Low-rank solvers for Uncertainty Quantification and parameter estimation

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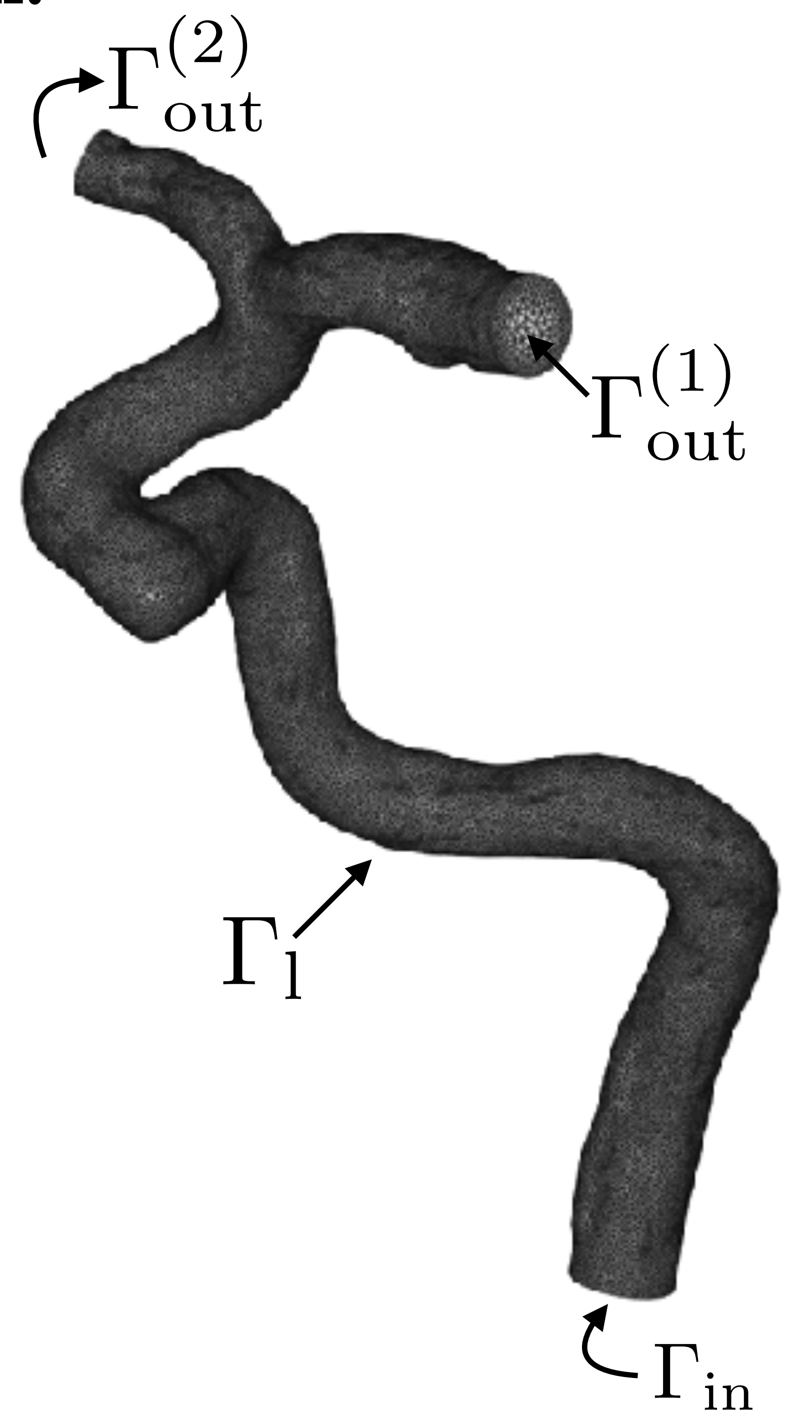
Motivation

- **Simulation of the blood flow inside a carotid siphon:**
  - Uncertainty in the material parameters
  - Geometry acquired through medical imaging (uncertain)

$$\Omega \subset \mathbb{R}^3 \qquad x \in \Omega$$

$$\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{l}} \cup \Gamma_{\text{out}}^{(1)} \cup \Gamma_{\text{out}}^{(2)}$$

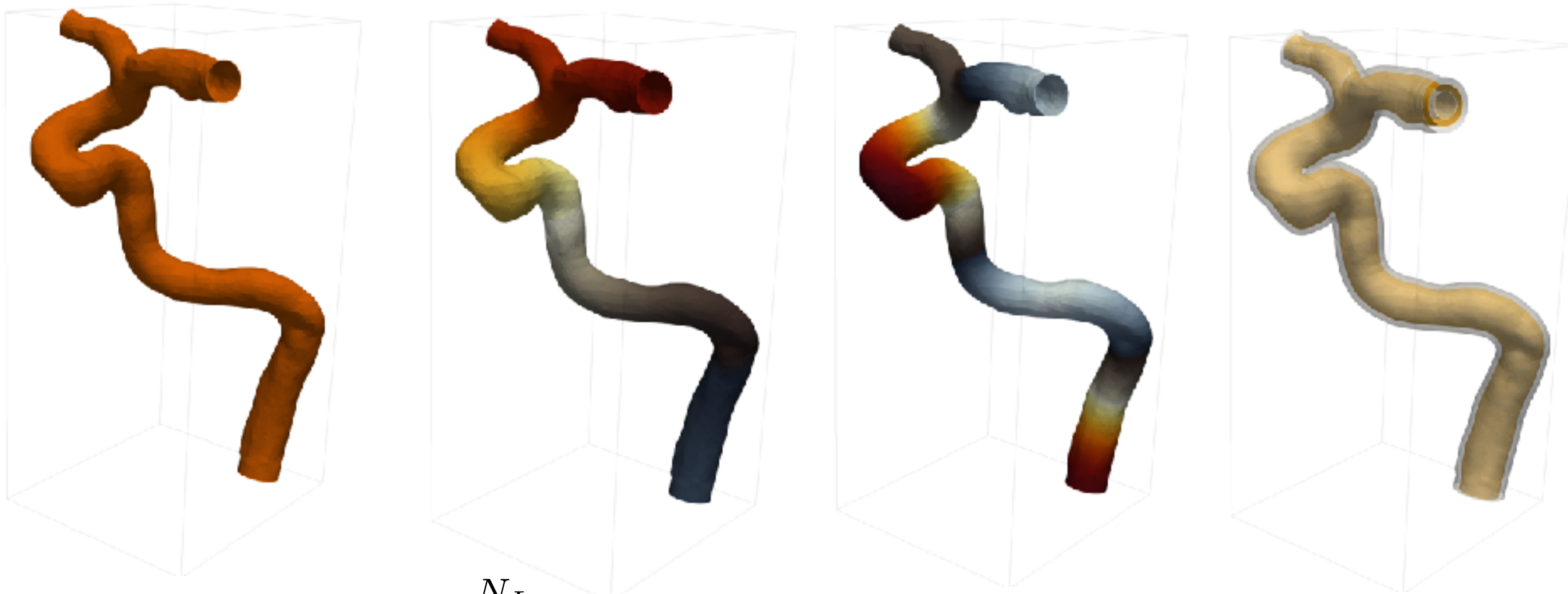
$$\Theta \subseteq \mathbb{R}^p$$



- **Model:**
  - Incompressible Navier-Stokes equations
  - Fluid-structure interaction

Motivation

- **Geometry perturbation: Laplace-Beltrami modes**



$$d = \xi \mathbf{n} \qquad \xi(x) = \sum_{i=1}^{N_L} c_i \xi_i(x)$$

$$\{\xi_i\}_{i\geq 1} \in \mathcal{C}^\infty(\Gamma_l) \qquad c_i \propto \mathcal{U}(-1/\lambda_i, 1/\lambda_i) \qquad \{c_i\}_{1\leq i\leq N_L} \in \Theta$$

Hiptmair, R., Scarabosio, L., Schillings, C., & Schwab, C. (2018). Large deformation shape uncertainty quantification in acoustic scattering. *Advances in Computational Mathematics*, *44*, 1475-1518.

Aylwin, R., Jerez-Hanckes, C., Schwab, C., & Zech, J. (2020). Domain uncertainty quantification in computational electromagnetics. *SIAM/ASA Journal on Uncertainty Quantification*, *8*(1), 301-341.

Discretisation

- **Equations and discretisation:**

$$u = (u_x, u_y, u_z, p) \in [H^1(\Omega)]^3 \otimes L^2(\Omega)$$

$$\mathbf{u} = (u_x, u_y, u_z)$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\varrho} \nabla p + \nu \Delta \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u} = \mathbf{u}_{\text{in}} \text{ on } \Gamma_{\text{in}}$$

$$\boxed{\mathbf{u} + \xi \partial_n \mathbf{u} = 0 \text{ on } \Gamma_{\text{l}}}$$

First order transpiration conditions

- **Semi-discretisation in time:**

$$u^{(n)}(x, \vartheta) \approx u(x, t_n, \vartheta)$$

$$u^{(n+1)} = u^{(n)} + \Delta t \mathcal{F}(u^{n+1}; t, \vartheta)$$

Discretisation

- Let us decompose the equation into two parts: linear and non-linear:

$$u^{(n+1)} = u^{(n)} + \Delta t \left(\mathcal{A}(t,\vartheta) u^{(n+1)} + \mathcal{G}(u^{(n+1)}, t, \vartheta) \right)$$

- Fixed-point:

$$u^{(n+1,k+1)} = u^{(n)} + \Delta t \left(\mathcal{A}(t,\vartheta) u^{(n+1,k+1)} + \mathcal{G}(u^{(n+1,k)}, t, \vartheta) \right)$$

$$\left(I - \Delta t \mathcal{A}(t,\vartheta)\right) u^{(n+1,k+1)} = u^{(n)} + \mathcal{G}(u^{(n+1,k)}, t, \vartheta)$$

$$u^{(n+1,0)} = u^{(n)}$$

- Classical discretisation in space, collocation in parameters

$$V_{N_x} \subset \mathcal{V}_x = \mathrm{span}\left\{v_1, \ldots, v_{N_x}\right\}$$

$$\left\{\vartheta^{(j)}\right\}_{1 \le j \le N_\vartheta} \in \Theta \qquad\qquad 1 \le j \le N_\vartheta$$

$$u^{(n)}(x, \vartheta^{(j)}) = \sum_{i=1}^{N_x} \hat{u}_{ij}^{(n)} v_i(x) \qquad\qquad \hat{u}_{ij}^{(n)} = \sum_{k=1}^{n(t_n)} \Phi_{ik}^{(n)} [S_{jk}^{(n)}]^T$$

Low-rank solver

- At every iteration of fixed-point we get the following problem:

$$\sum_{m=1}^{M} \left[A_m^{(x)} \otimes A_m^{(\vartheta)}\right] \hat{u} = b$$

- Fast application of the operators: Krylov methods

$$\sum_{m=1}^{M} \left[A_m^{(x)} \otimes A_m^{(\vartheta)}\right] \hat{u} = \sum_{m=1}^{M} \sum_{k=1}^{n(t_n)} \left(A_m^{(x)} \Phi_{\cdot k}\right) \left(A_m^{(\vartheta)} S_{\cdot k}^T\right)$$

Grasedyck, L., Kressner, D., & Tobler, C. (2013). A literature survey of low-rank tensor approximation techniques. *GAMM-Mitteilungen*, *36*(1), 53-78.

Kressner, D., & Tobler, C. (2010). Krylov subspace methods for linear systems with tensor product structure. *SIAM journal on matrix analysis and applications*, *31*(4), 1688-1714.

Bader, B. W. (2005). Tensor-Krylov methods for solving large-scale systems of nonlinear equations. *SIAM journal on numerical analysis*, *43*(3), 1321-1347.

Savas, B., & Eldén, L. (2013). Krylov-type methods for tensor computations I. *Linear Algebra and its Applications*, *438*(2), 891-918.

Dolgov, S. V. (2013). TT-GMRES: solution to a linear system in the structured tensor format. *Russian Journal of Numerical Analysis and Mathematical Modelling*, *28*(2), 149-172.

Iannacito, M., Agullo, E., Coulaud, O., Giraud, L., Marait, G., & Schenkels, N. (2022, September). GMRES in variable accuracy: a case study in low rank tensor linear systems. In *GAMM-Workshop on Applied and Numerical Linear Algebra 2022*.

Low-rank solver

Algorithm 1 Preconditioned GMRES algorithm

Require: $\mathcal{A} \in \mathbb{R}^{n \times n \times m}$, $\mathbf{X}_{k-1} \in \mathbb{R}^{n \times m}$, $\mathbf{B}_k \in \mathbb{R}^{n \times m}$, $\mathbf{P} \in \mathbb{R}^{n \times n}$ and $\varepsilon \in [0, 1]$

Ensure: $\mathbf{X}_k \in \mathbb{R}^{n \times m}$

$\boxed{\mathbf{R} = \mathbf{P}^{-1}\left(\mathbf{B}_k - \mathcal{A}(\mathbf{X}_{k-1})\right)}$

$\mathbf{Q}_1 = \mathbf{R} / \left\|\mathbf{R}\right\|_F$

$\boldsymbol{\beta} = [\left\|\mathbf{R}\right\|_F, 0, \ldots, 0] \in \mathbb{R}^q$

for $j = 1, \ldots, q$ **do**

    $\boxed{\mathbf{R} = \mathbf{P}^{-1} A(\mathbf{Q}_j)}$ Preconditioner

    for $i = 1, \ldots, j$ **do**

        $H_{i,j} = \langle \mathbf{Q}_i, \mathbf{R} \rangle_F$

        $\mathbf{R} = \mathbf{R} - H_{i,j}\mathbf{Q}_i$

    end for

    $H_{j+1,j} = \left\|\mathbf{R}\right\|_F$

    $\mathbf{Q}_{j+1} = \mathbf{R} / H_{j+1,j}$

end for

Find $\boldsymbol{\omega} \in \mathbb{R}^q$ minimizing $\left\|\mathbf{H}\boldsymbol{\omega} - \boldsymbol{\beta}\right\|_2$

$\mathbf{X}_k = \mathbf{X}_{k-1} + \sum_{j=1}^{q} \omega_j \mathbf{Q}_j$

Preconditioning

Weinhandl, Roman, Peter Benner, and Thomas Richter. "Low-rank linear fluid-structure interaction discretizations." *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik* 100.11 (2020): e201900205.

Venkovic, Nicolas. *Preconditioning strategies for stochastic elliptic partial differential equations*. Diss. Université de Bordeaux, 2023.

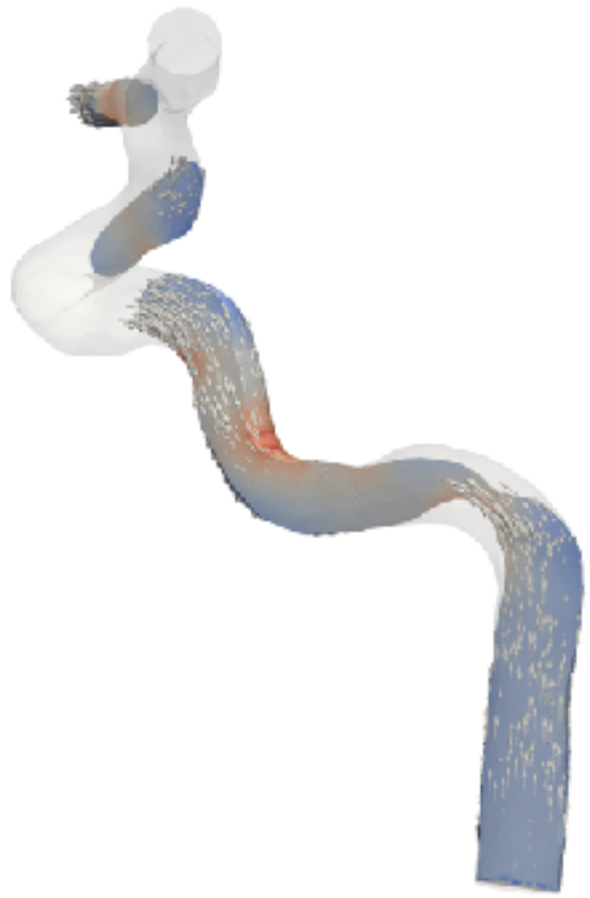
- Preliminary study on three different preconditioning strategies.

  Lombardi, D., & Riffaud, S. (2024). Preconditioners for multilinear problems arising in parametric Partial Differential Equations.

  - Numerical results exceed theoretical expectations.
  - Need to better understand the preconditioning step, to tailor it to the problem at hand.

Results

Pressure



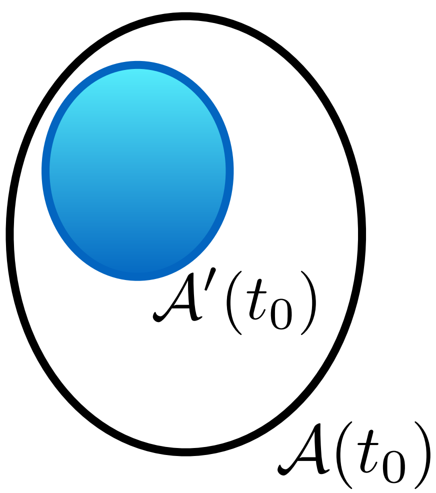
Velocity

$$N_x \approx 5 \cdot 10^5$$
$$N_\vartheta \approx 10^3$$
$$\Delta t = 10^{-2}$$

- Rank: ≈ 27
- When including material properties + other B.C. uncertainty; rank: ≈ 120

Partial Conclusions

- **Tensor methods for UQ**
  - In general, rank might be large: need of developing novel approximation formats
  - For some applications, we have some ***measurements*** on the system
    - Solution set: $\mathcal{A}(t_0) = \{v \in \mathcal{V}_x, v = u(x, t_0, \vartheta_*), \vartheta_* \in \Theta\}$
    - Kolmogorov widths: $d_n = \inf_{V_n} \sup_{w \in \mathcal{A}(t_0)} \inf_{v \in V_n} \|w - v\|_{\mathcal{V}_x}$



$$\mathcal{A}'(t_0) = \{v \in \mathcal{V}_x, v = u(x, t_0, \vartheta_*), \vartheta_* \in \Theta' \subset \Theta\}$$
$$\mathcal{A}'(t_0) \subset \mathcal{A}(t_0) \Rightarrow d_n' \leq d_n$$

- **Tensor methods for UQ + sequential data assimilation**
  - It might happen that the rank is lower, for all time instants!

Parameter estimation

- **State** $u : \Omega \times \mathbb{R}^+ \times \Theta \to \mathbb{R}^d$ $\quad u \in \mathcal{V}$
  $(x,t,\vartheta) \mapsto u(x,t,\vartheta)$
- **Observable** $y \in \mathbb{R}^m \qquad H : \mathcal{V} \to \mathbb{R}^m$
- **Model** $\mathcal{F}(u;t,\vartheta) = 0$

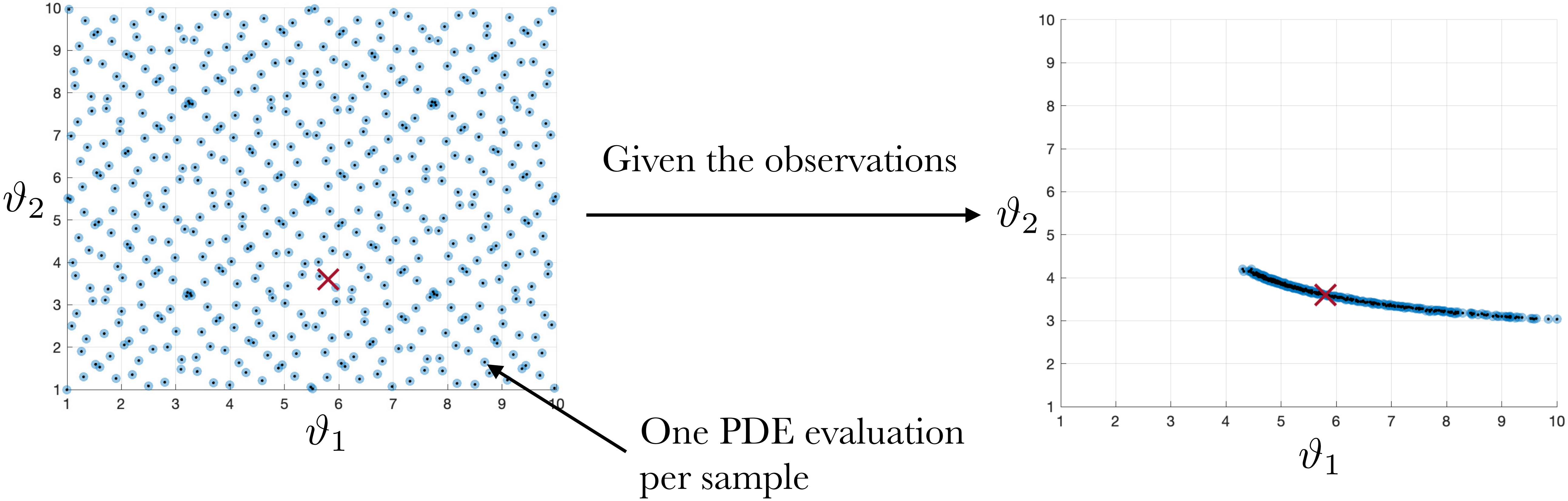
- Determine the parameters, given the observations:
  - ***Deterministic*** $\vartheta^* = \arg \inf_{\vartheta \in \Theta} \operatorname{dist}(y, H(u))$
  - ***Bayesian*** $p(\vartheta|y)$

- Challenges:
  - ***Structural identifiability***: injectivity of parameters-to-observable map

    Bellman, R., & Åström, K. J. (1970). On structural identifiability. *Mathematical biosciences*, *7*(3-4), 329-339.
  - ***Practical identifiability***: Bayesian methods make it possible to have an insight

    Wieland, F. G., Hauber, A. L., Rosenblatt, M., Tönsing, C., & Timmer, J. (2021). On structural and practical identifiability. *Current Opinion in Systems Biology*, *25*, 60-69.
  - ***Computational burden***

- Bayesian estimation:



- Computational burden:
  - Memory: $N_x \cdot N_\vartheta$
  - Number of operations: $\propto N_x^\beta N_\vartheta$

- Can we use ***tensor methods*** to enable ***sequential Bayesian estimation*** of the parameters?

Doucet et al.(2009). An overview of sequential Monte Carlo methods for parameter estimation in general state-space models. *IFAC Proceedings Volumes*

Arnold, A. (2022). When artificial parameter evolution gets real: particle filtering for time-varying parameter estimation in deterministic dynamical systems. *Inverse Problems*, *39*(1), 014002.

Sequential Bayesian estimation

t_0 t_1 t_2 t_3

$$y = \left(z^{(t_1)}, \dots, z^{(t_n)}\right)$$

- $\Theta^{(t_0)} = \left\{\vartheta^{(i,t_0)}\right\}_{1 \le i \le N_\vartheta}$
- Compute the solution till t_1

- Get the first observation $z^{(t_1)}$
- MH $\Theta^{(t_1)} = \left\{\vartheta^{(i,t_1)}\right\}_{1 \le i \le N_\vartheta}$
- Compute the solution till t_2

- Observations $z^{(t_1)}, z^{(t_2)}$
- MH $\Theta^{(t_2)} = \left\{\vartheta^{(i,t_2)}\right\}_{1 \le i \le N_\vartheta}$
- Compute the solution till t_3

Sequential Bayesian estimation

- Use Metropolis Hastings to distribute the samples in high-likelihood regions

$$\tilde{\vartheta}^{(j)} = \vartheta^{(j)} + \gamma \Delta\vartheta \qquad \Delta\vartheta \sim \mathcal{N}(0, C)$$

- Need to evaluate the solution ***from initial time*** to current time, for the candidate parameter sample!

- The low-rank solver makes it possible to build a projection based ROM:

  - $[t_0, t_1], p_0 \qquad \Phi^{(0)} \in \mathbb{R}^{N_x \times n(t_0)} \longrightarrow W_0 = \Phi^{(0)}$
  - $u \approx W_0 \tilde{s} \qquad [W_0^T A W_0]\tilde{s} = W_0^T f \xrightarrow{\text{MH}} U(t_1) = W_0 \tilde{S}_0^T$
  - $[t_1, t_2], p_1 \qquad U(t_1) \xrightarrow{\text{Low-rank solver}} \Phi^{(1)} \in \mathbb{R}^{N_x \times n(t_1)}$

$$W_1 = \text{update}(W_0, \Phi^{(1)})$$

- Update performed using Brand fast SVD update

Brand, M. (2006). Fast low-rank modifications of the thin singular value decomposition. *Linear algebra and its applications*, *415*(1), 20-30.

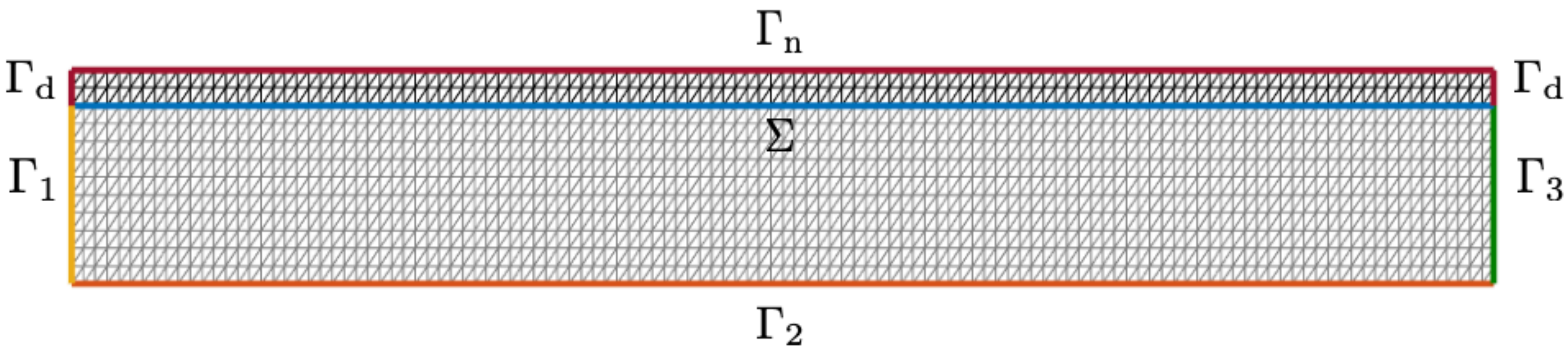
Sequential Bayesian estimation

Low-rank solver

- Memory reduction: $\approx 10^3$
- Speed-up: $\approx 10^1 - 10^2$

Projection-based ROM

- Construction: low (Brand+low-memory)
- Speed-up: $\approx 10^3$



$$\begin{cases} \rho_\mathrm{f}\partial_t \boldsymbol{u} - \operatorname{div} \boldsymbol{\sigma}_\mathrm{f}(\boldsymbol{u}, p) = 0 & \text{in} \quad \Omega_\mathrm{f} \times \mathbb{R}_+, \\ \operatorname{div} \boldsymbol{u} = 0 & \text{in} \quad \Omega_\mathrm{f} \times \mathbb{R}_+, \end{cases}$$

$$\begin{cases} \rho_\mathrm{s}\partial_t \dot{\boldsymbol{d}} - \operatorname{div} \boldsymbol{\sigma}_\mathrm{s}(\boldsymbol{d}) + \beta \boldsymbol{d} = 0 & \text{in} \quad \Omega_s \times \mathbb{R}_+, \\ \dot{\boldsymbol{d}} = \partial_t \boldsymbol{d} & \text{in} \quad \Omega_s \times \mathbb{R}_+. \end{cases}$$

$$\boldsymbol{\sigma}_\mathrm{f}(\boldsymbol{u}, p) := 2\mu_\mathrm{f}\boldsymbol{\epsilon}(\boldsymbol{u}) - p\mathbf{I},$$

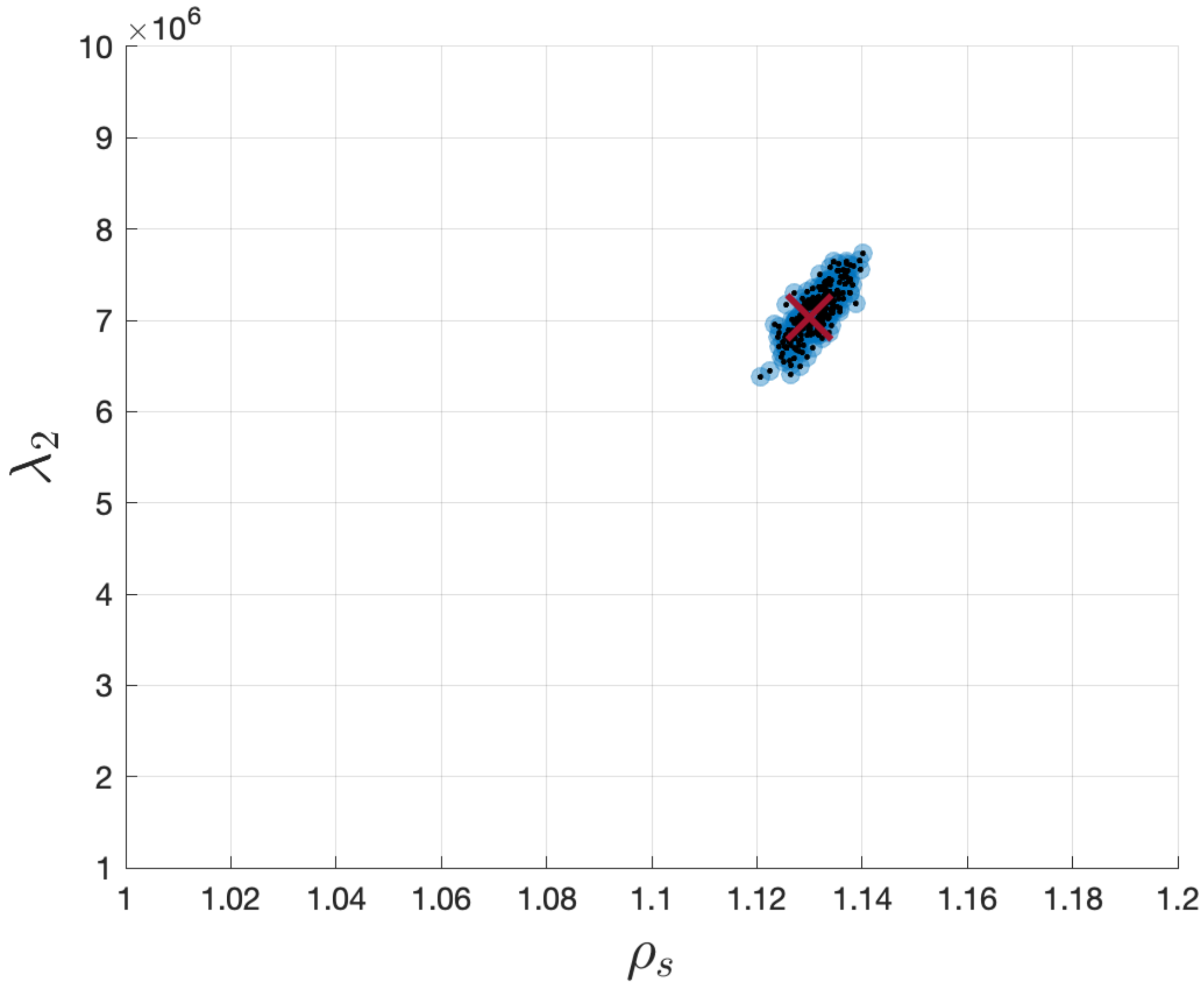
$$\boldsymbol{\sigma}_\mathrm{s}(\boldsymbol{d}) := 2\lambda_1\boldsymbol{\epsilon}(\boldsymbol{d}) + \lambda_2(\operatorname{div} \boldsymbol{d})\mathbf{I}.$$

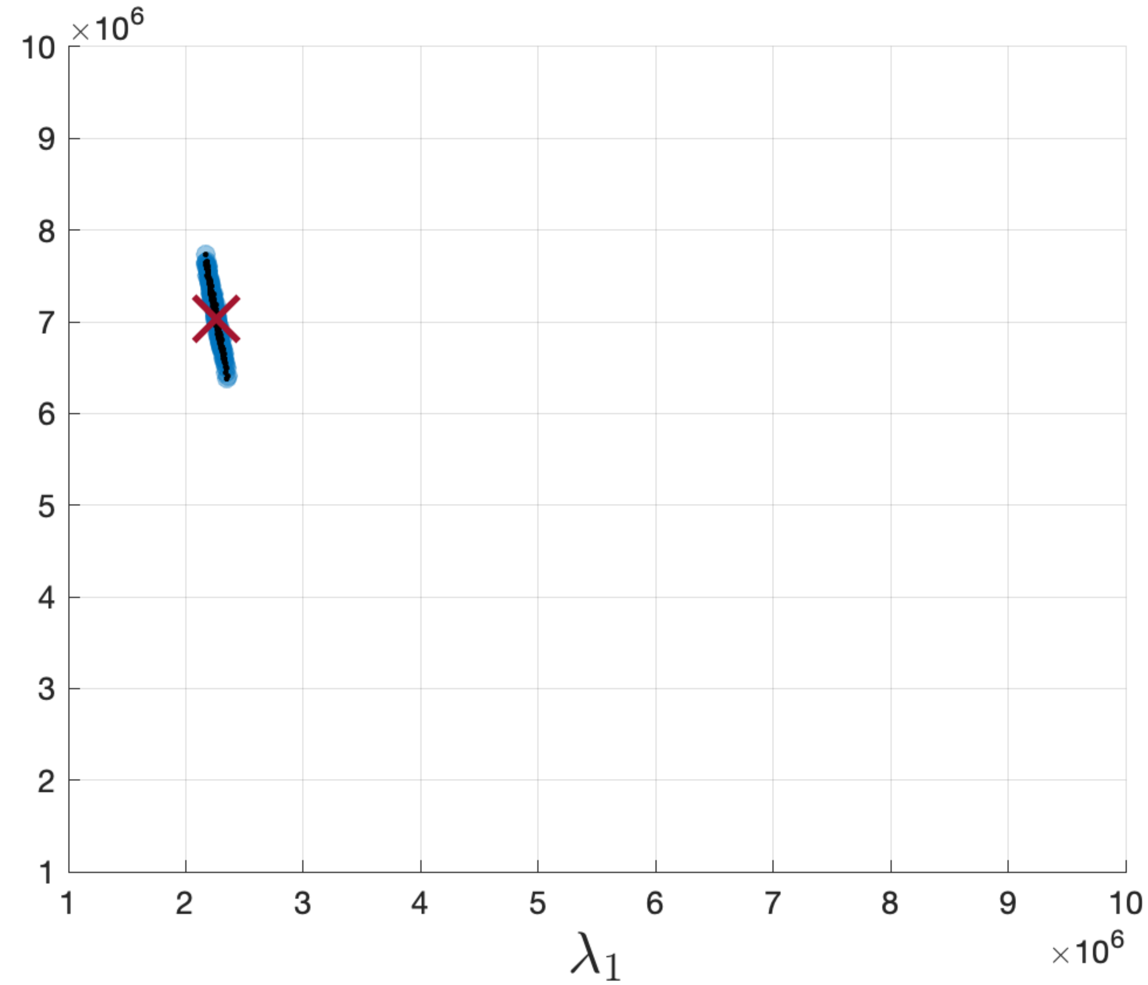
$$\begin{cases} \boldsymbol{u} = \dot{\boldsymbol{d}} & \text{on} \quad \Sigma \times \mathbb{R}_+, \\ \boldsymbol{\sigma}_\mathrm{f}(\boldsymbol{u}, p)\boldsymbol{n} = \boldsymbol{\sigma}_\mathrm{s}(\boldsymbol{d})\boldsymbol{n} & \text{on} \quad \Sigma \times \mathbb{R}_+, \end{cases}$$

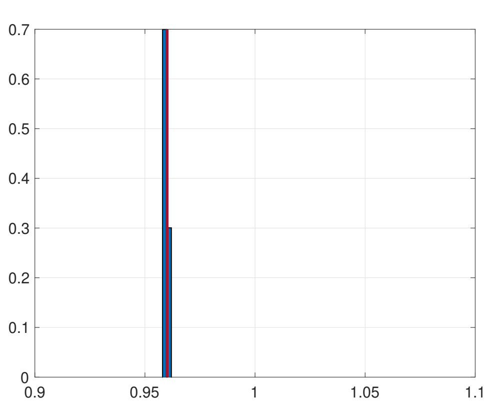
Observable: fluid velocity

ρ_f	μ_f	ρ_s	λ_1	λ_2
$[0.9, 1.1]$	$[0.03, 0.04]$	$[1, 1.2]$	$[10^6, 10^7]$	$[10^6, 10^7]$

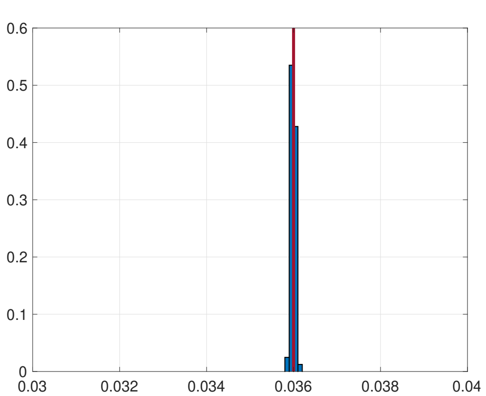
$$N_\theta \approx 250$$



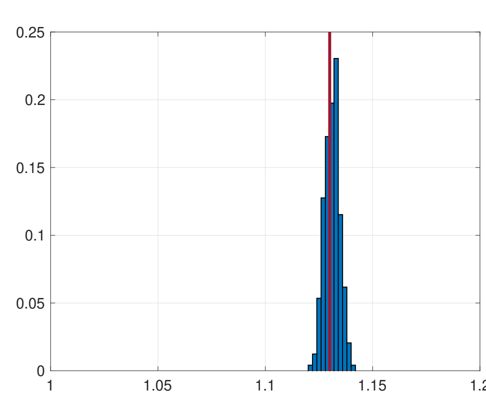




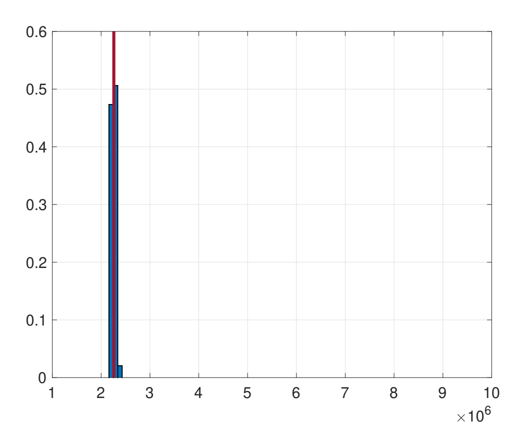
(a) ρ_f



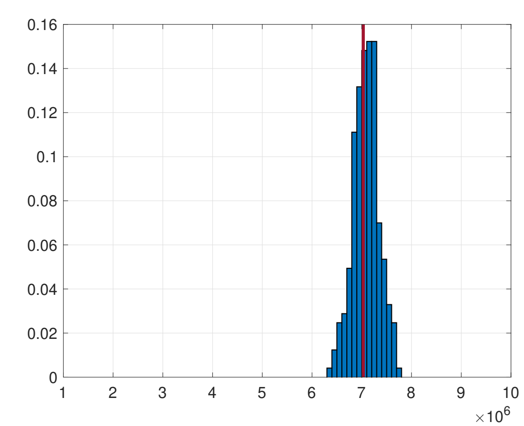
(b) μ_f



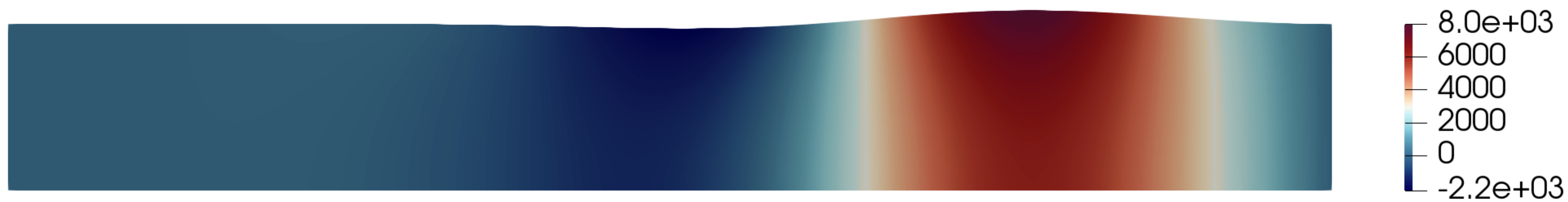
(c) ρ_s



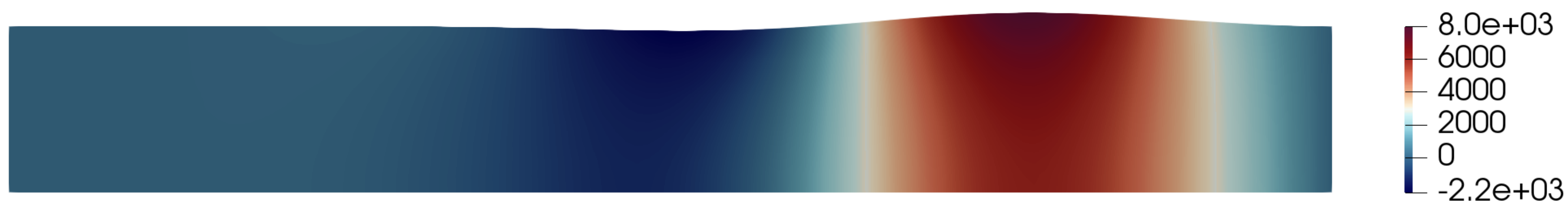
(d) λ_1



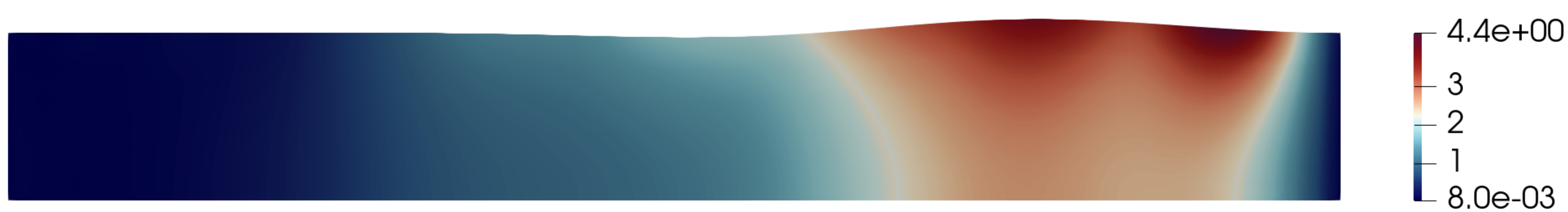
(e) λ_2



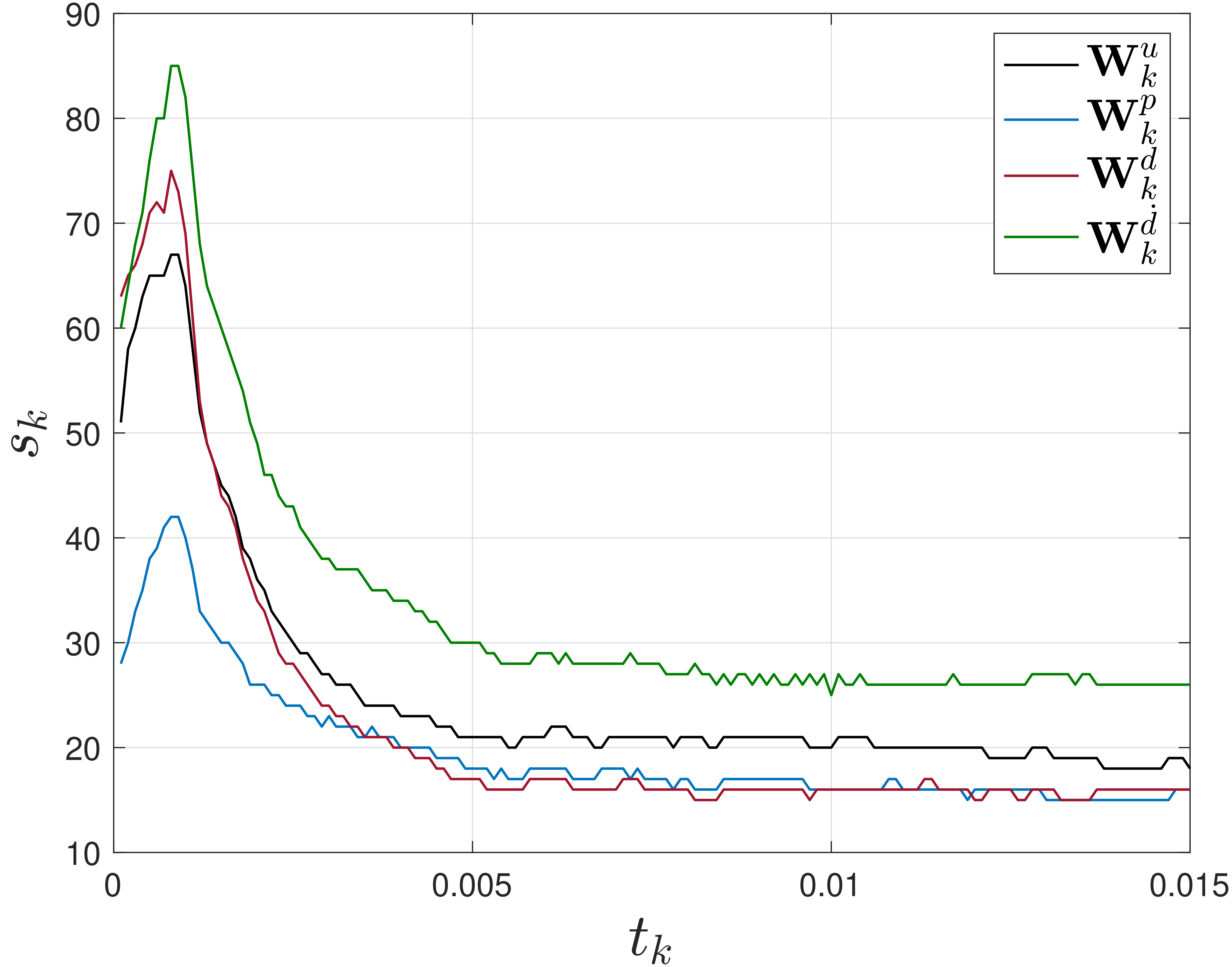
(a) Ground truth pressure p at $t = 0.015$.



(b) $\boldsymbol{\mu}_{\mathrm{qoi}}(0.015)$.

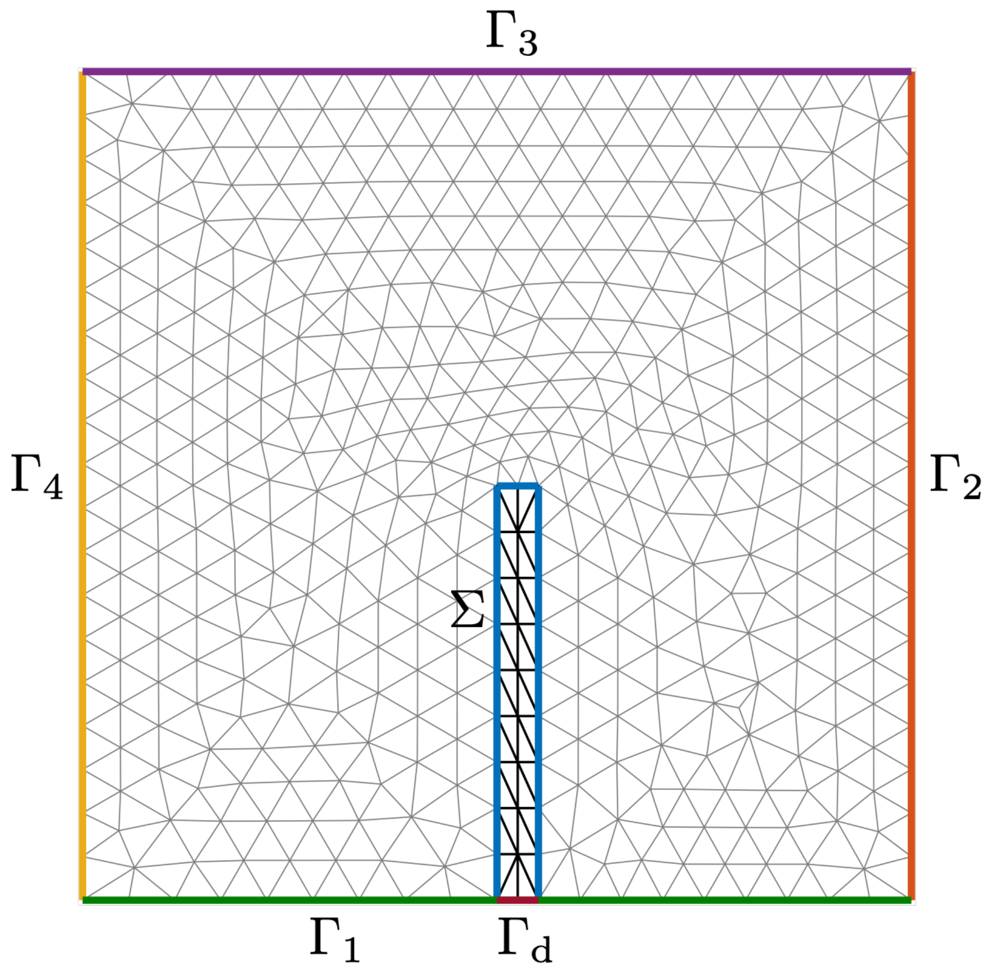


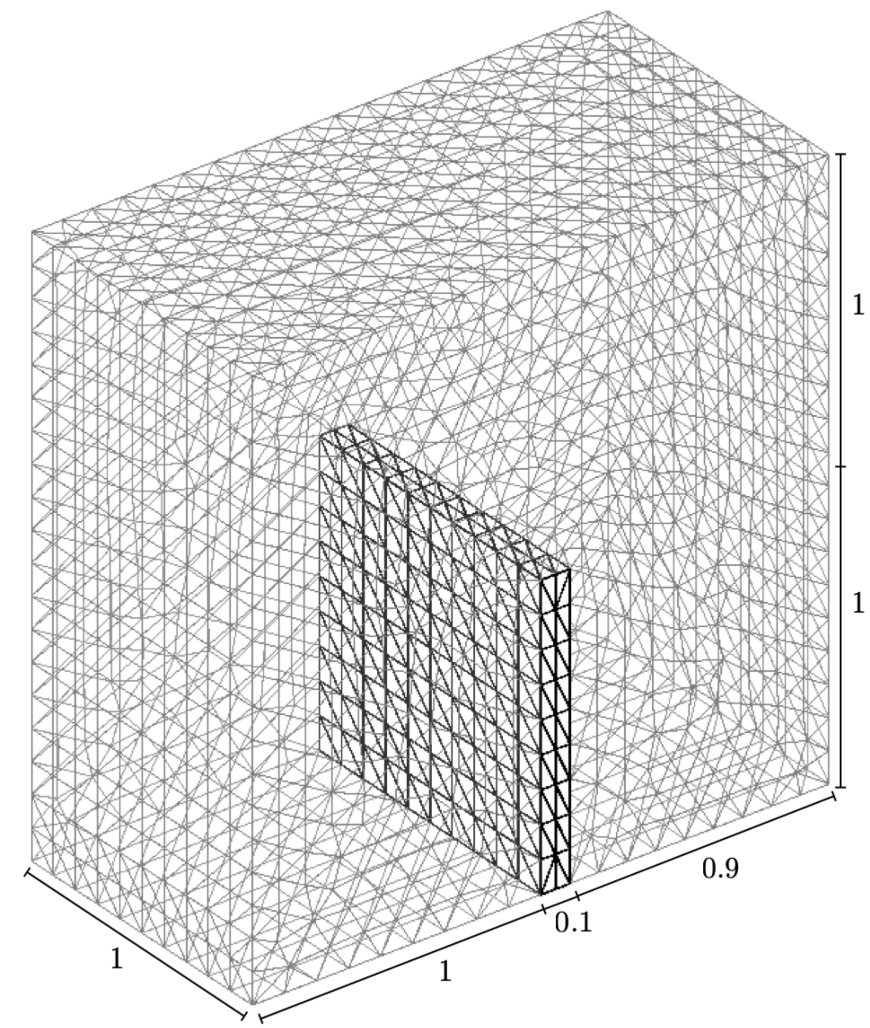
(c) $\boldsymbol{\sigma}_{\mathrm{qoi}}(0.015)$.



90
80
70
60
50
40
30
20
10
0
0.005
0.01
0.015
s_k
t_k
$\mathbf{W}_k^u$
$\mathbf{W}_k^p$
$\mathbf{W}_k^d$
$\mathbf{W}_k^{\dot{d}}$

Elstic 3d wall

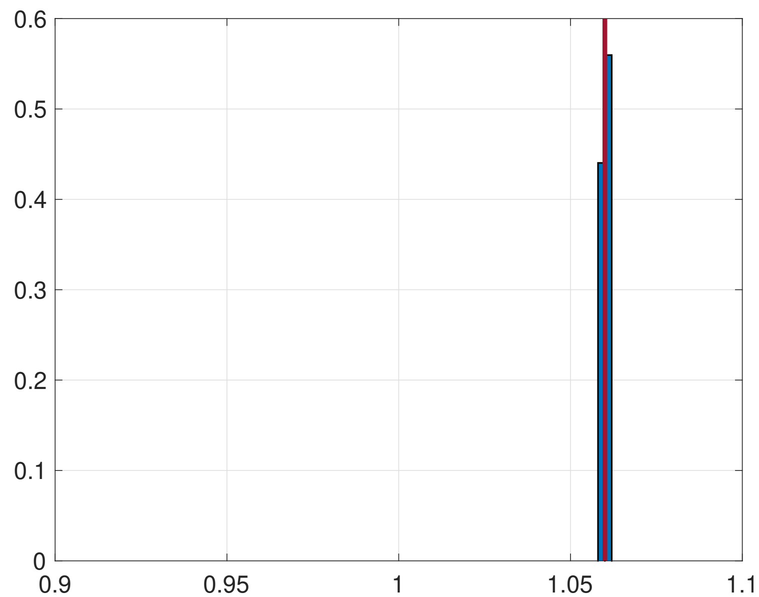




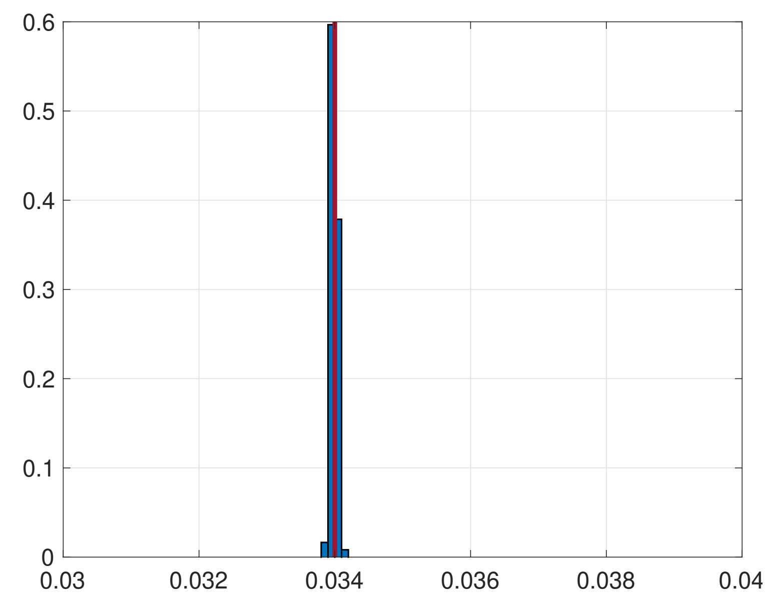
Observable: fluid velocity

ρ_f	μ_f	ρ_s	λ_1	λ_2
$[0.9, 1.1]$	$[0.03, 0.04]$	$[1, 1.2]$	$[10^5, 10^6]$	$[10^5, 10^6]$

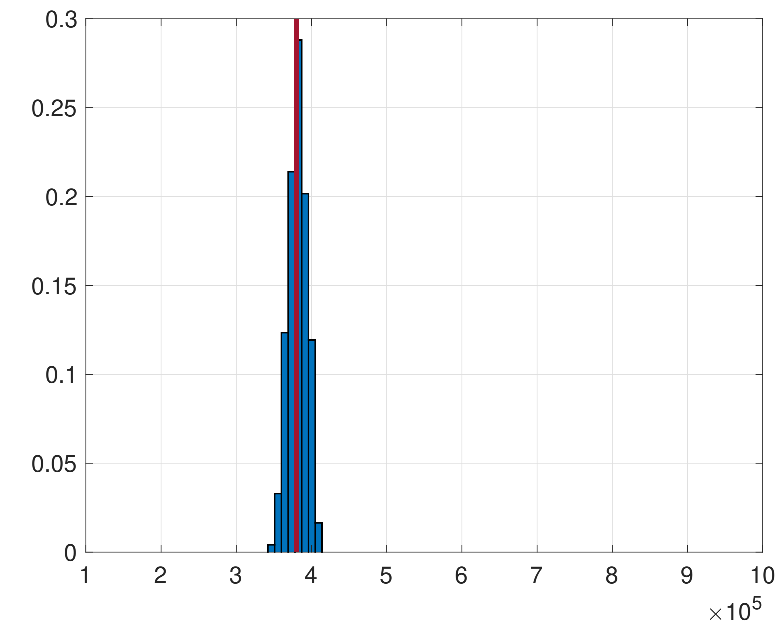
4d-flow MRI



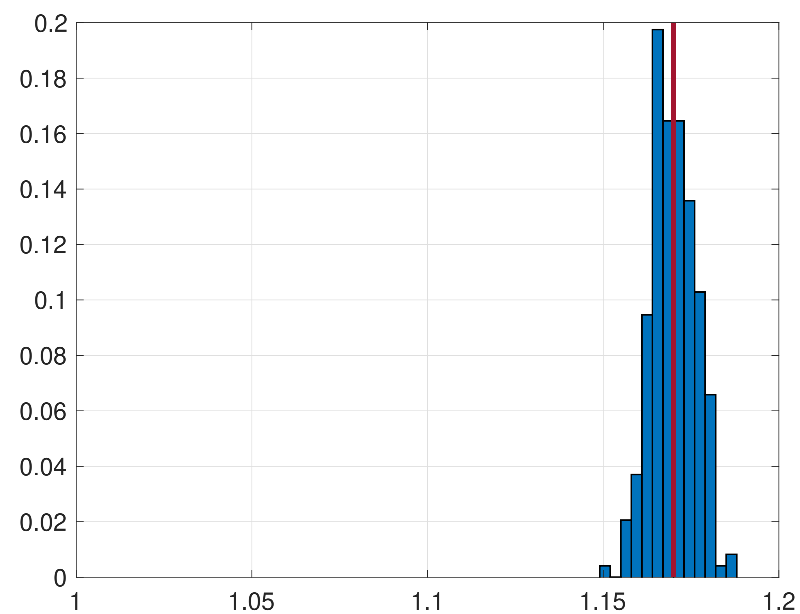
(a) ρ_f



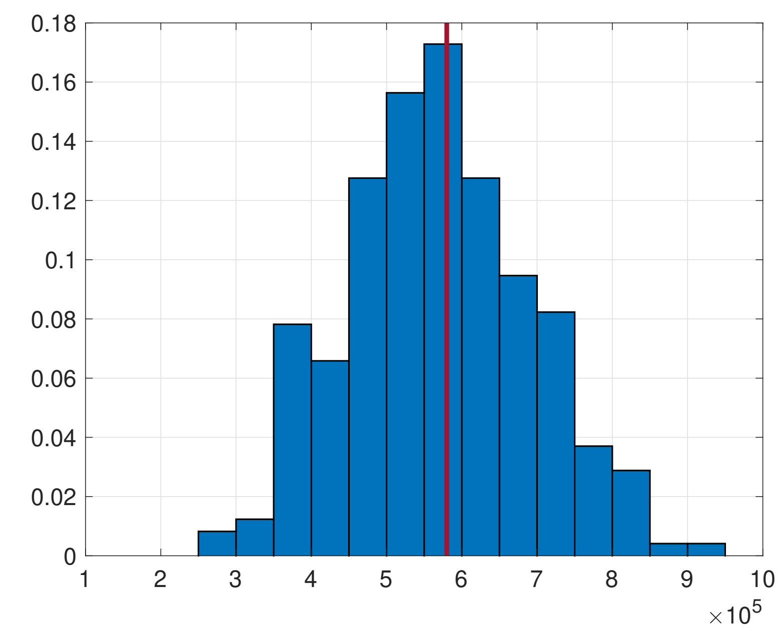
(b) μ_f



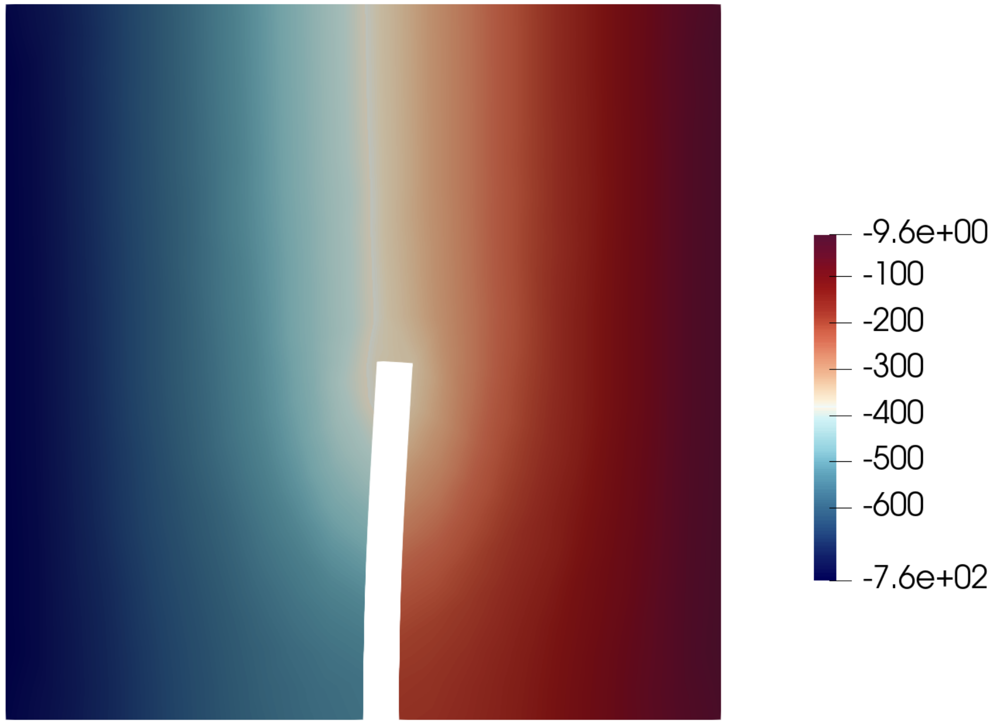
(d) λ_1



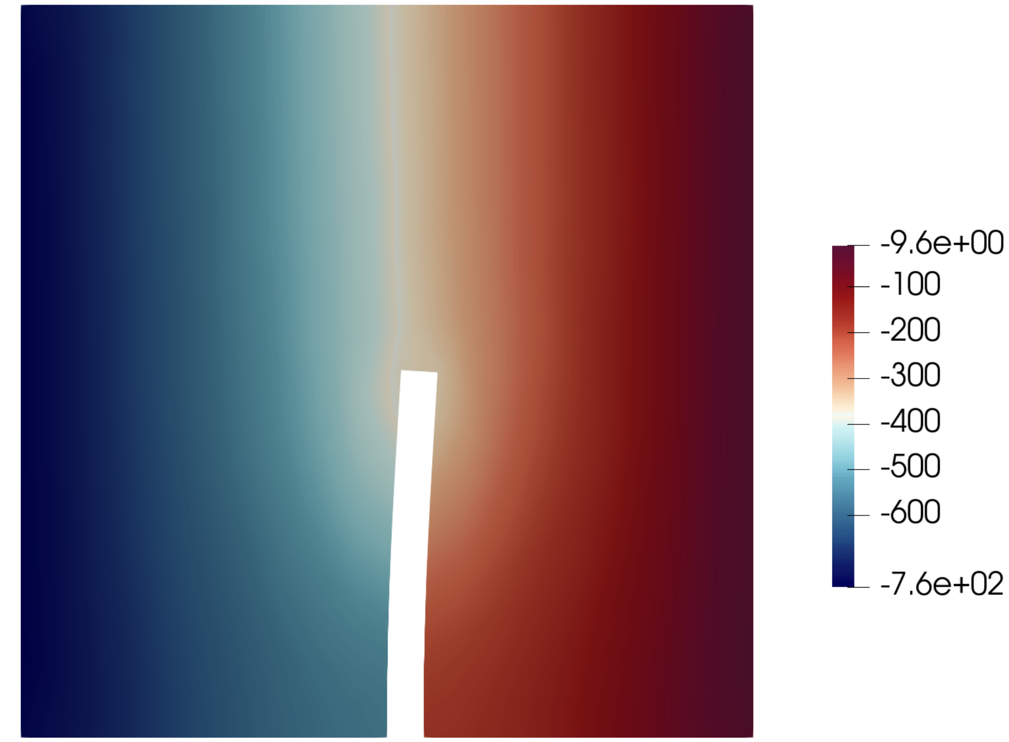
(c) ρ_s



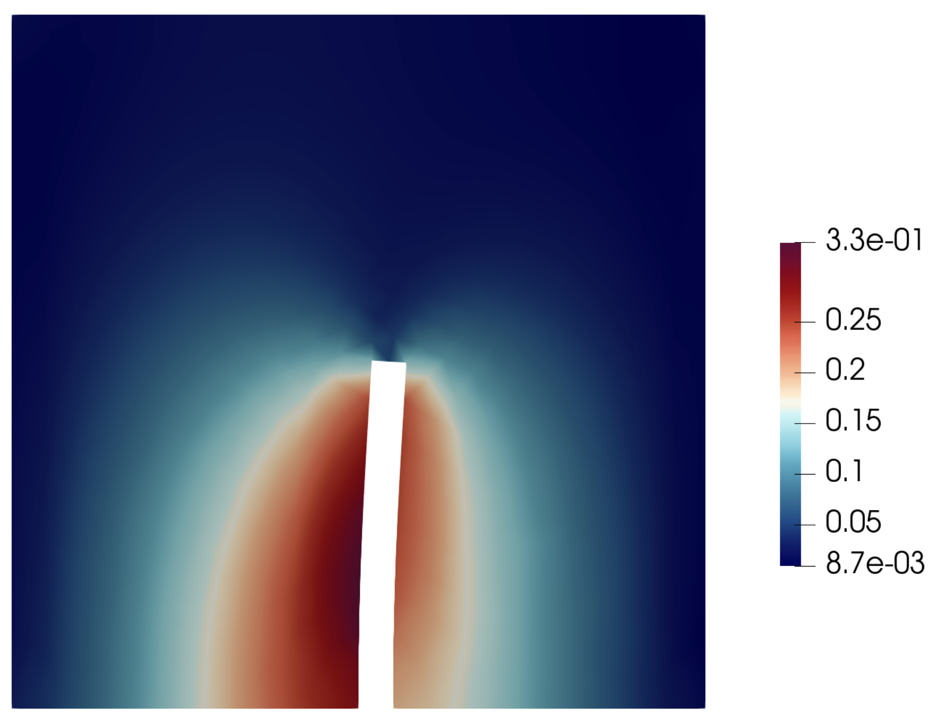
(e) λ_2



(a) Ground truth presure p at $t = 0.1$.



(b) $\boldsymbol{\mu}_{\mathrm{qoi}}$ at $t = 0.1$.



(c) $\boldsymbol{\sigma}_{\mathrm{qoi}}$ at $t = 0.1$.

Conclusions and Perspectives

- Parametric solvers:
  - Enabling MCMC: sequential Bayesian parameter estimation
  - Encouraging results on 3d examples

- State estimation:
  - Deterministic, optimal recovery based:

    Galarce, F., Lombardi, D., & Mula, O. (2021). Reconstructing haemodynamics quantities of interest from Doppler ultrasound imaging. *International Journal for Numerical Methods in Biomedical Engineering*, *37*(2), e3416.

    Galarce, F., Gerbeau, J. F., Lombardi, D., & Mula, O. (2021). Fast reconstruction of 3D blood flows from Doppler ultrasound images and reduced models. *Computer Methods in Applied Mechanics and Engineering*, *375*, 113559.

    Galarce, F., Lombardi, D., & Mula, O. (2022). State estimation with model reduction and shape variability. Application to biomedical problems. *SIAM Journal on Scientific Computing*, *44*(3), B805-B833.

    Damiano, L. (2022). State estimation in nonlinear parametric time dependent systems using tensor train. *International Journal for Numerical Methods in Engineering*, *123*(20), 4935-4956.

  - With G. Le Ruz and P. Moireau: Mortensen observer for dynamical systems on manifolds

  - With C. James and M. Boulakia: exploiting population data

    Boulakia, M., James, C., & Lombardi, D. (2024). Numerical approximation of the unique continuation problem enriched by a database for the Stokes equations.

Thank you