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Application of the reduced basis method to compressible single-phase flows in porous media

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Doctoral dissertation supervised by

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Outline

1 Introduction

- Modeling a CO₂ storage area
- Objectives

2 Application of RB methods to single-phase flow problems

- Definition of the problem
- State of the art on RB methods and contribution
- Application to SPF problems
- Numerical tests

3 Conclusion and perspectives

Outline

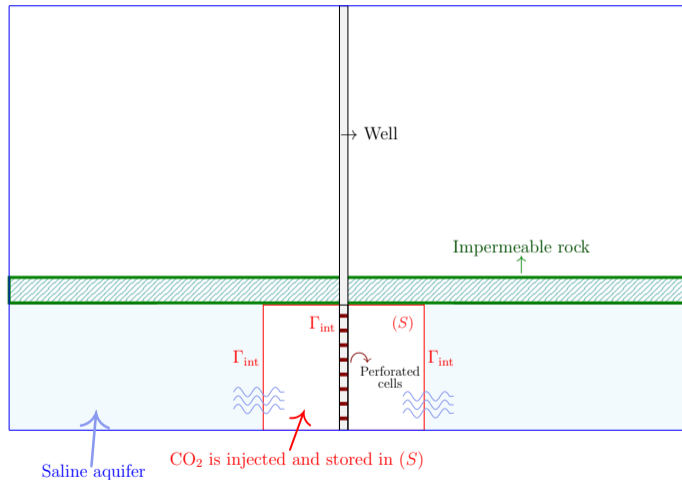
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Modeling a CO₂ storage area

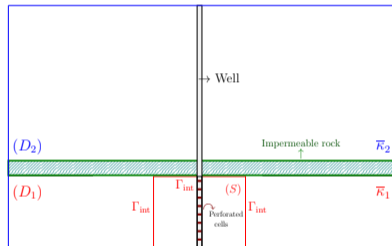


- CO₂ storage in saline aquifers
- Large-scale induced motions
- Large extended domain

Parametrized problem

- Uncertainty regarding certain parameters
 - Numerical resolution using a flow simulator
 - Several runs for *different* parameter values, e.g.,

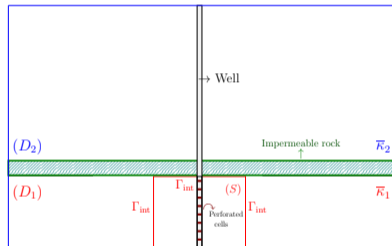
$$\bar{\kappa}(\mathbf{x}) = \bar{\kappa}_1 \mathbb{1}_{D_1}(\mathbf{x}) + \bar{\kappa}_2 \mathbb{1}_{D_2}(\mathbf{x})$$



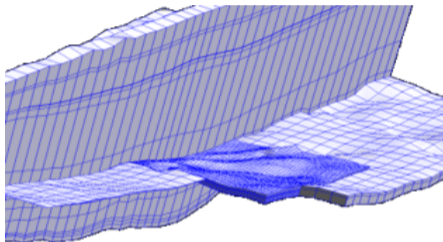
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A possible way to handle large space domain



- Local grid refinement near the injection zone
- Still very **costly** computational effort

Methodology

- Reduced systems for *single-phase flow*
 - Lower **simulation costs** of many simulations for many parameters
 - Control errors in parameter **independent** norms
 - Control **linear** outputs of the solutions p and u

Strategy

- Advantages of (RB) method
 - Replace **high-fidelity** calls by less expensive surrogate calls

Offline stage

- Use of high-fidelity solutions
 - Many degrees of freedom \mathcal{N}
- Construct **reduced bases**
 - POD-Greedy process

Online stage

- Construct reduced solutions
 - Construct a Galerkin system of small dimension N
- Provide **cheap** *output* of interest

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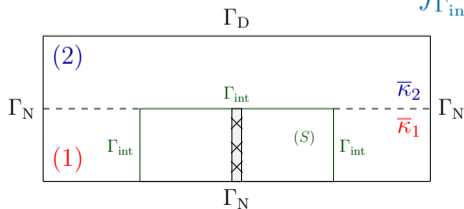
Single-phase flow

Model

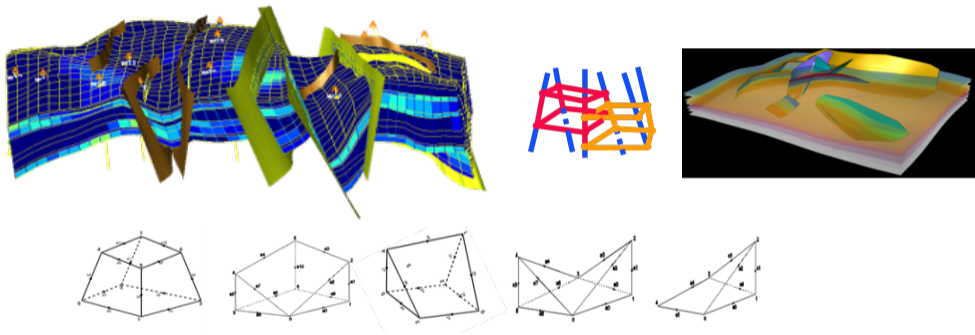
$$\begin{aligned}
 c_{\Phi} \partial_t p - \nabla \cdot (\mathbf{\Lambda}(\nabla p + \rho g \nabla z)) &= q(p) && \text{in }]0, T] \times \Omega \\
 \mathbf{\Lambda}(\nabla p + \rho g \nabla z) \cdot \mathbf{n} &= 0 && \text{on }]0, T] \times \Gamma_N \\
 p &= p_D && \text{on }]0, T] \times \Gamma_D \\
 p(x, t = 0) &= p^0(x) && \text{in } \Omega
 \end{aligned}$$

with **uncertainty** on $\mathbf{\Lambda} = \bar{\kappa}(\mathbf{x})/\mu$

- Predict the impact of $\bar{\kappa}$ on the **flux** $s = - \int_{\Gamma_{\text{int}}} \mathbf{\Lambda}(\bar{\kappa})(\nabla p + \rho g \nabla z) \cdot \mathbf{n}$



Complex meshes in porous medium simulations



- Geological layers using folders in a mesh of CPG-type

Discretization

- Time: Implicit Euler discretization
- Space: Average multi-point finite volume method
- Discrete high-fidelity system:

- $\Delta t = \frac{T}{N}$
- A parameter ξ

$$(M + \Delta t A(\xi)) \mathbf{p}_{\mathcal{M}}^{n+1} = M \mathbf{p}_{\mathcal{M}}^n + \Delta t \mathbf{b}(\xi) \quad n = 0, \dots, N-1$$

$$s^{n+1} = \mathbf{l}^T(\xi) \mathbf{p}_{\mathcal{M}}^{n+1}$$

$$\begin{pmatrix} M + \Delta t A & 0 & 0 & \dots & \dots & 0 \\ -M & M + \Delta t A & \ddots & \ddots & & \vdots \\ 0 & -M & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & \dots & 0 & -M & M + \Delta t A \end{pmatrix} \begin{pmatrix} \mathbf{p}_{\mathcal{M}}^1 \\ \mathbf{p}_{\mathcal{M}}^2 \\ \vdots \\ \vdots \\ \mathbf{p}_{\mathcal{M}}^{N-1} \\ \mathbf{p}_{\mathcal{M}}^N \end{pmatrix} = \Delta t \begin{pmatrix} \mathbf{b} + M \mathbf{p}_{\mathcal{M}}^0 \\ \mathbf{b} \\ \vdots \\ \vdots \\ \mathbf{b} \\ \mathbf{b} \end{pmatrix}$$

State of the art and contribution

State of the art

- A goal oriented version of the RB method
 - Grepl & Patera. A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations. M2AN, 2005
 - Haasdonk & Ohlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. M2AN, 2008

Contribution

- New discrete a posteriori error estimations
- Reduction error estimated using the *same norm* of $L^2([0, T]; H^1(\Omega))$ -type for all parameter values
 - Tarhini, Boyaval, Enchéry & Tran, preprint, June 2024

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Discrete Dual Problem

■ $\forall n = N, \dots, 0$

$$M\Psi^N = -l(\xi)$$

$$(M + \Delta t A^T(\xi))\Psi^n = M\Psi^{n+1}$$

$$\begin{pmatrix} M + \Delta t A & -M & 0 & \dots & \dots & 0 \\ 0 & M + \Delta t A & \ddots & \ddots & & \vdots \\ 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & -M \\ 0 & \dots & \dots & 0 & 0 & M + \Delta t A \end{pmatrix}^T \begin{pmatrix} \Psi^{N-1} \\ \Psi^{N-2} \\ \vdots \\ \vdots \\ \Psi^1 \\ \Psi^0 \end{pmatrix} = \begin{pmatrix} -l \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

Galerkin projection

Primal reduced problem

- Galerkin projection using $\mathbf{Z} \in \mathbb{R}^{\mathcal{N}, N_{\text{pr}}}$

$$\mathbf{Z}^T (\mathbf{M} + \Delta t \mathbf{A}(\xi)) \mathbf{Z} \tilde{\mathbf{p}}^{n+1} = \mathbf{Z}^T \mathbf{M} \mathbf{Z} \tilde{\mathbf{p}}^n + \Delta t \mathbf{Z}^T \mathbf{b}(\xi)$$

⇒ Reduced solution: $\mathbf{p}^{N, n+1} \approx \mathbf{Z} \tilde{\mathbf{p}}^{n+1}$

Dual reduced problem

- Galerkin projection using $\mathbf{Z}_{\text{du}} \in \mathbb{R}^{\mathcal{N}, N_{\text{du}}}$

$$(\mathbf{Z}_{\text{du}}^T \mathbf{M} \mathbf{Z}_{\text{du}} + \Delta t \mathbf{Z}_{\text{du}}^T \mathbf{A}^T(\xi) \mathbf{Z}_{\text{du}}) \tilde{\Psi}^n = \mathbf{Z}_{\text{du}}^T \mathbf{M} \mathbf{Z}_{\text{du}} \tilde{\Psi}^{n+1}$$

$$\mathbf{Z}_{\text{du}}^T \mathbf{M} \mathbf{Z}_{\text{du}} \tilde{\Psi}^N = -\mathbf{Z}_{\text{du}}^T \mathbf{l}(\xi)$$

⇒ Reduced solution: $\Psi^{N_{\text{du}}, n} = \mathbf{Z}_{\text{du}} \tilde{\Psi}^n$

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A posteriori error estimation for primal problem

- Reduction error $e^n = p_{\mathcal{M}}^n - p^{N,n}$
- A new space-time energy norm $\|\cdot\|_{\text{pr}}$ independent of ξ

$$\|e^N\|_{\text{pr}} := \left(\sum_{n=1}^N \langle e^n, G^* e^n \rangle \right)^{1/2} \leq \Delta_{\text{pr}}^N := \left(\frac{\Delta t}{\alpha_{G,\text{LB}} \alpha_{A_{\text{sym},\text{LB}}}} \sum_{n=1}^N (N+2-n) \|r^n\|_{-1}^2 \right)^{1/2}$$

Primal residual

$$r^{n+1} = \frac{1}{\Delta t} [(M + \Delta t A)p^{N,n+1} - Mp^{N,n} - \Delta t b]$$

$$\alpha_{A_{\text{sym},\text{LB}}}(\xi) \leq \inf_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T A_{\text{sym}}(\xi)v}{\|v\|_{G^*}^2} := \alpha_{A_{\text{sym}}}(\xi) \quad \blacksquare \quad G^* = M + \Delta t A_{\text{sym}}(\xi^*)$$

$$\alpha_{G,\text{LB}}(\xi) \leq \inf_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T (M + \Delta t A_{\text{sym}}(\xi))v}{\|v\|_{G^*}^2} := \alpha_G(\xi) \quad \blacksquare \quad \|r^n\|_{-1} = \sup_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T r^n}{\|v\|_{G^*}}$$

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A posteriori error estimation for dual problem

- Reduction error $\epsilon_{\text{du}}^n = \Psi_{\mathcal{M}}^n - \Psi^{\text{Ndu},n}$
- Energy norm

$$\|\epsilon^N\|_{\text{du}} := \left(\sum_{n=1}^N \langle e^n, \mathbf{G}^* e^n \rangle \right)^{1/2} \leq \Delta_{\text{du}}^N$$

$$\Delta_{\text{du}}^N := \left(\frac{\Delta t}{\alpha_{\mathbf{A}_{\text{sym},\text{LB}}} \alpha_{\mathbf{G},\text{LB}}} \sum_{m=0}^{N-1} (m+2) \|\varrho^m\|_{-1}^2 + \frac{(T + \Delta t)}{\Delta t} \frac{\|\varrho^N\|_{-1}^2}{\alpha_M \alpha_{\mathbf{G},\text{LB}}} \right)^{1/2}$$

$$\blacksquare \varrho^n = \frac{1}{\Delta t} (M + \Delta t A^T) \Psi^{\text{Ndu},n} - M \Psi^{\text{Ndu},n+1} \quad n = N-1, \dots, 0$$

$$\triangleright \varrho^N = -l - M \Psi^{\text{Ndu},N} \quad \triangleright \|\varrho^m\|_{-1} = \sup_{v \in \mathbb{R}^{\mathcal{N}}} \frac{\langle \varrho^m, v \rangle}{\|v\|_{G^*}} \quad \triangleright \alpha_M := \inf_{v \in \mathbb{R}^{\mathcal{N}}} \frac{v^T M v}{\|v\|_{G^*}^2}$$

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A posteriori error estimation for QOI

- Under the equality

$$\langle \boldsymbol{l}, \boldsymbol{p}_{\mathcal{M}}^n - \boldsymbol{p}^{\text{Npr},n} \rangle = \Delta t \sum_{k=0}^{n-1} \langle \boldsymbol{r}^{k+1}, \boldsymbol{\varepsilon}^{N-n+k} \rangle + \Delta t \sum_{k=0}^{n-1} \langle \boldsymbol{r}^{k+1}, \boldsymbol{\Psi}^{\text{Ndu},N-n+k} \rangle$$

- Reduced output

$$s^{\text{Ns},n} = \langle \boldsymbol{l}, \boldsymbol{p}^{\text{Npr},n} \rangle + \Delta t \sum_{n'=0}^{n-1} \langle \boldsymbol{r}^{n'+1}, \boldsymbol{\Psi}^{\text{Ndu},N-n+n'} \rangle$$

- Estimation

$$|s^N - s^{\text{Ns},N}| \leq \Delta t \left(\sum_{n=1}^N \|\boldsymbol{r}^n\|_{-1}^2 \right)^{1/2} \Delta_{\text{du}}^N =: \Delta_s^N$$

EIM and SCM

- Δ_{pr}^N has to be
 - reliable: $\|e^N\|_{\text{pr}} \leq \Delta_{\text{pr}}^N$
 - $c := \frac{\Delta_{\text{pr}}^N}{\|e^N\|_{\text{pr}}}$ depends weakly on ξ
 - computationally cheap
- EIM for $\mathbf{A}^N = \mathbf{Z}^T \mathbf{A}(\xi) \mathbf{Z}$, $\mathbf{b}^N(\xi) = \mathbf{Z}^T \mathbf{b}$

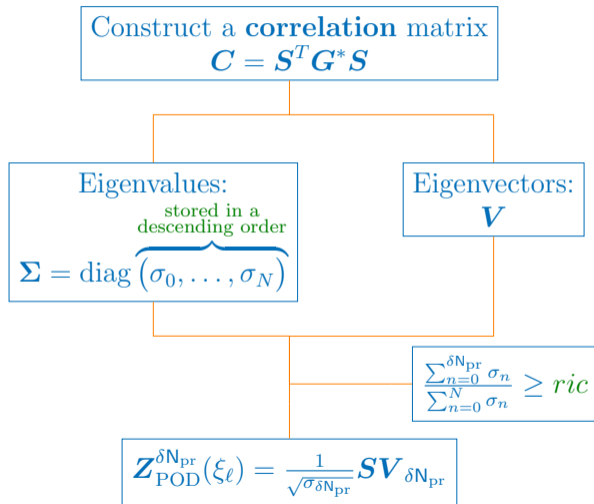
$$\mathbf{A}(\xi) \approx \sum_{d=1}^{D_a} \theta_d^a(\xi) \mathbf{A}_d, \quad \mathbf{b}(\xi) \approx \sum_{d=1}^{D_b} \theta_d^b(\xi) \mathbf{b}_d$$

- SCM on $\alpha_{\mathbf{A}_{\text{sym}}}(\xi)$

$$\alpha_{\mathbf{A}_{\text{sym, LB}}}(\xi) \leq \alpha_{\mathbf{A}_{\text{sym}}}(\xi) \leq \alpha_{\mathbf{A}_{\text{sym, UB}}}(\xi)$$

POD method

- S : snapshots matrix
- $ric \in [0, 1]$



POD-Greedy algorithm

Algorithm 1: POD-greedy algorithm using Δ_{pr}^N

Input: $N_{\text{max}}, \epsilon_{\text{tol}}, \Xi, ric$

Data: $N_{\text{pr}} = 1, \delta^{\text{Npr}} = \epsilon_{\text{tol}} + 1$
 $\xi \in \Xi, \ell = 1, \Xi^\ell = \{\xi_1\}$

Initialize:

Compute $\mathbf{p}_{\mathcal{M}}^n(\xi_1)$ **for** $0 \leq n \leq N$

Set

$$\mathbf{S}_{\text{pr}} = \left(\mathbf{p}_{\mathcal{M}}^0(\xi_1) \quad \Big| \quad \dots \quad \Big| \quad \mathbf{p}_{\mathcal{M}}^N(\xi_1) \right)$$

Set $\mathbf{Z}^{\text{Npr}} = \text{POD}(\mathbf{S}_{\text{pr}}, \mathbf{G}^*, ric)$

$$\delta^{\text{Npr}} = \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \xi_{\ell+1} = \arg \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \Xi^{\ell+1} \leftarrow \Xi^\ell \cup \{\xi_{\ell+1}\}$$

POD-Greedy algorithm

while $\delta^{N_{\text{pr}}} > \epsilon_{\text{tol}}$, $N_{\text{pr}} < N_{\text{max}}$ **do**

 Compute $\mathbf{p}_{\mathcal{M}}^n(\xi_\ell)$ for $0 \leq n \leq N$

 Set

$$\mathbf{S}_{\text{pr}} := [\mathbf{p}_{\mathcal{M}}^0(\xi_\ell) - \text{Proj}_{\mathbf{Z}_{\text{pr}}}(\mathbf{p}_{\mathcal{M}}^0(\xi_\ell)) \mid \dots \mid \mathbf{p}_{\mathcal{M}}^N(\xi_\ell) - \text{Proj}_{\mathbf{Z}_{\text{pr}}}(\mathbf{p}_{\mathcal{M}}^N(\xi_\ell))]$$

 Compute $[z_1 \mid \dots \mid z_{\delta N_{\text{pr}}}] = \text{POD}(\mathbf{S}_{\text{pr}}, G^*, \text{ric})$

 Define $\mathbf{Z}^{N_{\text{pr}} + \delta N_{\text{pr}}} := \text{orthonormalize}(\mathbf{Z}^{N_{\text{pr}}} \cup [z_1 \mid \dots \mid z_{\delta N_{\text{pr}}}])$

$$\delta^{N_{\text{pr}}} = \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \xi_{\ell+1} = \arg \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \Xi^{\ell+1} \leftarrow \Xi^\ell \cup \{\xi_{\ell+1}\}$$

$$N_{\text{pr}} \leftarrow N_{\text{pr}} + \delta N_{\text{pr}} \quad \ell \leftarrow \ell + 1$$

end

POD-Greedy algorithm

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$$\mathbf{S}_{\text{pr}} := [\mathbf{p}_{\mathcal{M}}^0(\xi_\ell) - \text{Proj}_{\mathbf{Z}_{\text{pr}}}(\mathbf{p}_{\mathcal{M}}^0(\xi_\ell)) \mid \dots \mid \mathbf{p}_{\mathcal{M}}^N(\xi_\ell) - \text{Proj}_{\mathbf{Z}_{\text{pr}}}(\mathbf{p}_{\mathcal{M}}^N(\xi_\ell))]$$

 Compute $[z_1 \mid \dots \mid z_{\delta N_{\text{pr}}}] = \mathbf{POD}(\mathbf{S}_{\text{pr}}, \mathbf{G}^*, \text{ric})$

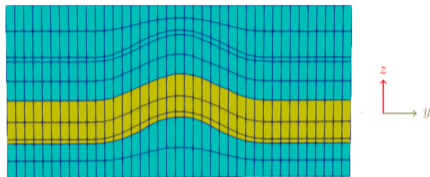
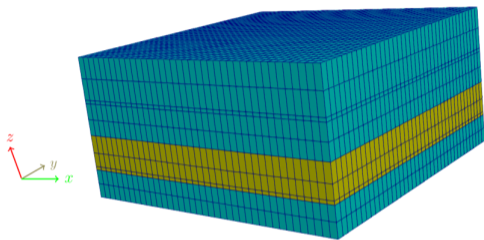
 Define $\mathbf{Z}^{N_{\text{pr}} + \delta N_{\text{pr}}} := \text{orthonormalize}(\mathbf{Z}^{N_{\text{pr}}} \cup [z_1 \mid \dots \mid z_{\delta N_{\text{pr}}}])$

$$\delta^{N_{\text{pr}}} = \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \xi_{\ell+1} = \arg \max_{\xi \in \Xi} \Delta_{\text{pr}}^N \quad \Xi^{\ell+1} \leftarrow \Xi^\ell \cup \{\xi_{\ell+1}\}$$

$$N_{\text{pr}} \leftarrow N_{\text{pr}} + \delta N_{\text{pr}} \quad \ell \leftarrow \ell + 1$$

end

Numerical tests



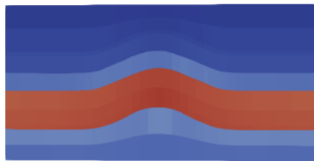
- Number of cells $\mathcal{N} = 15210$
- Yellow zone:
 $\kappa_1 \in [10^{-14} \text{ m}^2, 10^{-12} \text{ m}^2]$
- Blue zone: $\kappa_2 \in [10^{-17} \text{ m}^2, 10^{-15} \text{ m}^2]$
- $T = 200$ days, $\Delta t = 10$ days
- *Dirichlet* condition: $p_D = 10^5$ Pa
- Well pressure: $p_{bh} = 4.3 \times 10^7$ Pa

Pressure profile

$$\kappa_1 = 10^{-12}, \kappa_2 = 10^{-16}$$



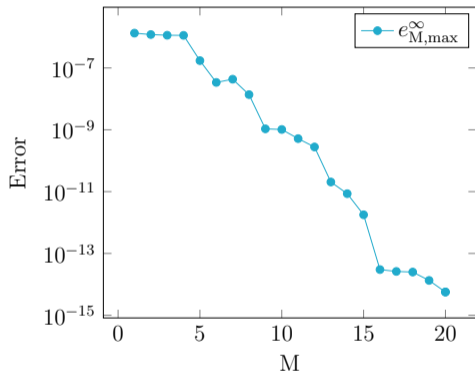
$$\kappa_1 = 10^{-13}, \kappa_2 = 10^{-16}$$



$$\kappa_1 = 10^{-13}, \kappa_2 = 3 \times 10^{-17}$$



Numerical tests: EIM



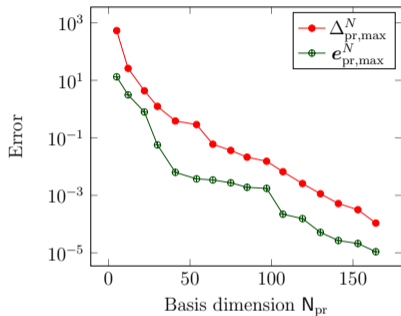
■ $\Xi_{\text{training}} \in \mathbb{R}^{2 \times 100}$

■ $e_{M,\max}^{\infty} = \max_{\xi \in \Xi_{\text{training}}} \frac{\|\hat{\mathbf{v}}(\xi) - \mathcal{I}_M[\hat{\mathbf{v}}(\xi)]\|_{L^\infty}}{\|\hat{\mathbf{v}}(\xi)\|_{L^\infty}}$

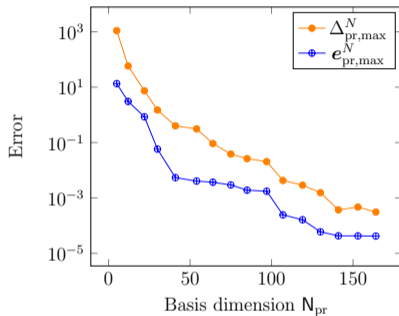
■ $\hat{\mathbf{v}} = ((\alpha_{K,\sigma\sigma'})_{K \in \mathcal{T}, \sigma \in \mathcal{E}_K, \sigma' \in \mathcal{S}_{K,\sigma}}, (\alpha_{K,\sigma\sigma'} \omega_{M,\sigma'})_{K \in \mathcal{T}, M \in \mathcal{T}_{\sigma'}, \sigma \in \mathcal{E}_K, \sigma' \in \mathcal{S}_{K,\sigma}, \sigma' \in \mathcal{E}_{\text{int}}}, (\mathbf{WI})_{K \in \mathcal{T}})$

Numerical tests

Offline stage



Online stage



■ $\xi = \{\kappa_1, \kappa_2\}, \Xi_{\text{training}} \in \mathbb{R}^{2 \times 100}, \Xi_{\text{test}} \in \mathbb{R}^{2 \times 100}$

■ $e_{pr,max}^N = \max_{\xi} \|\| e^N \|\|_{pr}$

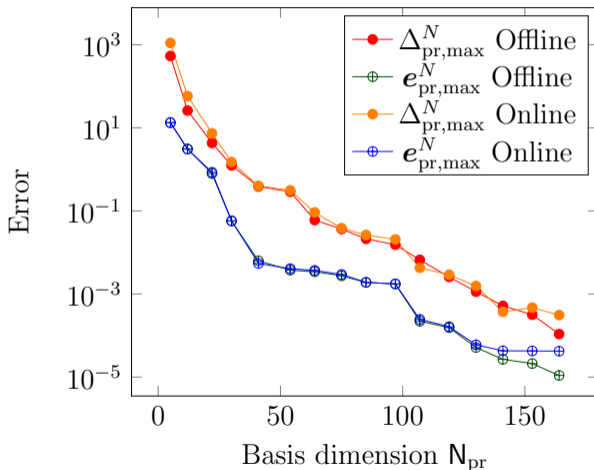
■ $\Delta_{pr,max}^N = \max_{\xi} \Delta_{pr}^N$

■ $\eta_{pr,max}^N = \max_{\xi} \frac{\Delta_{pr}^N}{\|\| e^N \|\|_{pr}}$

$\Rightarrow N_{pr} = 164, E_{pr,max}^N = 7 \cdot 10^{-10}$

$\Rightarrow \eta_{pr,max}^N \approx 10^3$

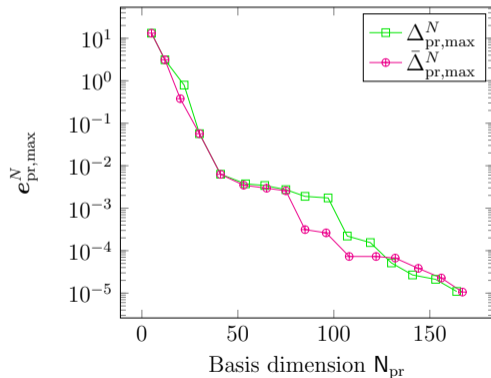
Numerical tests



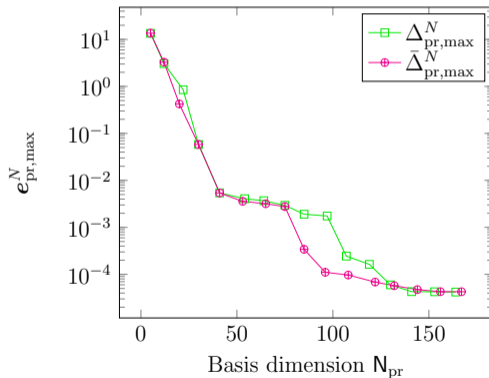
Numerical tests

■ $\bar{\Delta}_{\text{pr,max}} = \max_{\xi} \left(\frac{\Delta t}{\alpha_{A_{\text{sym, LB}}}} \sum_{n=1}^N \|\mathbf{r}^n\|_{-1}^2 \right)^{1/2}$ (M. A. Grepl and A. T. Patera, 2005)

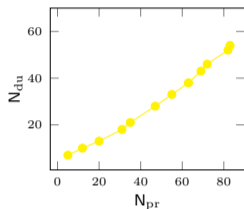
Offline stage



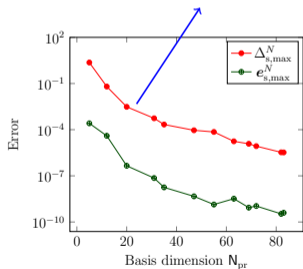
Online stage



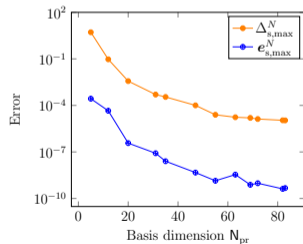
Numerical tests



- $e_s^N = |s^N - s^{N_s, N}|$
- $e_{s, \max}^N = \max_{\xi} |s^N - s^{N_s, N}|$
- $\Delta_{s, \max}^N = \max_{\xi} \Delta_s^N$
- $\eta_{s, \max}^N = \max_{\xi} \frac{\Delta_s^N}{e_s^N}$



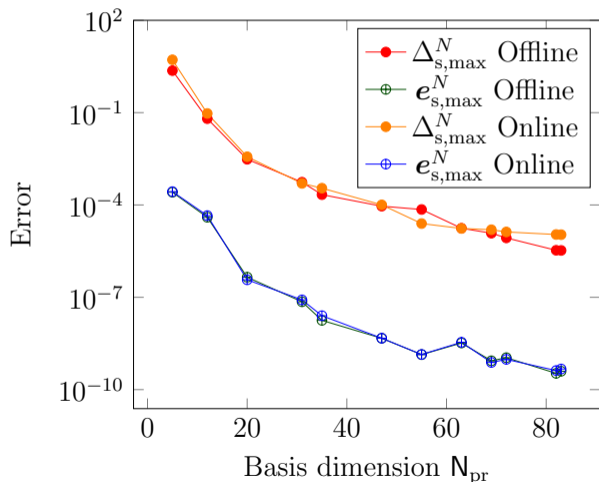
(a) Offline phase



(b) Online phase

Effectivities $\eta_{s, \max}^N \approx 10^6$

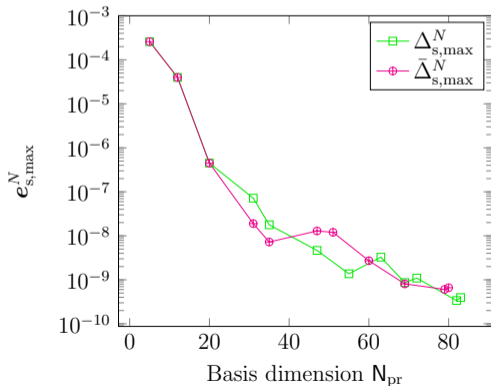
Numerical tests



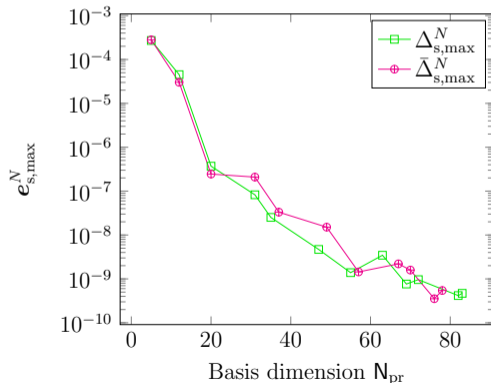
Numerical tests

- $\bar{\Delta}_{s,\max} = \left(\sum_{n=1}^N \frac{\Delta t}{\alpha_{\mathbf{A}_{\text{sym, LB}}}} \|\mathbf{r}^n\|_{-1}^2 \sum_{n=1}^N \frac{\Delta t}{\alpha_{\mathbf{A}_{\text{sym, LB}}}} \|\mathbf{q}^n\|_{-1}^2 \right)^{1/2}$ (M. A. Grepl and A. T. Patera, 2005)

Offline stage



Online stage



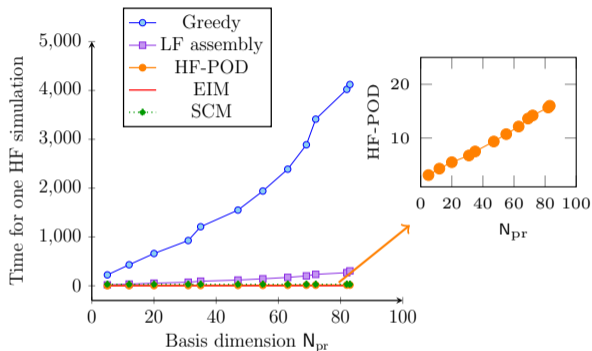
Numerical tests

Offline stage

- Time computation of "Greedy" increases with respect to N_{pr}
- Time computation of "POD" linear with respect to N_{pr}

Online stage

- Time computation reduced by a factor of $\frac{20 \text{ s}}{1.17 \text{ s}} = 17$



Outline

- 1 Introduction
- 2 Application of RB methods to single-phase flow problems
- 3 Conclusion and perspectives

RB for SPF problem

- A space-time energy norm independent of the parameters
- A posteriori estimation for *linear* QOIs
- Submitted paper: Reduced Basis method for finite volume simulations of parabolic PDEs applied to porous media flows

SPF problem

- Modify the definition of the estimator for better efficiency ?
- Estimate different types of QOIs
- Consider a time-varying source term

Thank you for your attention!

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