

Sensitivity analysis with the non-intrusive reduced basis 2-grid method

MAP5 Groupe de travail Modélisation, Analyse & Simulation

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Introduction

Non-Intrusive Reduced Basis 2-grid (NIRB) method

- ▶ Several numerical analyses of the 2-grid method
 - FEM context
 - FV schemes
 - Parabolic equations
- ▶ Development of new NIRB methods
- ▶ Non-intrusive implementation in a Python module
- ▶ Application to offshore wind turbines



Introduction

- ▶ Meniscus tissue regeneration
- ▶ Parameter identification & Sensitivity analysis
- ▶ NIRB method with parabolic equations
- ▶ NIRB method in the context of sensitivity analysis

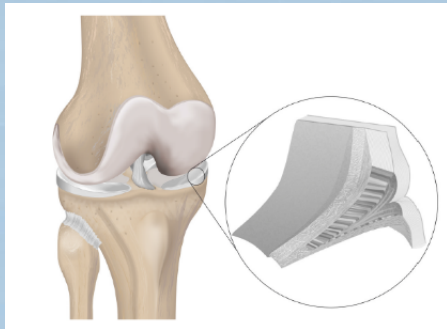


Figure: Meniscus

Motivation

- ▶ Meniscectomy leads to premature osteoarthritis of the knee joint
- ▶ New paradigm of healing by repair and regeneration of meniscus tissue
- ▶ Replacement tissue for cartilage is successfully generated based on cell cultured scaffolds



Motivation

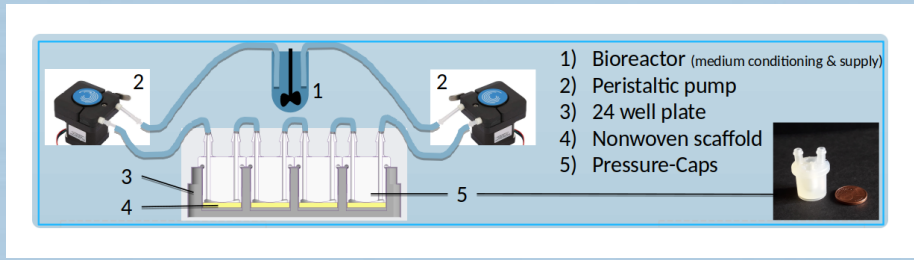


Figure: Cell cultured scaffold

Motivation

- Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration

$$\partial_t \rho_1 = \underbrace{\text{motility}}_{\text{(nonlinear/myopic) diffusion+chemo- and/or haptotaxis}} + \mu_1(\rho_1, \rho_2, Q, r)\zeta(S)$$

$$\partial_t \rho_2 = \text{motility} + \mu_2(\rho_1, \rho_2, Q, r)\eta(S)$$

$$\partial_t Q = \text{production by chondrocytes} - \text{degradation/proteolysis}$$

$$\partial_t r = \text{linear diffusion+decay/uptake by cells}$$

$$S = \frac{|\gamma|}{\alpha} + \frac{|v_f|}{\beta}$$

incompressible flow with velocity v_f (or Darcy law)

ρ_1 density of ADSCs

ρ_2 density of chondrocytes

Q macroscopic tissue density

r concentration of chemoattractant

S mechanical stimulus

Figure: The macroscopic model ¹

¹C. Engwer, T. Hillen, M. Knappitsch, C. Surulescu Glioma follow white matter tracts: a multiscale DTI-based model. 2014.

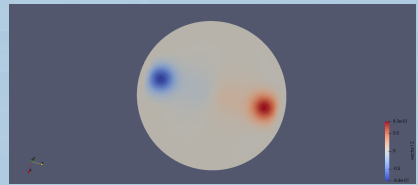
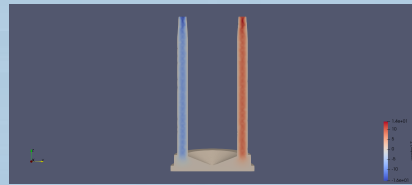
Motivation

- ▶ Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber

Density of the adipose tissue-derived stem cells
(FreeFem++)

Motivation

- Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber



Mechanical stimulus
(FreeFem++)

Motivation

- ▶ Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber
 - **Parameter identification**
 - **Sensitivity analysis**

Motivation

- ▶ Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber
 - Parameter identification
 - Sensitivity analysis

Geometry

Initial condition for the densities

Rates for ADSCs, chondrocytes and cartilage

Macroscopic density of scaffold fibers

Consumption of hyaluron by ADSCs

Stress

...

Motivation

- ▶ Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber
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Geometry
Initial condition for the densities
Rates for ADSCs, chondrocytes and cartilage
Macroscopic density of scaffold fibers
Consumption of hyaluron by ADSCs
Stress
...

Initial condition for the interstitial fluid
Porosity
Fluid density
Young's modulus
Poisson's ratio
Lamé coefficients
Dynamic viscosity
Permeability
...

Motivation

- Identification of crucial stimuli for chondrocytes and stem cells (ADSCs) w.r.t. cell proliferation, differentiation, and migration
 - Forward simulation of scaffold and cell colonization in perfusion chamber
 - Parameter identification
 - Sensitivity analysis

Non-Intrusive Reduced Basis 2-grid (NIRB) method ² with parabolic equations ³

²R. Chakir, Y. Maday, A two-grid finite-element/reduced basis scheme for the approximation of the solution of parameter dependent PDE. 2009.

³E. G., Y. Maday, Error estimate of the Non-Intrusive Reduced Basis (NIRB) two-grid method with parabolic equations. 2022.

Parametric problem

NIRB &
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Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

Parameter identification & Sensitivity analysis

Parametric problem

IVP

$$\mathcal{P} : (u^0, t, x, p) \rightarrow u(t, x; p), \quad t \in [0, T] \ x \in \Omega, \ p \in \mathbb{R}^P.$$

Numerical solution

$$\mathcal{P}_h : (u_h^0, t^k, x, p) \rightarrow u_h^k(x; p), \quad k \in 0, \dots, N_T, \ x \in \Omega, \ p \in \mathbb{R}^P.$$

Measures with true parameter \bar{p}

$$\begin{cases} \bar{u}(t, x), & t \in]0, T], \quad x \in \Omega, \\ \bar{u}(0, x) = \bar{u}^0(x), & x \in \Omega. \end{cases}$$

Parameter identification

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Parameter
identification

Sensitivity
analysis

NIRB
method

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with parabolic
equations

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$$\mathcal{F}(p) = \sum_{k=1}^{T/\Delta t} \underbrace{\|u_h^k(p) - \bar{u}^k\|_{L^2}^2}_{\|\text{err}(t^k;p)\|_{L^2}^2},$$

Parameter identification

$$\mathcal{F}(p) = \sum_{k=1}^{T/\Delta t} \underbrace{\|u_h^k(p) - \bar{u}^k\|_{L^2}^2}_{\|\text{err}(t^k;p)\|_{L^2}^2}$$



Gauss – Newton



Gradient descent

Performance measure

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Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
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$$\mathcal{F}(p) = \sum_{k=1}^{T/\Delta t} g^k u_h^k(p),$$

Sensitivities

$$\Psi_j^k(\mathbf{x}; \mathbf{p}) := \frac{\partial u_h^k}{\partial p_j}(\mathbf{x}; \mathbf{p}) \quad \text{or} \quad \frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p})$$

Normalized sensitivity coefficients (elasticity of \mathcal{P})

$$S_j = \frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p}) \times \frac{p_j}{\mathcal{F}(\mathbf{p})}, \quad j = 1, \dots, P.$$

Net change in performance measure

$$\Delta \mathcal{F} = \sum_{j=1}^P \frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p}) \times \Delta p_j, \quad j = 1, \dots, P.$$

⁴E. Borgonovo, E. Plischke, Sensitivity analysis: a review of recent advances. 2016.

$$\mathcal{P}_{IVP} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

Forward method

$$\left(\frac{\partial u}{\partial p_j} \right)_{j=1, \dots, P}$$

Sensitivity analysis

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

Forward method

$$\left(\frac{\partial u}{\partial p_j} \right)_{j=1, \dots, P}$$

$$\mathcal{P}_j \begin{cases} \frac{\partial \Psi_j}{\partial t} = \partial_u f \cdot \Psi_j + \partial_{p_j} f, & \text{in } \Omega \times]0, T], \\ \Psi_j(0) = \Psi_j^0, & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

Sensitivity analysis

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

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Backward method

$$\left(\frac{\partial \mathcal{F}}{\partial p_j}\right)_{j=1, \dots, P}$$

Sensitivity analysis

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, x; p) = f(u, t, x, p), & \text{in } \Omega \times]0, T], \\ u(0, x; p) = u^0(x, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

<p>Forward method</p> $\left(\frac{\partial u}{\partial p_j}\right)_{j=1, \dots, P}$	$\mathcal{P}_j \begin{cases} \frac{\partial \Psi_j}{\partial t} = \partial_u f \cdot \Psi_j + \partial_{p_j} f, & \text{in } \Omega \times]0, T], \\ \Psi_j(0) = \Psi_j^0, & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$
<p>Backward method</p> $\left(\frac{\partial \mathcal{F}}{\partial p_j}\right)_{j=1, \dots, P}$	$\mathcal{L}(u, \lambda; p) = \mathcal{F}(p) + \int_0^T \int_{\Omega} \lambda \cdot \left(f - \frac{\partial u}{\partial t}\right) dx dt$

Sensitivity analysis

$$\mathcal{P}_{IVP} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

<p>Forward method $(\frac{\partial u}{\partial p_j})_{j=1, \dots, P}$</p>	$\mathcal{P}_j \begin{cases} \frac{\partial \psi_j}{\partial t} = \partial_u f \cdot \psi_j + \partial_{p_j} f, & \text{in } \Omega \times]0, T], \\ \psi_j(0) = \psi_j^0, & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$
<p>Backward method $(\frac{\partial \mathcal{F}}{\partial p_j})_{j=1, \dots, P}$</p>	$\mathcal{P}^* \begin{cases} \frac{\partial \lambda}{\partial t} = -(\frac{\partial f}{\partial u})^T \lambda - 2(\frac{\partial \text{err}}{\partial u})^T, & \text{in } \Omega \times [0, T[, \\ \lambda(T) = 0, & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$

Sensitivity analysis

$$\mathcal{P}_{IVP} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), & \text{in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$$

<p>Forward method</p> $\left(\frac{\partial u}{\partial p_j}\right)_{j=1, \dots, P}$	$\mathcal{P}_j \begin{cases} \frac{\partial \Psi_j}{\partial t} = \partial_u f \cdot \Psi_j + \partial_{p_j} f, & \text{in } \Omega \times]0, T], \\ \Psi_j(0) = \Psi_j^0, & \text{in } \Omega, \\ +\text{BCs.} \end{cases}$
<p>Backward method</p> $\left(\frac{\partial \mathcal{F}}{\partial p_j}\right)_{j=1, \dots, P}$	$\frac{\partial \mathcal{F}}{\partial p_j} = \frac{\partial \mathcal{L}}{\partial p_j} = \int_0^T \int_{\Omega} \lambda_j \cdot \frac{\partial f}{\partial p_j} \, dx \, dt$

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; p) = f(u, t, \mathbf{x}, p), \text{ in } \Omega \times]0, T], \\ u(0, \mathbf{x}; p) = u^0(\mathbf{x}, p), \text{ in } \Omega, \\ +\text{BCs.} \end{cases}$$

Forward method $(\frac{\partial u}{\partial p_j})_{j=1, \dots, P}$	IVP + P systems to solve ...
Backward method $(\frac{\partial \mathcal{F}}{\partial p_j})_{j=1, \dots, P}$	IVP + 1 system to solve ...

How to Reduce the computational costs of these
parameter-dependent problems?

Reduced basis methods

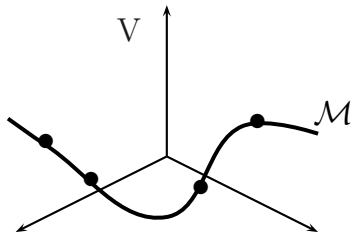


Figure: Solution manifold

$$\mathcal{M} = \{u(\mu) \in V \mid \mu \in \mathcal{G}\} \subset V.$$

- ▶ Parameter: $\mu = (t, p) \in \mathcal{G}$,
- ▶ Solution: $u(\mu) \in V$.

Introduction to the NIRB methods

Reduced basis methods

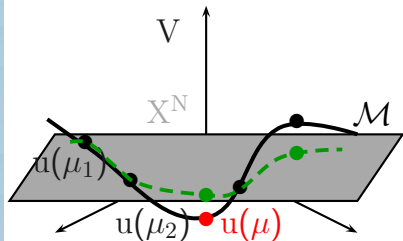


Figure: Solution manifold

$$\mathcal{M} = \{u(\mu) \in V \mid \mu \in \mathcal{G}\} \subset V.$$

- ▶ X^N Reduced basis space,
- ▶ Parameters $\mu_1, \dots, \mu_N \in \mathcal{G}$,
- ▶ Snapshots $u(\mu_1), \dots, u(\mu_N) \in V_h$,
- ▶ Projected snapshots onto X^N .
- ▶ Projected new solution onto X^N .

Introduction to the NIRB methods

Reduced basis methods

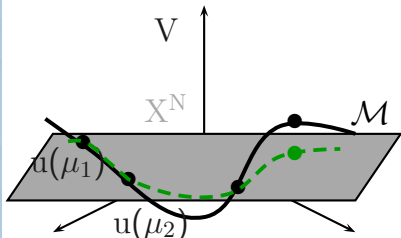


Figure: Solution manifold

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- ▶ X^N Reduced basis space,
- ▶ Parameters $\mu_1, \dots, \mu_N \in \mathcal{G}$,
- ▶ Snapshots $u(\mu_1), \dots, u(\mu_N) \in V$,
- ▶ Projected snapshots onto X^N .

$$\inf_{\dim(X^N)=N} \text{dist}(\mathcal{M}, X^N).$$

Kolmogorov n-width must be small ⁵

⁵ P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, P. Wojtaszczyk, Convergence rates for greedy algorithms in reduced basis methods. 2011.

Introduction to the NIRB methods

Reduced basis methods

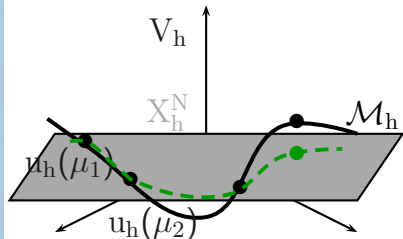


Figure: Solution manifold

$$\mathcal{M}_h = \{u_h(\mu) \in V_h \mid \mu \in \mathcal{G}\} \subset V_h.$$

- ▶ X_h^N Reduced basis space,
- ▶ Parameters $\mu_1, \dots, \mu_N \in \mathcal{G}$,
- ▶ Snapshots $u_h(\mu_1), \dots, u_h(\mu_N) \in V_h$,
- ▶ Projected snapshots onto X_h^N .

Kolmogorov n-width must be small ⁵

⁵ P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, P. Wojtaszczyk Convergence rates for greedy algorithms in reduced basis methods. 2011.

Introduction to the NIRB methods

NIRB &
Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

Reduced basis methods

Intrusive methods

Non-Intrusive Reduced basis methods (NIRB)

Industrial context → **black box solver**



A model problem

Introduction to the two-grid method within the parabolic context

$$\begin{cases} \frac{\partial u}{\partial t} - \nabla \cdot (A(\mathbf{p})\nabla u) = f, & \text{in } \Omega \times]0, T], \\ u(\mathbf{x}, 0) = u^0(\mathbf{x}), & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, t \in [0, T], \end{cases}$$

- ▶ $\mu = (t, \mathbf{p}) \in \mathcal{G} \subset \mathbb{R}^+ \times \mathbb{R}^P$: Variable parameter
- ▶ $u(t, \mathbf{x}; \mathbf{p})$: Unknowns

A model problem

Offline stage

$u_h^n(p^k) = u_h(p^k, t^n) \in V_h$, for $n = 1, \dots, N_T$: Snapshots on \mathcal{T}_h
(HF code).

Online stage

$u_H^m(p) = u_H(p, \tilde{t}^m) \in V_H$, for $m = 1, \dots, M_T$: Coarse solution on \mathcal{T}_H ,
 $H \gg h$.

⁶R. Chakir, Y. Maday, A two-grid finite-element/reduced basis scheme for the approximation of the solution of parameter dependent PDE. 2009.

⁷E. G., Y. Maday, error estimate of the non-intrusive reduced basis method with finite volume schemes. 2021.

⁸E. G., Y. Maday, Error estimate of the Non-Intrusive Reduced Basis (NIRB) two-grid method with parabolic equations. 2022.

Separation of variables

$$u_h(x, t^n; p) = \sum_{j=1}^N a_j^h(p, t^n) \Phi_j^h(x), \quad n = 1, \dots, N_T$$

$(\Phi_j^h)_{j=1, \dots, N} \in X_h^N$: L^2 -orthonormalized basis functions (modes)

Coefficients $a_j^h(\mu) = a_j^h(p, t^n)$

- Optimal coefficients: $(u_h(p, t^n), \Phi_j^h(x))$,
- Our choice: $(I_n(u_H(p, \tilde{t}^m)), \Phi_j^h(x))$, $m=1, \dots, M_T$

Greedy algorithm

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Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

→ L^2 orthonormalization

+ Eigenvalue problem: $\forall v \in X_h^N, \int_{\Omega} \nabla \Phi_h \cdot \nabla v = \lambda \int_{\Omega} \Phi_h \cdot v$

→ $L^2(\Omega)$ and $H^1(\Omega)$ orthogonalization.

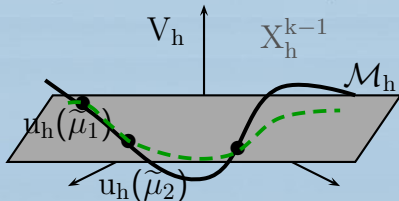
$$X_h^N = \text{Span}\{\Phi_1^h, \dots, \Phi_N^h\}$$

⁹B. Haasdonk, Convergence rates of the pod-greedy method, 2013.

Greedy algorithm

for $k = 1, \dots, N$:

$$\tilde{p}^k = \arg \max_{p \in \mathcal{G}} \|u_h(p, t^n) - P^{k-1}(u_h(p, t^n))\|_{1^\infty(1, \dots, N_T; L^2(\Omega))}$$



⁹B. Haasdonk, Convergence rates of the pod-greedy method, 2013.

FEM Error estimates within the elliptic context

Energy error estimate with P_1 FE (elliptic equations)

$$\|u(p) - u_{Hh}^N(p)\|_{H^1} \leq \overbrace{\varepsilon(N)}^{T_1} + \underbrace{C_1 h}_{T_2} + \overbrace{C_2(N)H^2}^{T_3} \sim Ch \text{ if } H^2 \sim h$$

where C_1, C_2 are constants independent of h and H .⁵

¹⁰R. Chakir, Y. Maday. A two-grid finite-element/reduced basis scheme for the approximation of the solution of parameter dependent PDE. 2009

FEM Error estimates within the elliptic context

Energy error estimate with P_1 FE (elliptic equations)

$$\|u(p) - u_{Hh}^N(p)\|_{H^1} \leq \overbrace{\varepsilon(N)}^{T_1} + \underbrace{C_1 h}_{T_2} + \overbrace{C_2(N)H^2}^{T_3} \sim Ch \text{ if } H^2 \sim h$$

where C_1, C_2 are constants independent of h and H .⁵

Aubin-Nitsche's Lemma (P_1 FE).

$$\|u - u_H\|_{L^2} \leq CH \|u - u_H\|_{H^1}.$$

¹⁰R. Chakir, Y. Maday. A two-grid finite-element/reduced basis scheme for the approximation of the solution of parameter dependent PDE. 2009

FEM Error estimates

Theorem [E G.-Y M.] (H^1 error estimate)

$$\forall n, \|u(t^n)(p) - u_{Hh}^{N,n}(p)\|_{H^1(\Omega)} \leq \overbrace{\varepsilon(N)}^{T_1} + \underbrace{C_1(p)h + C_2(p)\Delta t_F}_{T_2} + \overbrace{C(N)(H^2 + \Delta t_G^2)}^{T_3}$$

C, C_1, C_2 : Constants independent of h and H .

¹¹V. Thomée, Galerkin finite element methods for parabolic problems, 1984.

FEM Error estimates

Theorem [E G.-Y M.] (H^1 error estimate)

▶ With L^2 -orthonormalized modes:

$$\forall n, \|u(t^n)(p) - u_{\text{Hh}}^{N,n}(p)\|_{H^1(\Omega)} \leq \overbrace{\varepsilon(N)}^{T_1} + \underbrace{C_1(p)h + C_2(p)\Delta t_F}_{T_2} + \overbrace{C\sqrt{\lambda_N}\sqrt{N}(H^2 + \Delta t_G^2)}^{T_3}$$

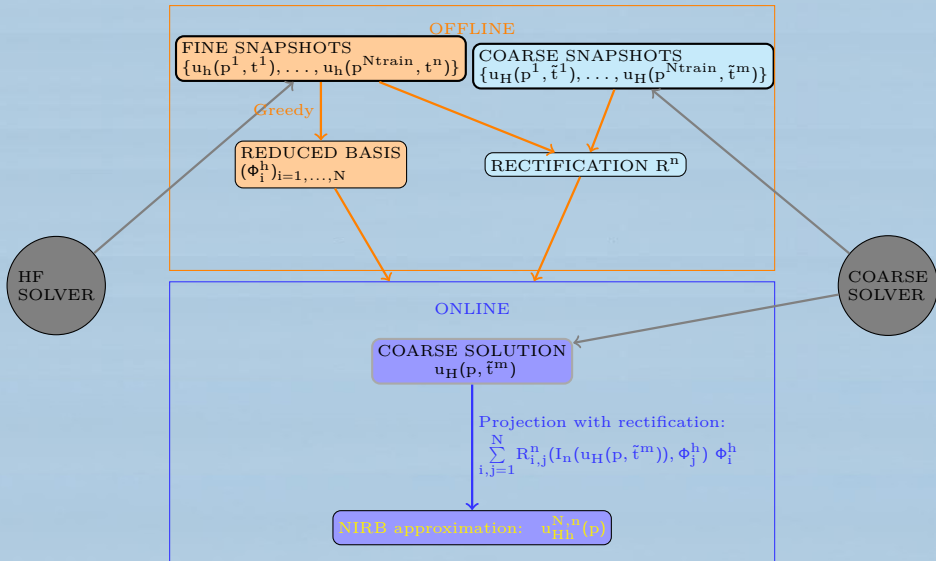
▶ With H^1 and L^2 orthogonalization

$$\forall n, \|u(t^n)(p) - u_{\text{Hh}}^{N,n}(p)\|_{H^1(\Omega)} \leq \overbrace{\varepsilon(N)}^{T_1} + \underbrace{C_1(p)h + C_2(p)\Delta t_F}_{T_2} + \overbrace{C\sqrt{\lambda_N}(H^2 + \Delta t_G^2)}^{T_3}$$

$$\lambda_N: \quad \forall v \in X_h^N, \int_{\Omega} \nabla \Phi_h \cdot \nabla v = \lambda \int_{\Omega} \Phi_h \cdot v,$$

C, C_1, C_2 : Constants independent of h, H and N .

NIRB – OFFLINE/ONLINE



The rectification post-treatment

Fine coefficients

$$a_j^h(p^i, t^n) = (u_h(p^i, t^n), \Phi_j)$$

Coarse coefficients

$$b_j^H(p^i, t^n) = (I_n(u_H(p^i, \tilde{t}^m), \Phi_j))$$

The rectification post-treatment

Post-Treatment: The rectification method ¹²

$$b_j^H(p^i, t^n) \rightarrow a_j^h(p^i, t^n)$$

$\forall n = 1, \dots, N_T, j = 1, \dots, N, i = 1, \dots, N_{\text{train}}$:

$$A_{i,j}^n = a_j^h(p^i, t^n),$$

$$B_{i,j}^n = b_j^H(p^i, t^n).$$

$$R_i^n = (A^T A + \varepsilon I_N)^{-1} A^T B_i, \quad \forall i = 1, \dots, N.$$

$$u_{\text{Hh}}^N(p, t^n) = \sum_{i,j=1}^N R_{ij}^n b_j^H(p, t^n) \Phi_i$$

For $p \in \mathcal{G} = [0.5, 9.5]$,

$$\begin{cases} \frac{\partial u}{\partial t} - p\Delta u = f, & \text{in } \Omega \times]0, T], \\ u(x, 0) = u^0(x), & \text{in } \Omega, \\ u = 0, & \text{on } \partial\Omega, t \in [0, T], \end{cases}$$

$$u(t, \mathbf{x}; 1) = 10 t x_1^2(1 - x_1)^2 x_2^2(1 - x_2)^2, \quad t \geq 0, \quad \mathbf{x} \in [0, 1]^2.$$

Numerical results

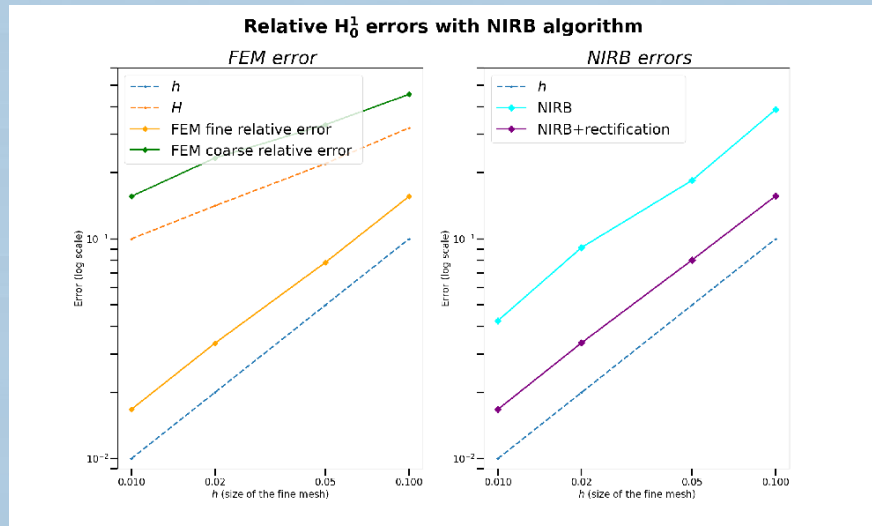


Figure: $l^\infty(1, 2; H_0^1(\Omega))$ with $p = 1$, $\Delta t_G^2 \simeq H^2 \simeq h \simeq \Delta t_F$, $N_{\text{train}} = 18$, $N = 3$

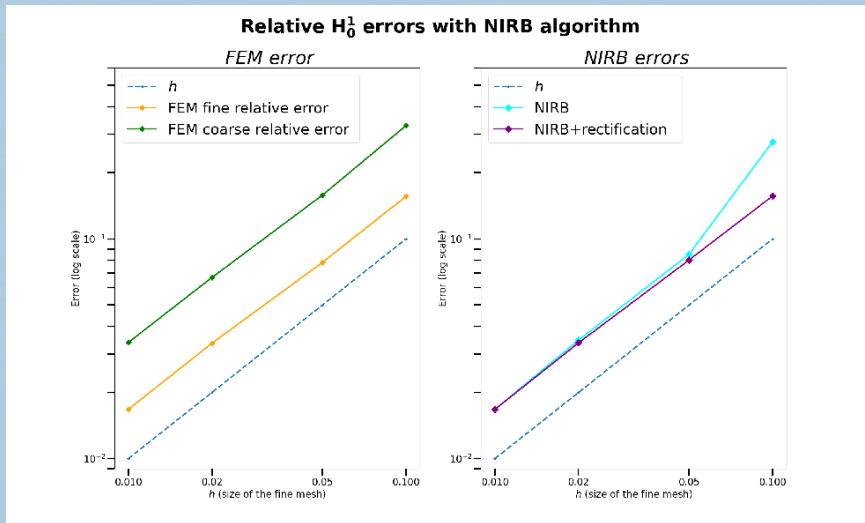


Figure: $l^\infty(1, 2; H_0^1(\Omega))$ with $p = 1$, $\Delta t_G \simeq H \simeq 2h \simeq 2\Delta t_F$, $N_{\text{train}} = 18$, $N = 3$

NIRB method on the sensitivity analysis

Online sensitivity analysis

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial u}{\partial t}(t, \mathbf{x}; \mathbf{p}) = f(u, t, \mathbf{x}, \mathbf{p}), \text{ in } \Omega \times]0, T], \\ u(0, \mathbf{x}; \mathbf{p}) = u^0(\mathbf{x}, \mathbf{p}), \text{ in } \Omega, \\ + \text{BCs.} \end{cases}$$

<p>Forward method $(\frac{\partial u}{\partial p_j})_{j=1, \dots, P}$</p>	<p>IVP + P systems to solve ...</p>
<p>Backward method $(\frac{\partial \mathcal{F}}{\partial p_j})_{j=1, \dots, P}$</p>	<p>IVP + 1 system to solve ...</p>

Forward method

NIRB &
Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

$$\begin{cases} \frac{\partial_t \Psi}{\partial t} - p \Delta \Psi = \Delta u, & \text{in } \Omega \times]0, T] \\ \Psi(x, 0) = 0, & \text{in } \Omega, \\ \Psi = 0, & \text{on } \partial\Omega, t \in [0, T]. \end{cases}$$

Forward method

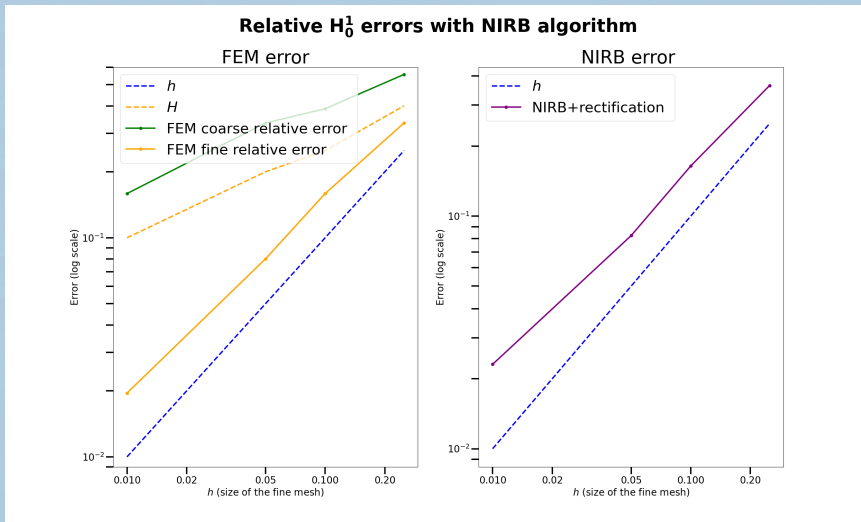


Figure: $l^\infty(1, 2; H_0^1(\Omega))$ with $p = 1$, $\Delta t_G^2 \simeq H^2 \simeq h \simeq \Delta t_F$, $N_{\text{train}} = 18$, $N = 3$

The new rectification post-treatment

Fine coefficients

$$a_j^h(p^i, t^n) = (\Psi_k(p^i, t^n), \zeta_j^k)$$

Coarse coefficients

$$b_j^H(p^i, t^n) = (I_n(u_H(p^i, \tilde{t}^m), \Phi_j))$$

The new rectification post-treatment

$$\mathcal{P}_{\text{IVP}} : \begin{cases} \frac{\partial \mathbf{u}}{\partial t}(t, \mathbf{x}; \mathbf{p}) = f(\mathbf{u}, t, \mathbf{x}, \mathbf{p}), & \text{in } \Omega \times]0, T], \\ \mathbf{u}(0, \mathbf{x}; \mathbf{p}) = \mathbf{u}^0(\mathbf{x}, \mathbf{p}), & \text{in } \Omega, \\ + \text{BCs.} \end{cases}$$

<p>Forward method</p> $\left(\frac{\partial \mathbf{u}}{\partial p_j} \right)_{j=1, \dots, P}$	<p>IVP + 1 systems to solve ...</p>
<p>Backward method</p> $\left(\frac{\partial \mathcal{F}}{\partial p_j} \right)_{j=1, \dots, P}$	<p>IVP + 1 system to solve ...</p>

Brusselator equations

NIRB &
Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

$$\partial_t u = a + uv^2 - (b + 1)u + \alpha \Delta u$$

$$\partial_t v = bu - uv^2 + \alpha \Delta v.$$

- ▶ $(u(x, t; p), v(x, t; p))$: Unknowns
- ▶ $\mu = (t, a, b, \alpha) \in \mathbb{R}^4$: Variable parameter

Numerical results on the state solution (u, v)

NIRB &
Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

For $p \in \mathcal{G} = [2, 4] \times [1, 4] \times [0.001, 0.05]$,
 $T = [0, 5]$

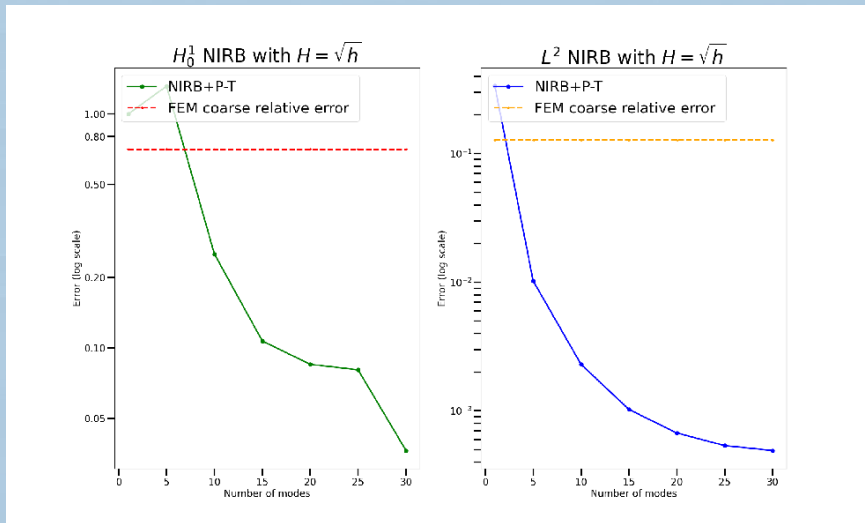
Numerical results on the state solution (u, v) 

Figure: $l^\infty(0, 5; H_0^1(\Omega))$ with $p = (3, 2, 0.008)$, $\Delta t_G^2 \simeq H^2 \simeq h \simeq \Delta t_F$

Parameter identification results

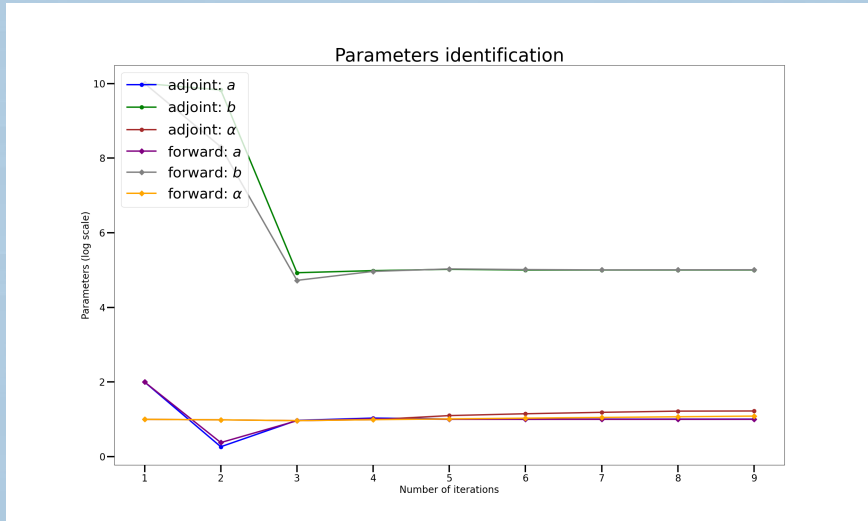


Figure: Identification of $a = 1$, $b = 5$ and $\alpha = 2$

Parameter identification results

FEM (fine/HF)	02:43
FEM (coarse)	00:03

Table: FEM runtimes

Adjoint method	Direct method	Direct method with new rectification
00:06	00:13	00:08

Table: Runtimes of the NIRB online part (min:sec) with $h = 0.02$, $H = 0.1$

¹³Y. Maday, A. T Patera, J. D. Penn, M. Yano, A parameterized-background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics.2015.

Conclusions & Perspectives

- ▶ Sensitivity analysis & NIRB with parabolic equations

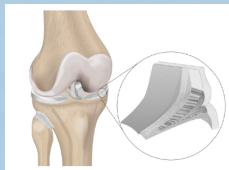


Figure: Meniscus tissue

Perspectives

- ▶ Automatic differentiation
- ▶ Sensitivity analysis on the meniscus tissue problem
- ▶ Two-grid a-posteriori & rectification error estimates

Conclusions & Perspectives

NIRB &
Sensitivity
analysis

Elise
Grosjean

Meniscus
Tissue
regeneration

Parameter
identifica-
tion

Sensitivity
analysis

NIRB
method

NIRB method
with parabolic
equations

NIRB method
on sensitivity
analysis

- ▶ Sensitivity analysis & NIRB with parabolic equations

Merci !

Perspectives

- ▶ Automatic differentiation
- ▶ Sensitivity analysis on the meniscus tissue problem
- ▶ Two-grid a-posteriori & rectification error estimates

Optimization algorithms

$$\text{err}(\mathbf{p}) = (\text{err}(0; \mathbf{p}), \dots, \text{err}(T; \mathbf{p})) \in \mathbb{R}^{T/\Delta t \times \mathcal{N}}$$

$$\text{err}(t; \mathbf{p}) \in \mathbb{R}^{\mathcal{N}}$$

Optimization algorithms

$$\text{err}(\mathbf{p}) = (\text{err}(0; \mathbf{p}), \dots, \text{err}(T; \mathbf{p})) \in \mathbb{R}^{T/\Delta t \times \mathcal{N}}$$

Gauss-Newton

$$\mathbf{p}^{s+1} = \mathbf{p}^s - (\mathbf{J}^T \mathbf{J})^{-1} \mathbf{J}^T \text{err}(\mathbf{p}^s),$$

$$\mathbf{J}_{i,j} = \frac{\partial \text{err}^i}{\partial p_j}(\mathbf{p}^s), \quad i = 0, \dots, T/\Delta t \times \mathcal{N}, \quad j = 1, \dots, P.$$

Optimization algorithms

$$\text{err}(\mathbf{p}) = (\text{err}(0; \mathbf{p}), \dots, \text{err}(T; \mathbf{p})) \in \mathbb{R}^{T/\Delta t \times \mathcal{N}}$$

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Gradient descent

$$\mathbf{p}^{s+1} = \mathbf{p}^s - \alpha \cdot \nabla \mathcal{F}(\mathbf{p}^s),$$

$$\frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p}^s) = 2 \sum_{k=1}^{T/\Delta t} \int_{\Omega} \text{err}(t^k, \mathbf{x}; \mathbf{p}^s) \frac{\partial u_h^k}{\partial p_j}(\mathbf{x}; \mathbf{p}^s) \, dx.$$

Optimization algorithms

$$\text{err}(p) = (\text{err}(0; p), \dots, \text{err}(T; p)) \in \mathbb{R}^{T/\Delta t \times \mathcal{N}}$$

Gauss-Newton

$$p^{s+1} = p^s - (J^T J)^{-1} J^T \text{err}(p^s),$$

$$J_{i,j} = \frac{\partial \text{err}^i}{\partial p_j}(p^s), \quad i = 0, \dots, T/\Delta t \times \mathcal{N}, \quad j = 1, \dots, P.$$

Gradient descent

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Sensitivities

Optimization algorithms

$$\text{err}(\mathbf{p}) = (\text{err}(0; \mathbf{p}), \dots, \text{err}(T; \mathbf{p})) \in \mathbb{R}^{T/\Delta t \times \mathcal{N}}$$

Gauss-Newton

$$\mathbf{p}^{s+1} = \mathbf{p}^s - (\mathbf{J}^T \mathbf{J})^{-1} \mathbf{J}^T \text{err}(\mathbf{p}^s),$$

$$\mathbf{J}_{i,j} = \frac{\partial \text{err}^i}{\partial p_j}(\mathbf{p}^s), \quad i = 0, \dots, T/\Delta t \times \mathcal{N}, \quad j = 1, \dots, P.$$

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$$\mathbf{p}^{s+1} = \mathbf{p}^s - \alpha \cdot \nabla \mathcal{F}(\mathbf{p}^s),$$

$$\frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p}^s) = 2 \sum_{k=1}^{T/\Delta t} \int_{\Omega} \text{err}(t^k, \mathbf{x}; \mathbf{p}^s) \frac{\partial u_h^k}{\partial p_j}(\mathbf{x}; \mathbf{p}^s) \, dx.$$

Sensitivities:

$$\frac{\partial u_h^k}{\partial p_j}(\mathbf{x}; \mathbf{p}^s) \quad \text{or} \quad \frac{\partial \mathcal{F}}{\partial p_j}(\mathbf{p}^s)$$