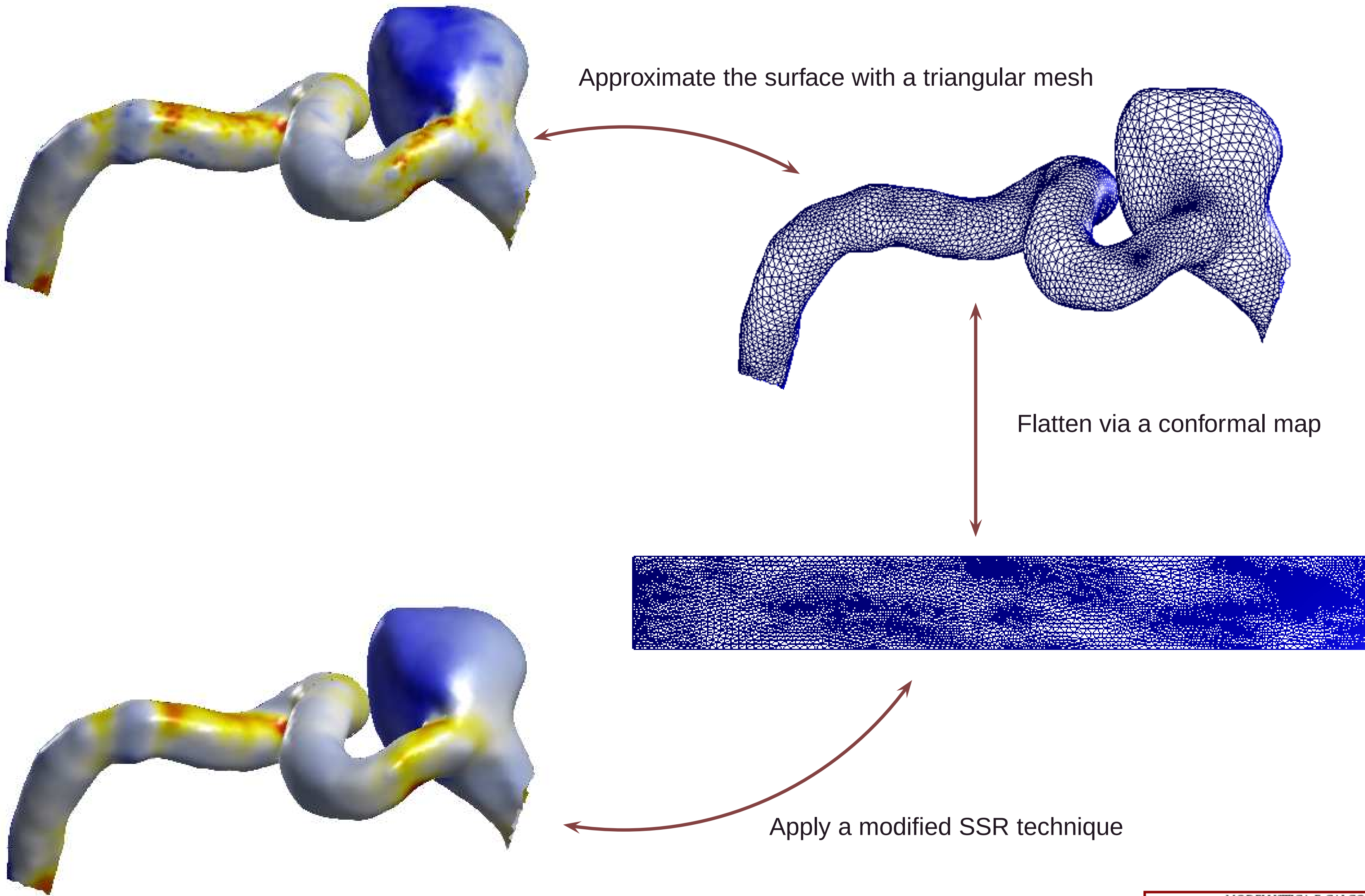

Approximate the surface with a triangular mesh
Flatten via a conformal map

The plan



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The flattening map

We define a map X such that

$$\begin{aligned} X : \Omega &\to \Sigma \\ \mathbf{u} = (u, v) &\mapsto \mathbf{x} = (x_1, x_2, x_3) \end{aligned}$$

where Ω is an open, convex and bounded set in $\mathbb{R}^2$.

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X_u and X_v - column vectors of first order partial derivatives of X with respect to u and v.

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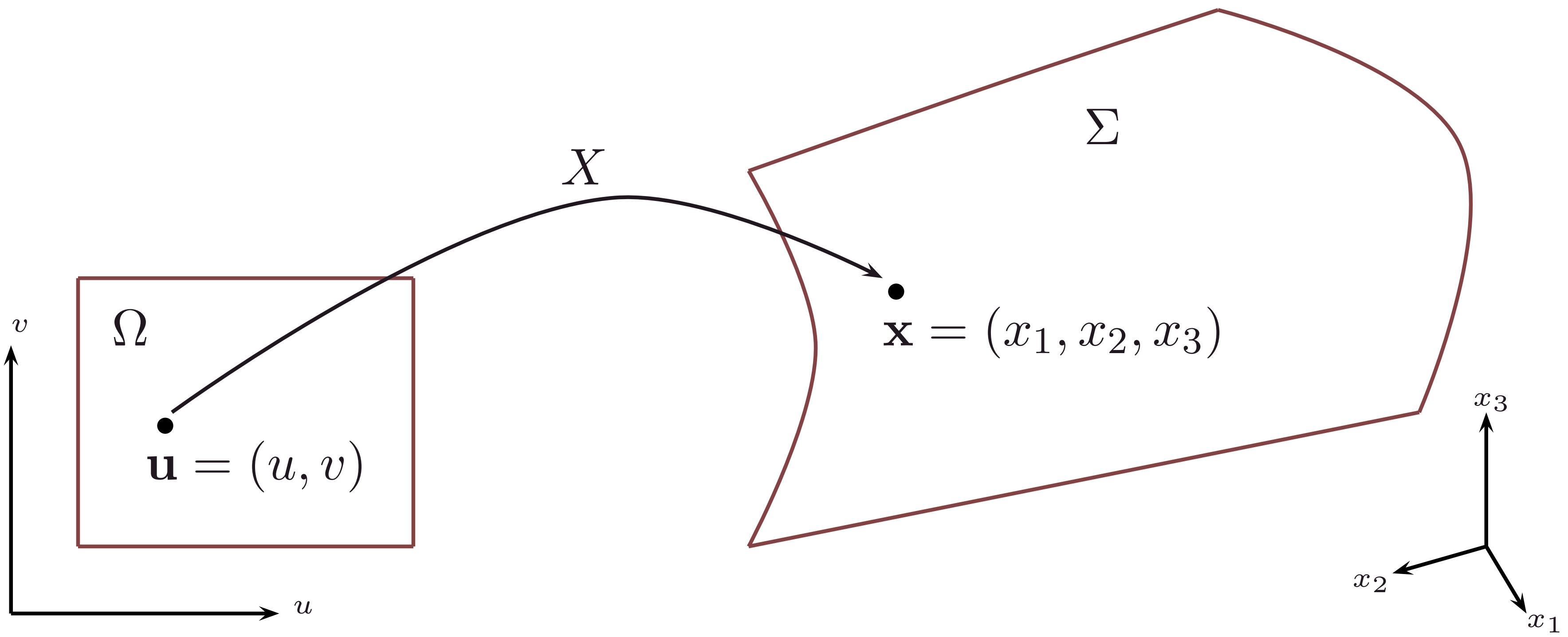
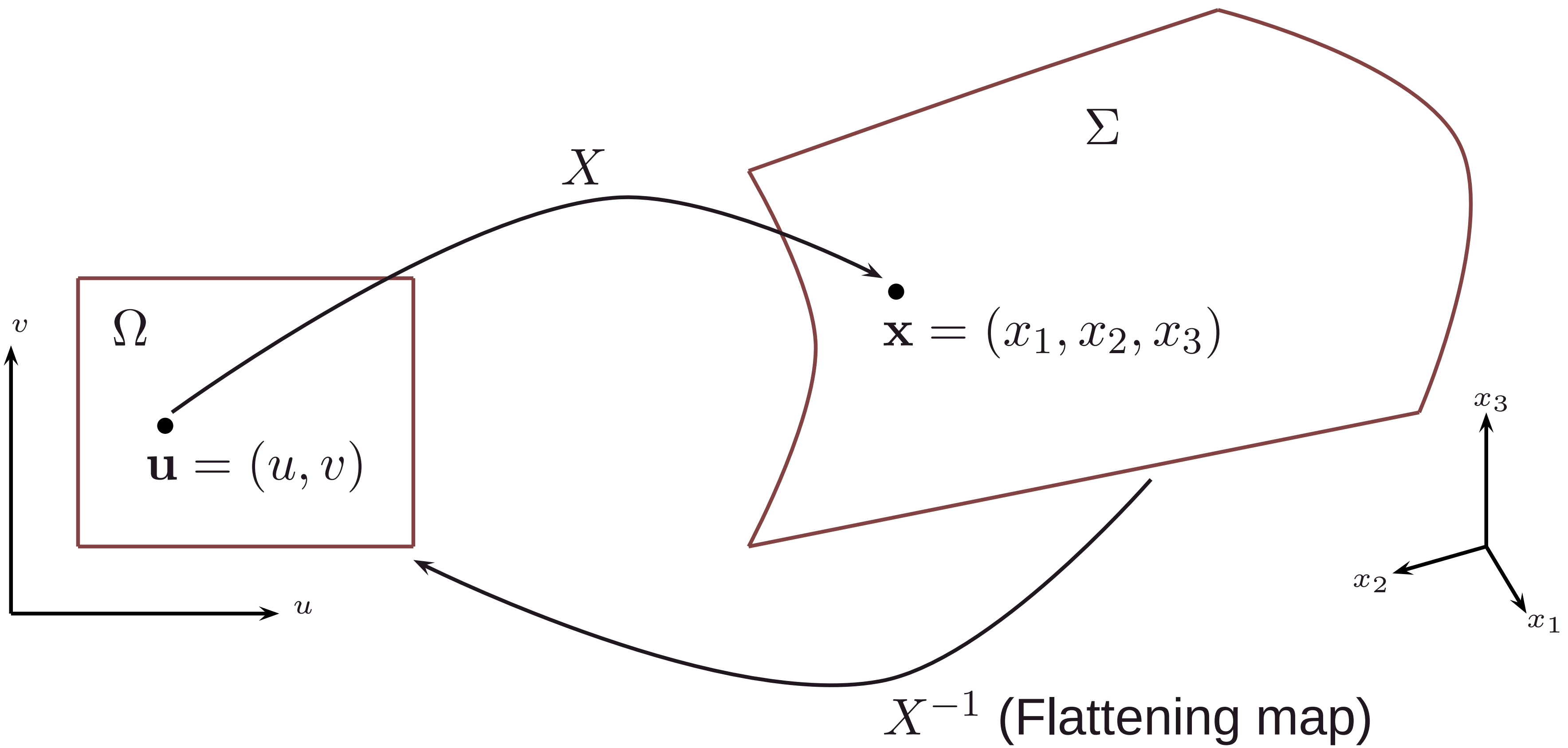
X_u and X_v - column vectors of first order partial derivatives of X with respect to u and v.

For the map X to be conformal:

1. $\|X_u\| = \|X_v\|$
2. $\langle X_u, X_v \rangle = 0$


X
Σ
Ω
v
u
$\mathbf{u} = (u, v)$
$\mathbf{x} = (x_1, x_2, x_3)$
x_3
x_2
x_1



X
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$\mathbf{u} = (u, v)$
u
$\mathbf{x} = (x_1, x_2, x_3)$
x_3
x_2
x_1
X^{-1} (Flattening map)

Flattening method

(Haker et al., [5])

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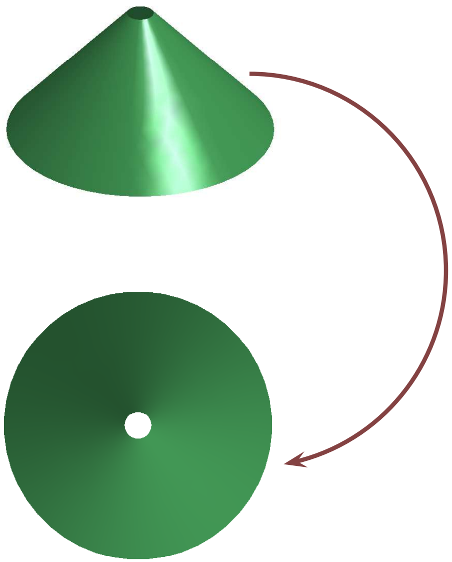
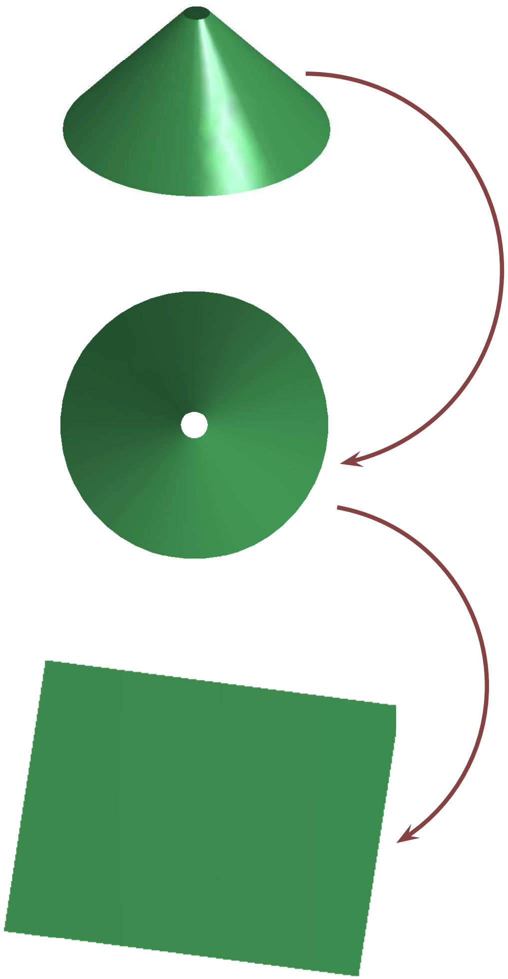


$$\begin{cases} -\Delta_\Sigma u = 0 \text{ on } \Sigma \\ u = 0 \text{ on } \sigma_0 \\ u = 1 \text{ on } \sigma_1 \end{cases}$$

Flattening method

(Haker et al., [5])



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$$\begin{cases} -\Delta_\Sigma v = 0 \text{ on } \Sigma \\ v(\zeta) = \int_{\zeta_0}^{\zeta} \frac{\partial u}{\partial \nu} \, ds \ \text{ on } B \end{cases}$$

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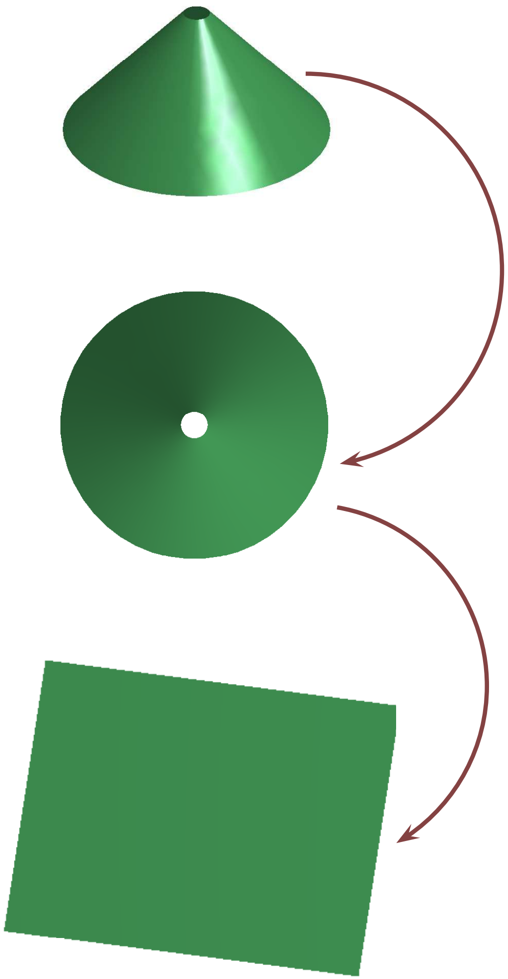

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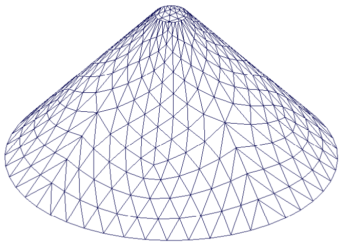

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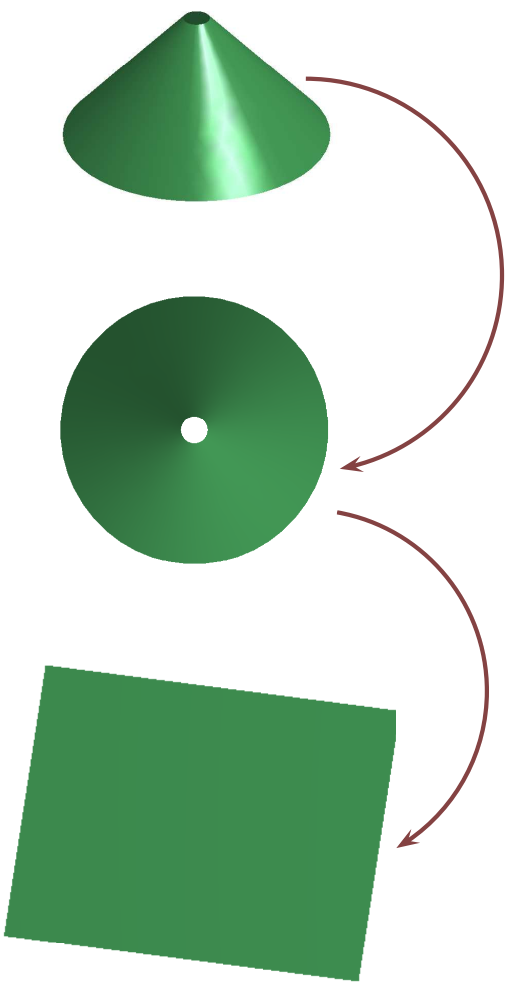

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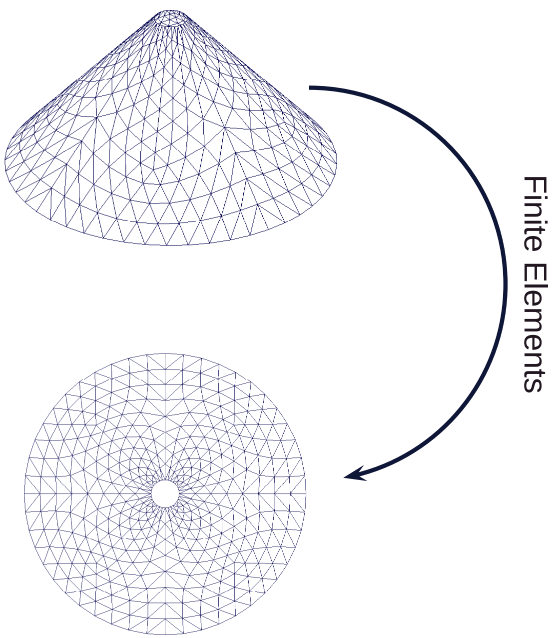

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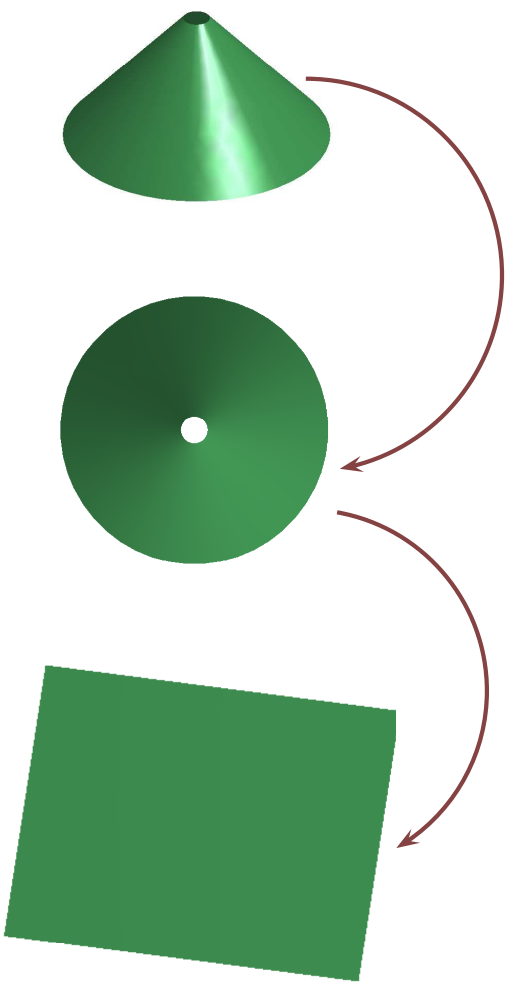

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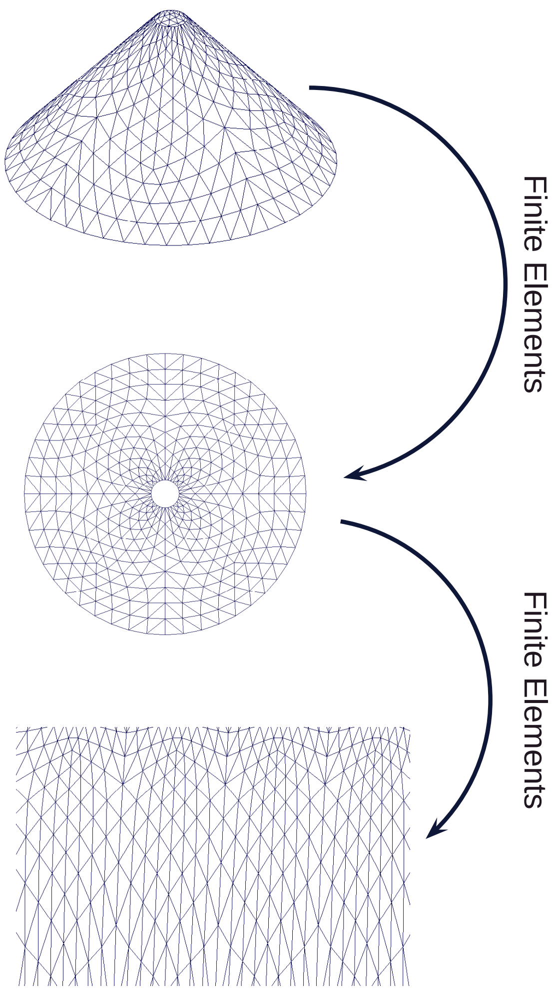

Laplace-Beltrami operator

$$G := (\nabla X)' \, \nabla X = \begin{pmatrix} \|X_u\|^2 & \langle X_u, X_v \rangle \\ \langle X_v, X_u \rangle & \|X_v\|^2 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}$$

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Keep in mind:

$$G(\mathbf{u}) := (\nabla X(\mathbf{u}))' \, \nabla X(\mathbf{u}) = \begin{pmatrix} \|X_u(\mathbf{u})\|^2 & \langle X_u(\mathbf{u}), X_v(\mathbf{u}) \rangle \\ \langle X_v(\mathbf{u}), X_u(\mathbf{u}) \rangle & \|X_v(\mathbf{u})\|^2 \end{pmatrix}$$

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For $(f \circ X) \in \mathcal{C}^2(\Omega)$:

$$\Delta_\Sigma f(\mathbf{x}) = \frac{1}{\mathcal{W}} \sum_{i,j=1}^{2} \partial_i (a_{ij} \partial_j (f \circ X))$$

a_{ij} are the components of the positive definite symmetric matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \mathcal{W} G^{-1}.$$

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Flattened model

Over the planar domain Ω:

$$J_\lambda(f \circ X) = \sum_{i=1}^{n} \big(z_i - f(X(\mathbf{u}_i))\big)^2 + \lambda \int_\Omega \left[\frac{1}{\mathcal{W}} \sum_{i,j=1}^{2} \partial_i (a_{ij} \partial_j (f \circ X)) \right]^2 \mathcal{W} d\Omega$$

where $X(\mathbf{u}_i) = \mathbf{x}_i$.

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Conformal coordinates:

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Properties

Proposition 1 (Existence and uniqueness)**.** *The estimator $\hat{f} \circ X$ that minimizes $J_\lambda(f \circ X)$ over $H^2_{n0}(\Omega)$ satisfies the following relation*

$$\boldsymbol{\mu}_n' \mathbf{z} = \boldsymbol{\mu}_n' \hat{\mathbf{f}}_n + \lambda \int_\Omega \left(\frac{1}{\mathcal{W}} \Delta(\mu \circ X) \right) \left(\frac{1}{\mathcal{W}} \Delta(\hat{f} \circ X) \right) \mathcal{W} d\Omega$$

for all μ with $\mu \circ X \in H^2_{n0}(\Omega)$. Moreover, the estimate $\hat{f} \circ X$ is unique.

Reformulation in $H^1_{n0}(\Omega) \implies$ Finite Element Solution

$$\boldsymbol{\mu}_n' \hat{\mathbf{f}}_n - \lambda \int_\Omega \nabla(\gamma \circ X)\, \nabla(\mu \circ X)\, d\Omega = \boldsymbol{\mu}_n' \mathbf{z}$$

$$\int_\Omega (\xi \circ X)(\gamma \circ X) \mathcal{W} d\Omega + \int_\Omega \nabla(\xi \circ X) \nabla(\hat{f} \circ X) d\Omega = 0.$$

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Uncertainty quantification

Inferential tools for the model:

- pointwise (simultaneous) confidence bands for f
- prediction intervals for new observations
- Generalized-Cross-Validation for the selection of λ

Test functions

(1) (2) (3)

50 test functions of the form:

$$f(x, y, z) = a_1 \sin(2\pi x) + a_2 \sin(2\pi y) + a_3 \sin(2\pi z) + 1$$

Coefficients: a_1, a_2 and a_3 randomly generated from i.i.d. $N(1, 1)$.

Noisy data

(1)

(2)

(3)

$$z_i = f(\mathbf{x}_i) + \epsilon_i$$

$$\epsilon_i \overset{i.i.d.}{\sim} N(0, 0.5)$$

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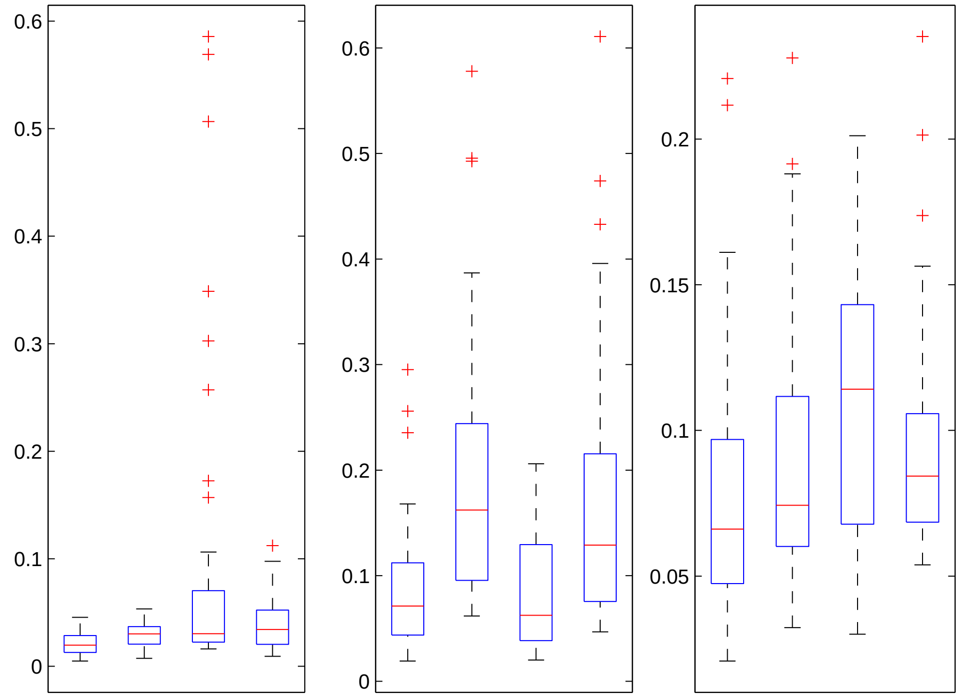
Simulations

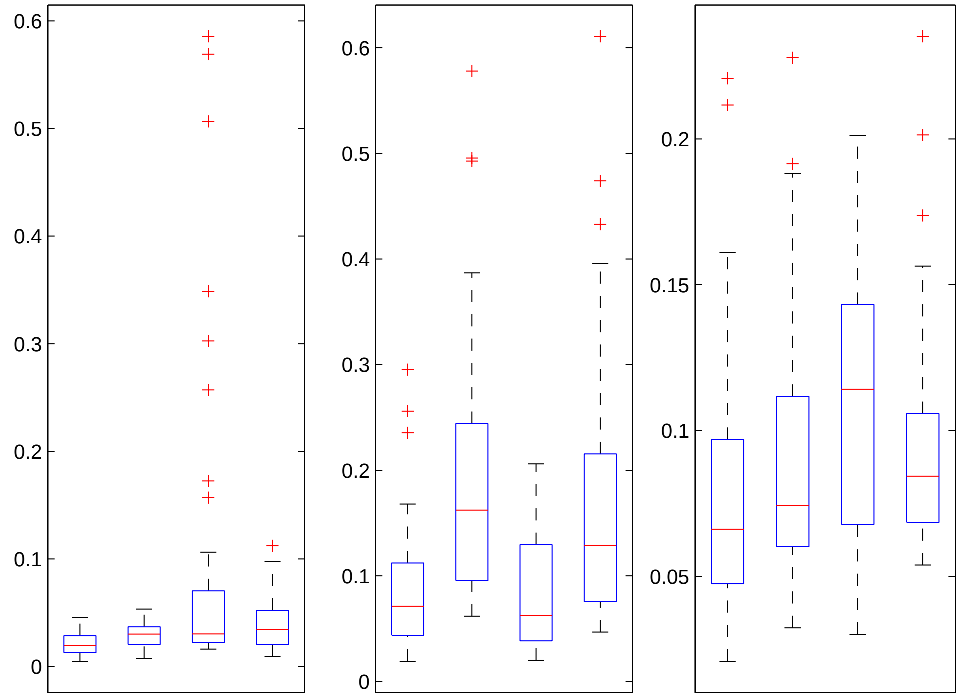
1. SSR models for non-planar domains
2. angular map + SSR models for planar domains
3. Iterative heat kernel smoothing
4. angular map+ Multivariate kernel smoothing regression

SSR model for non-planar domains fit



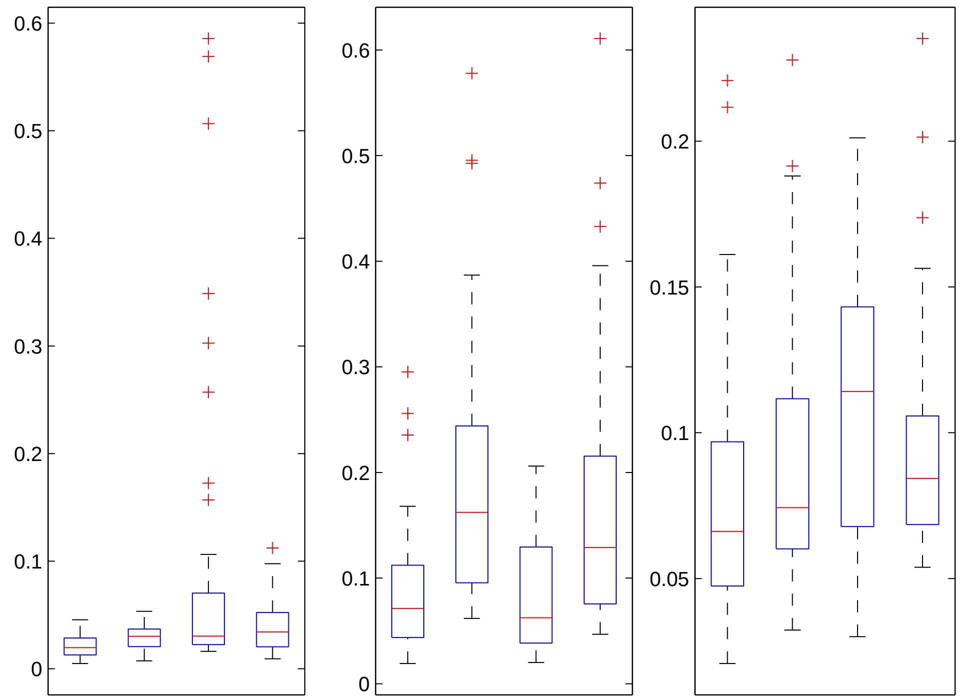
MSE	Geometry 1	Geometry 2	Geometry 3
SSR over non-planar domains	0.0196(0.0157)	0.0712(0.0677)	0.0661(0.0491)
SSR over planar domains	0.0301(0.0160)	0.1623(0.1463)	0.0743(0.0512)
Iterative Heat Kernel Smoothing	0.0303(0.0448)	0.0625(0.0897)	0.1142(0.0748)
Multivariate Kernel Smoothing	0.0343(0.0313)	0.1290(0.1380)	0.0843(0.0357)

SSR model for non-planar domains fit



p-values	Geometry 1	Geometry 2	Geometry 3
SSR over non-planar vs. SSR over planar	4.965×10^{-10}	3.894×10^{-10}	3.395×10^{-4}
SSR over non-planar vs. Iterative Heat Kernel	1.542×10^{-9}	0.8101	3.1×10^{-10}
SSR over non-planar vs. Multivariate Kernel	3.895×10^{-10}	3.895×10^{-10}	4.449×10^{-8}

SSR model for non-planar domains fit



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Iterative Heat Kernel vs. SSR over non-planar p-value = 0.1925

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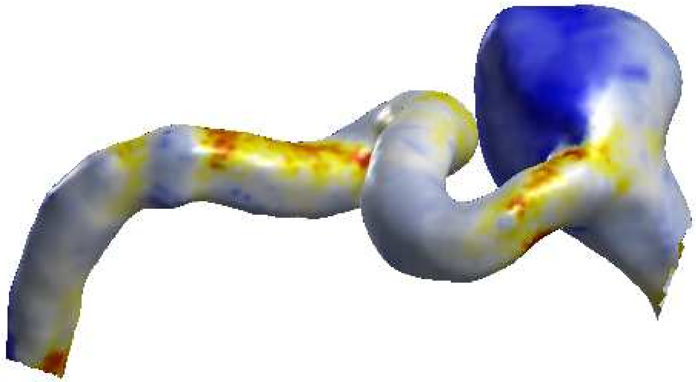
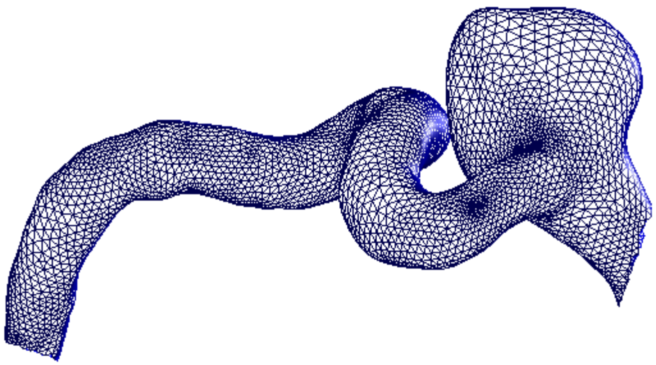
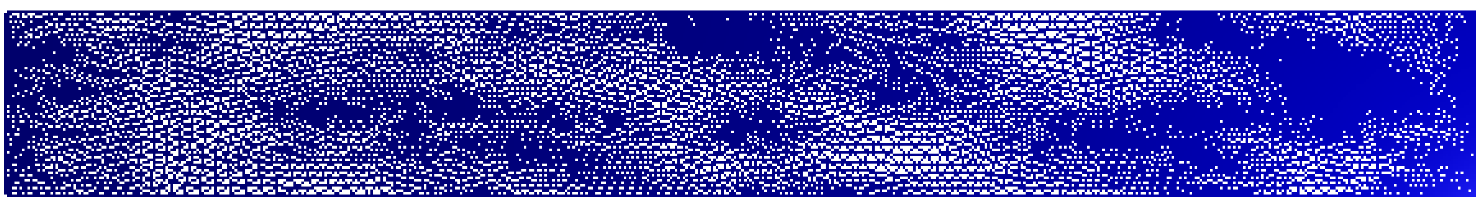
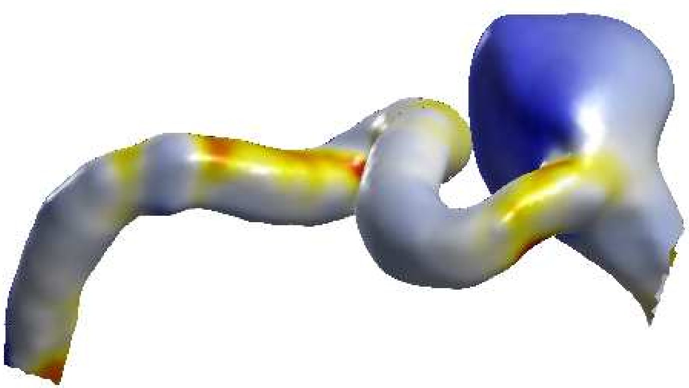
Application to hemodynamic data









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Future projects

0. include covariates in the model

$$z_i = \mathbf{w}_i' \boldsymbol{\beta} + f(x_i) + \epsilon_i$$

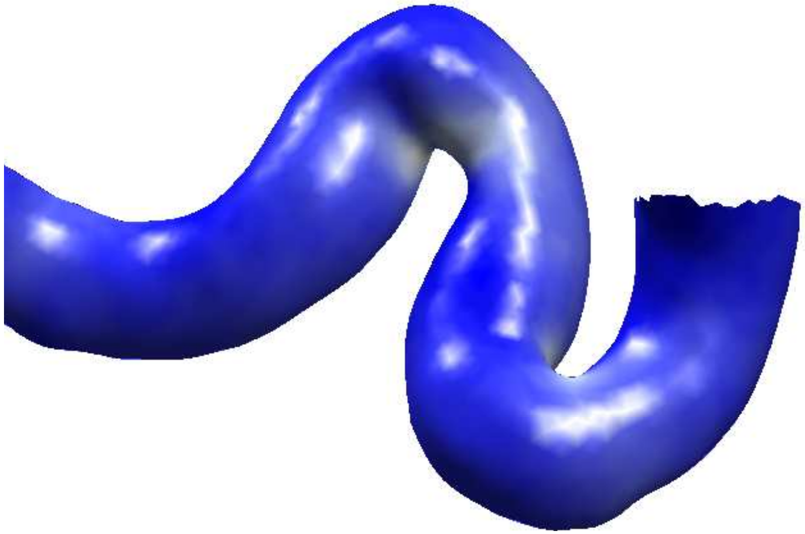
Future projects

$$\sum_{i=1}^{n} (z_i - f(\mathbf{x}_i))^2 + \lambda \int_{\Sigma} \text{PDE}_{\Sigma} \, d\Sigma$$

0. include covariates in the model

1. change penalty

Future projects



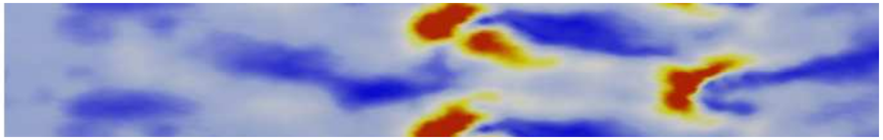
0. include covariates in the model

1. change penalty

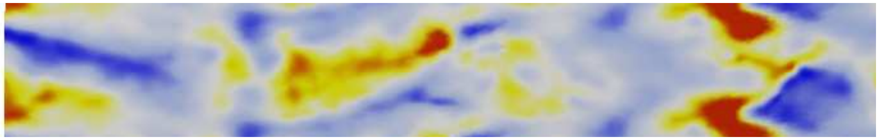
2. dynamic in time

Future projects

- Patient 1:



- Patient 2:



0. include covariates in the model

1. change penalty

2. dynamic in time

3. across patient variability

Grazie!

[1] Chung, M.K., Robbins, S.M., Dalton, K.M., Davidson, R.J., Alexander, A.L., Evans, A.C. (2005), “Cortical thickness analysis in autism with heat kernel smoothing,” *NeuroImage,* 25, 1256-1265.

[2] B. Ettinger, S. Perotto and L.M. Sangalli. *Regression models for data distributed over non-planar domains.* Tech. rep. N. 22/2012,MOX, Dipartimento di Matematica “F.Brioschi,”Politecnico di Milano, Available at http://mox.polimi.it/it/progetti/pubblicazioni. Submitted.

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