Model Reduction Methods

Linear Affine Parabolic Problems

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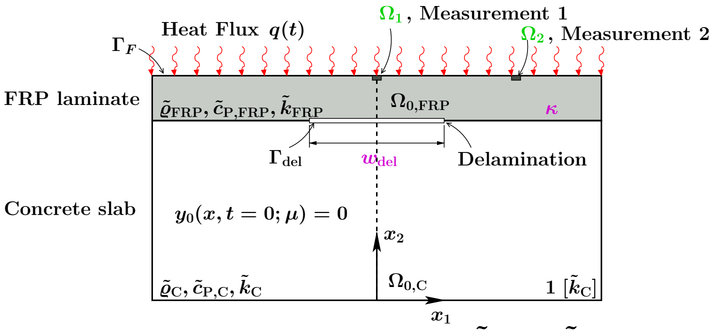
Concrete Delamination [HJN], [S]



Input (parameter): $\mu \equiv (w_{\mathrm{del}}/2, \kappa \equiv \tilde{k}_{\mathrm{FRP}}/\tilde{k}_{\mathrm{C}})$

Output of interest: $s_i(t;\mu) = \int_{\Omega_i} y_0(x,t;\mu), \; i = 1, 2$

Concrete Delamination – Problem Statement

Given $(\mu_1, \mu_2) \in \mathcal{D} \equiv [1, 10] \times [0.4, 1.8]$, evaluate the outputs,

for $k = 1, \ldots, 200$, $(\Delta t = 0.05, t^k \in (0, 10])$,

$$\mathrm{S}_i(t^k; \mu) = \frac{1}{|\Omega_i|} \int_{\Omega_i} y_0(t^k; \mu), \; i = 1, 2$$

$$\mathrm{TS}(t^k; \mu) = \mathrm{S}_1(t^k; \mu) - \mathrm{S}_2(t^k; \mu) ,$$

where $y_0(t^k; \mu) \in X_0(\Omega_0(\mu_1))$ satisfies†

† Here, $X_0 \equiv \{v \in H^1(\Omega_0(\mu_1)) |\; v|_{\Gamma_{\text{bottom}}} = 0\}$; $y_0(t^0; \mu) = 0$.

Concrete Delamination – Problem Statement

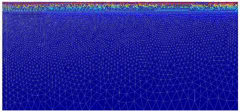
$$\frac{1}{\Delta t}\int_{\Omega_0(\mu_1)} \left(y_0(t^k;\mu) - y_0(t^{k-1};\mu)\right) v_0 + \mu_2 \int_{\Omega_{0,\mathrm{FRP}}(\mu_1)} \nabla y_0(t^k;\mu)\cdot\nabla v_0 + \int_{\Omega_{0,\mathrm{C}}(\mu_1)} \nabla y_0(t^k;\mu)\cdot\nabla v_0 = u(t^k)\int_{\Gamma_\mathrm{F}} v_0 \ , \quad \forall v_0 \in X_0,$$

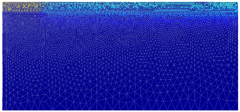
where $u(t^k)$ is specified "in the field."

Concrete Delamination – Results

Temperature distribution: $\boldsymbol{w_{\text{del}}/2 = 5}$, $\boldsymbol{\kappa = 1}$

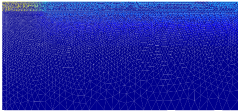
$\boldsymbol{k = 10}$

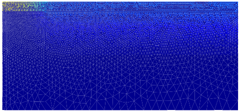




$\boldsymbol{k = 20}$

$\boldsymbol{k = 40}$



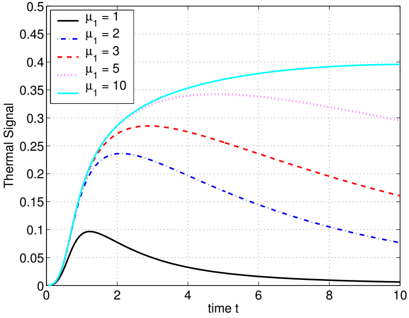


$\boldsymbol{k = 60}$

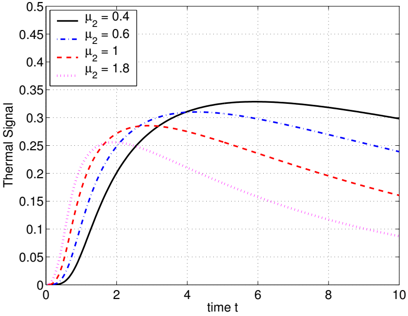
Concrete Delamination – Results

Thermal signal $\mathbf{TS}^{\mathrm{e}}(t^k; \mu)$

$\kappa = 1$



$w_{\mathrm{del}}/2 = 3$



Concrete Delamination – Parameter Estimation

In the "field," can we deduce

- the delamination width, w_{del}, and
- uncertainty with respect to κ,

from noisy measurements of

- the averaged surface temperatures?

Contexts: Real-time & Many Query

$\Rightarrow$ Premium: Marginal & Asymptotic Average Cost.

MATLAB DEMO

Reduced Basis Methods for Time-dependent Problems

New ingredients/challenges:

- Simultaneous dependence on both time and parameters.
  - "Time" as an additional (albeit special) parameter.
- Output, $s = s(t; \mu)$, is a function of time (and parameter).
  - Important for applications, e.g., control.
  - *A posteriori* error bounds (no "compliance" $\Rightarrow$ dual problem).
- Sampling procedure.
  - Greedy algorithm for parameter-time case.
  - Unknown "control" input.
- Dimension N of RB space.
  - Advection-dominated problems.

Problem Statement

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\quad t \in (0, t_f]$

$$s^{\mathrm{e}}(t;\mu) = \ell(u^{\mathrm{e}}(x;t;\mu);\mu)$$

where $u^{\mathrm{e}}(x;t;\mu) \in L^2(0, t_f; X^{\mathrm{e}}(\Omega))$ satisfies $\quad u_0 = 0$

$$m\left(\frac{\partial u^{\mathrm{e}}}{\partial t}(x;t;\mu), v;\mu\right) + a(u^{\mathrm{e}}(x;t;\mu), v;\mu) = f(v;\mu)\, g(t), \quad \forall\, v \in X^{\mathrm{e}}.$$

Note: For now, we assume $u_0 = 0$ – extension to nonzero initial conditions are briefly discussed below.

Definitions

μ: input parameter - $\mu = (\mu_1, \mu_2, \ldots, \mu_P)$; P-tuple

$\mathcal{D}$: parameter domain in $\mathbb{R}^P$;

Ω: spatial domain in $\mathbb{R}^d$;

s^e: output;

ℓ: output functional;

u^e: field variable;

X^e: function space $(H_0^1(\Omega))^\nu \subset X^e \subset (H^1(\Omega))^\nu$ †,
with inner product $(w, v)_{X^e}, \quad \forall w, v \in X^e$,
and induced norm $\|w\|_{X^e} = \sqrt{(w, w)_{X^e}}, \quad \forall w \in X^e$.

† For simplicity we assume $\nu = 1$.

Reference Geometry

Note Ω is parameter-independent:

- the reduced basis requires a common spatial configuration, i.e., a reference domain Ω_{ref}
- Introduce a piecewise affine mapping $\mathcal{T}(\cdot;\mu) : \Omega \to \Omega_o(\mu)$

$$a_o(w_o, v_o; \mu) \text{ over } \Omega_o(\mu)$$
$$\Downarrow$$
$$\mathcal{T}(\cdot;\mu)^{-1} : \Omega_o(\mu) \to \Omega_{\text{ref}} \equiv \Omega \qquad (\Omega_{\text{ref}} = \Omega_o(\mu_{\text{ref}}))$$
$$\Downarrow$$
$$a(w, v; \mu) \text{ over } \Omega$$

where $a(w, v; \mu) = a_o(w_o \circ \mathcal{T}_\mu, v_o \circ \mathcal{T}_\mu; \mu)$

We henceforth assume that the problem is already mapped to the reference domain.

Hypotheses

Linear forms and functions

$f(\cdot;\mu)$: linear, affine in μ,
X^{e}-bounded, $\forall \mu \in \mathcal{D}$

$g(\cdot)$: $L^2(0, t_f)$ "control" input

$\ell(\cdot;\mu)$: linear, affine in μ,
$L^2(\Omega)$-bounded, $\forall \mu \in \mathcal{D}$

Hypotheses

$$a(\cdot,\cdot;\mu): \quad \begin{array}{l} \text{bilinear, affine in } \mu, \\ \text{symmetric,} \\ X^e\text{-continuous,} \\ X^e\text{-coercive form,} \qquad \forall \mu \in \mathcal{D}; \end{array}$$

$$m(\cdot,\cdot;\mu): \quad \begin{array}{l} \text{bilinear, affine in } \mu, \\ \text{symmetric,} \\ L^2(\Omega)\text{-continuous,} \\ L^2(\Omega)\text{-coercive form,} \qquad \forall \mu \in \mathcal{D}; \end{array}$$

Extensions to non-symmetric, non-affine, non-linear are possible . . .
. . . and are partly discussed later on.

Hypotheses

$a(\cdot,\cdot;\mu)$: bilinear, affine in μ,
symmetric,
X^{e}-continuous,
X^{e}-coercive form, $\forall \mu \in \mathcal{D}$;

$m(\cdot,\cdot;\mu)$: bilinear, affine in μ,
symmetric,
$L^2(\Omega)$-continuous,
$L^2(\Omega)$-coercive form, $\forall \mu \in \mathcal{D}$;

Extensions to non-symmetric, non-affine, non-linear are possible . . .
. . . and are partly discussed later on.

Affine parameter dependence

Require also $\ell(v;\mu)$, $f(v;\mu)$

$$a(w,v;\mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, a^q(w,v),$$

$$m(w,v;\mu) = \sum_{q=1}^{Q_m} \Theta_m^q(\mu)\, m^q(w,v);$$

where

$\Theta_{a,m}^q : \mathcal{D} \to \mathbb{R}$, μ-dependent functions;
representing coefficients, geometry, . . .

a^q and m^q μ-independent forms.

Note: affine assumption may be relaxed [BMNP,GMNP].

Truth Approximation

- Spatial Discretization: Finite Element

$$X^{\mathcal{N}} \subset X \text{ with } \dim(X^{\mathcal{N}}) = \mathcal{N}$$

  for given $\mathcal{N}$ ($\mathcal{N} \to \infty$).

  We may also consider Finite Volume [HO]

- Temporal Discretization: Finite Difference

$$t^k = k\,\Delta t, \ \forall k \in \mathbb{K} \equiv \{(0), 1, 2, \ldots, K\}$$

  for given $\Delta t = t_f/K$ (fixed).

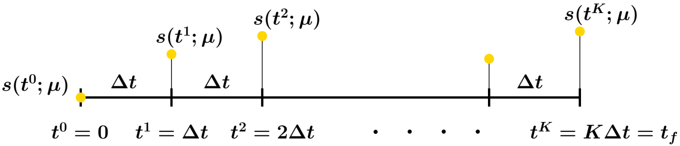
  We may also consider DG [RMM]

Truth Approximation

- Temporal Discretization: Finite Difference

$$\frac{\partial u}{\partial t}(t^k;\mu) \approx \frac{u(t^k;\mu) - u(t^{k-1};\mu)}{\Delta t}$$

  - Euler Backward
  - Crank-Nicolson (advection-dominated problems)



Problem Statement

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\quad \forall k \in \mathbb{K}$

$$s^k(\mu) \equiv s(t^k;\mu) = \ell(u(t^k;\mu);\mu)$$

where $u^k(\mu) \equiv u(t^k;\mu) \in X$ satisfies $\quad u_0 = 0$

$$m\left(\frac{u(t^k;\mu) - u(t^{k-1};\mu)}{\Delta t}, v;\mu\right) + a(u(t^k;\mu), v;\mu) = f(v;\mu)\, g(t^k), \quad \forall\, v \in X.$$

Note: We directly drop the superscript $\mathcal{N}$, i.e., $X = X^{\mathcal{N}}$, $u(t^k;\mu) = u^{\mathcal{N}}(t^k;\mu)$, $s(t^k;\mu) = s^{\mathcal{N}}(t^k;\mu)$.

Role

We shall

(*i*) *build* our reduced basis approximation upon "truth" solutions $\boldsymbol{u}(\boldsymbol{t}^{\boldsymbol{k}}; \boldsymbol{\mu}) \in \boldsymbol{X}$;

(*ii*) *measure* the error in the reduced basis approximation relative to the "truth" solution $\boldsymbol{u}(\boldsymbol{t}^{\boldsymbol{k}}; \boldsymbol{\mu}) \in \boldsymbol{X}$ (and $\boldsymbol{s}(\boldsymbol{t}^{\boldsymbol{k}}; \boldsymbol{\mu})$);

$\Rightarrow \boldsymbol{u}(\boldsymbol{t}^{\boldsymbol{k}}; \boldsymbol{\mu})$ is a *calculable surrogate* for $\boldsymbol{u}^{\mathrm{e}}(\boldsymbol{t}; \boldsymbol{\mu})$.

Parametric Manifold $\mathcal{M}^{\mathcal{N}K}$

We assume

- the form a is continuous and coercive (or inf-sup stable); and
- the form m is continuous and coercive; and
- the $\Theta^q_{m,a}(\mu)$, $1 \leq q \leq Q_{m,a}$, are smooth;

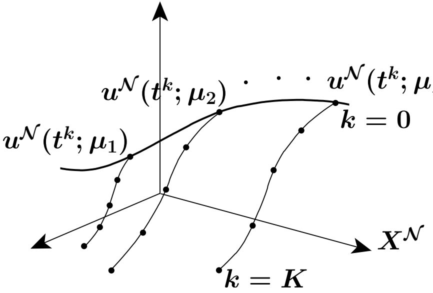
then

$$\mathcal{M}^{\mathcal{N}K} \equiv \{u(t^k;\mu) \,|\, 1 \leq k \leq K, \ \forall \mu \in \mathcal{D}\}$$

lies on a smooth $P+1$-dimensional manifold in X.

Parametric Manifold $\mathcal{M}^{\mathcal{N}K}$

To approximate $u(t^k;\mu)$, and hence $s(t^k;\mu)$,
we need not represent every possible function in $X^{\mathcal{N}}$.



$$X_N \subset \mathrm{span}\{u(t^k;\mu^m),\ 1\le k\le K,\ 1\le m\le M\};$$

Parametric Manifold $\mathcal{M}^{\mathcal{N}K}$

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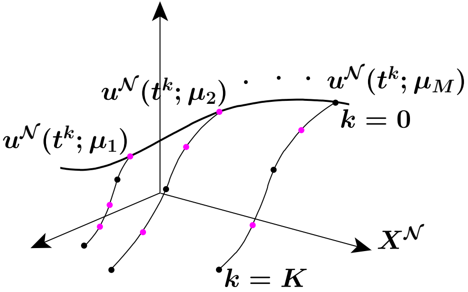

LOCALIZATION

Parametric Manifold $\mathcal{M}^{\mathcal{N}K}$

To approximate $u(t^k;\mu)$, and hence $s(t^k;\mu)$,
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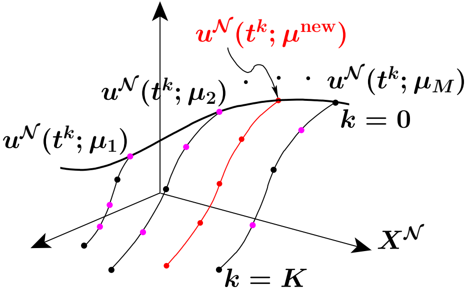

SMOOTHNESS

Reduced Basis Space

We define the Lagrangian RB space

$$X_N = \mathrm{span}\{\zeta^n,\ 1 \le n \le N\}, \quad 1 \le N \le N_{\max},$$

with mutually $(\cdot,\cdot)_X$-orthonormal basis functions

$$\zeta^n \in X, \quad 1 \le n \le N_{\max}.$$

We thus obtain

$$X_N \subset X, \quad \dim(X_N) = N, \quad 1 \le N \le N_{\max},$$

and hierarchical spaces

$$X_1 \subset X_2 \subset \ldots \subset X_{N_{\max}-1} \subset X_{N_{\max}} (\subset X).$$

The basis functions are constructed using a POD-Greedy algorithm outlined below.

Galerkin Projection

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\qquad \forall k \in \mathbb{K}$

$$s_N^k(\mu) \equiv s_N(t^k;\mu) = \ell(u_N(t^k;\mu);\mu)$$

where $u_N^k(\mu) \equiv u_N(t^k;\mu) \in X_N$ satisfies $\qquad u_{N,0} = 0$

$$m\left(\frac{u_N(t^k;\mu) - u_N(t^{k-1};\mu)}{\Delta t}, v;\mu\right) + a(u_N(t^k;\mu), v;\mu) = f(v;\mu)\,g(t^k), \quad \forall\, v \in X_N.$$

$\Rightarrow$ reduced basis inherits the fixed truth temporal discretization.

Field Variable

We expand $$u_N^k(\mu) = \sum_{j=1}^{N} u_{N\,j}^k(\mu)\zeta^j$$

and obtain $$v = \zeta^i,\ 1 \le i \le N$$

$$a(u_N^k(\mu), v; \mu) + \frac{1}{\Delta t} m(u_N^k(\mu), v; \mu) = \dots$$

$$\sum_{j=1}^{N} \left[a(\zeta^j, \zeta^i; \mu) + \frac{1}{\Delta t} m(\zeta^j, \zeta^i; \mu) \right] u_{N\,j}^k(\mu) = \dots$$

$$\sum_{j=1}^{N} \Bigg[\underbrace{\sum_{q=1}^{Q_a} \Theta_a^q(\mu) \underbrace{a^q(\zeta^j, \zeta^i)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_a N^2)} + \frac{1}{\Delta t} \underbrace{\sum_{q=1}^{Q_m} \Theta_m^q(\mu) \underbrace{m^q(\zeta^j, \zeta^i)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_m N^2)} \Bigg] u_{N\,j}^k(\mu) = \dots$$

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Field Variable

and $v = \zeta^i,\ 1 \le i \le N$

$$\ldots = \frac{1}{\Delta t} m(u_N^{k-1}(\mu), v; \mu) + f(v;\mu)\, g(t^k)$$

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$\Rightarrow$ solve for $u_{N\,j}^k(\mu),\ 1 \le j \le N,\ 1 \le k \le K.$

$$O(N^3 + KN^2)$$

Field Variable

and $\qquad v = \zeta^i, \; 1 \le i \le N$

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$\Rightarrow$ solve for $u_{N\,j}^k(\mu),\ 1 \le j \le N,\ 1 \le k \le K.$

$$O(N^3 + K N^2)$$

Output Evaluation

Given $u^k_{N\,j}(\mu)$, $1 \le j \le N$, evaluate the output from $\quad \forall k \in \mathbb{K}$

$$s^k_N(\mu) = \ell(u^k_N(\mu);\mu) = \sum_{j=1}^{N} u^k_{N\,j}(\mu)\ell(\zeta^j;\mu)$$

$$= \underbrace{\sum_{j=1}^{N} u^k_{N\,j}(\mu) \underbrace{\sum_{q=1}^{Q_\ell} \Theta^q_\ell(\mu) \underbrace{\ell^q(\zeta^j)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_\ell N)}}_{\text{ONLINE: } O(N)}$$

$\Rightarrow$ solve for $s^k_N(\mu)$, $1 \le k \le K$, in $O(KN)$.

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OFFLINE: $O(\mathcal{N})$

ONLINE: $O(Q_\ell N)$

ONLINE: $O(N)$

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$\Rightarrow$ solve for $s^k_N(\mu)$, $1 \le k \le K$, in $O(KN)$.

Output Evaluation

Given $u^k_{N\,j}(\mu)$, $1 \leq j \leq N$, evaluate the output from $\quad \forall k \in \mathbb{K}$

$$s^k_N(\mu) = \ell(u^k_N(\mu);\mu) = \sum_{j=1}^{N} u^k_{N\,j}(\mu)\ell(\zeta^j;\mu)$$

$$= \underbrace{\sum_{j=1}^{N} u^k_{N\,j}(\mu) \underbrace{\sum_{q=1}^{Q_\ell} \Theta^q_\ell(\mu) \underbrace{\ell^q(\zeta^j)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_\ell N)}}_{\text{ONLINE: } O(N)}$$

$\Rightarrow$ solve for $s^k_N(\mu)$, $1 \leq k \leq K$, in $O(KN)$.

Computational Cost

Summary computational cost: $(Q = Q_a + Q_m)$

OFFLINE — once, parameter *independent*

$$\underbrace{O(K N_{\max} \mathcal{N}^{\bullet})}_{\text{solve for } \zeta_n} + \underbrace{O(Q N_{\max}^2 \mathcal{N})}_{\text{form } \mu\text{-independent quantities}} ;$$

ONLINE — many times, parameter *dependent* μ^{new}

$$\underbrace{O(Q N^2)}_{\text{form RB matrices}} + \underbrace{O(N^3 + K N^2)}_{\text{solve for } u_{Nj}^k(\mu)} + \underbrace{O(K N)}_{\text{evaluate output}} ;$$

Online cost is independent of $\mathcal{N}$.

Stiffness Matrix

Evaluation of RB Stiffness Matrix $\underline{A}_N \in \mathbb{R}^{N\times N}$:

Parameter-independent matrices $\underline{\mathbb{A}}_N^q \in \mathbb{R}^{N\times N}$, $1 \le q \le Q_a$:

$$\begin{aligned} \mathbb{A}^q_{N\,n\,m} &= a^q(\zeta^m, \zeta^n) \\ &= \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \zeta_i^m \, a^q(\varphi_i^{\mathcal{N}}, \varphi_j^{\mathcal{N}}) \, \zeta_j^n, \quad 1 \le n, m \le N, \end{aligned}$$

thus

$$\underline{\mathbb{A}}_N^q = \mathbb{Z}_N^T \, \underline{\mathbb{A}}^{\mathcal{N}q} \, \mathbb{Z}_N.$$

We finally assemble

$$\underline{A}_N = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) \, \underline{\mathbb{A}}_N^q.$$

Here, $\mathbb{Z}_N = [\zeta^1 \, \zeta^2 \ldots \zeta^N] \in \mathbb{R}^{\mathcal{N}\times N}$.

Mass Matrix

Evaluation of RB Mass Matrix $\underline{M}_N \in \mathbb{R}^{N \times N}$:

Parameter-independent matrices $\underline{\mathbb{M}}_N^q \in \mathbb{R}^{N \times N}$, $1 \le q \le Q_m$:

$$\begin{aligned} \mathbb{M}^q_{N\,nm} &= m^q(\zeta^m, \zeta^n) \\ &= \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \zeta_i^m \, m^q(\varphi_i^{\mathcal{N}}, \varphi_j^{\mathcal{N}}) \, \zeta_j^n, \quad 1 \le n, m \le N, \end{aligned}$$

thus

$$\underline{\mathbb{M}}_N^q = \mathbb{Z}_N^T \, \underline{\mathbb{M}}^{\mathcal{N} q} \, \mathbb{Z}_N.$$

We finally assemble

$$\underline{M}_N = \sum_{q=1}^{Q_m} \Theta_m^q(\mu) \, \underline{\mathbb{M}}_N^q.$$

Load/Source Vector

Evaluation of RB Load/Source Vector $\underline{F}_N \in \mathbb{R}^N$:

Parameter-independent vectors $\underline{\mathbb{F}}_N^q \in \mathbb{R}^N$, $1 \le q \le Q_f$:

$$\begin{aligned} \mathbb{F}^q_{N\,n} &= f^q(\zeta^n) \\ &= \sum_{i=1}^{\mathcal{N}} \zeta_i^m \, f^q(\varphi_i^{\mathcal{N}}), \quad 1 \le n \le N, \end{aligned}$$

thus

$$\underline{\mathbb{F}}_N^q = \mathbb{Z}_N^T \, \underline{\mathbb{F}}^{\mathcal{N}q}.$$

We finally assemble

$$\underline{F}_N = \sum_{q=1}^{Q_f} \Theta_f^q(\mu) \, \underline{\mathbb{F}}_N^q.$$

Output Vector

Evaluation of RB Output Vector $\underline{L}_N \in \mathbb{R}^N$:

Parameter-independent vectors $\underline{\mathbb{L}}_N^q \in \mathbb{R}^N$, $1 \le q \le Q_\ell$:

$$\begin{aligned} \mathbb{L}_{N\,n}^q &= \ell^q(\zeta^n) \\ &= \sum_{i=1}^{\mathcal{N}} \zeta_i^m \, \ell^q(\varphi_i^{\mathcal{N}}), \quad 1 \le n \le N, \end{aligned}$$

thus

$$\underline{\mathbb{L}}_N^q = \mathbb{Z}_N^T \, \underline{\mathbb{L}}^{\mathcal{N} q}.$$

We finally assemble

$$\underline{L}_N = \sum_{q=1}^{Q_\ell} \Theta_\ell^q(\mu) \, \underline{\mathbb{L}}_N^q.$$

Summary

Given $\mu \in \mathcal{D}$, evaluate $\qquad \forall k \in \mathbb{K}$

$$s_N^k(\mu) = \underline{L}_N^T(\mu)\,\underline{u}_N^k(\mu)$$

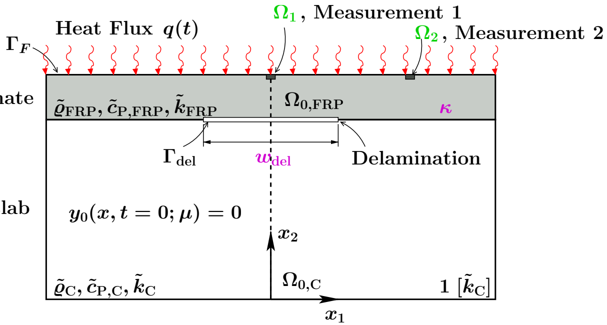
where $\underline{u}_N^k(\mu) \in \mathbb{R}^N$ satisfies $\qquad u_{N,0}(\mu) = 0$

$$\left(\underline{A}_N(\mu) + \frac{1}{\Delta t}\underline{M}_N(\mu)\right)\underline{u}_N^k(\mu) = \frac{1}{\Delta t}\underline{M}_N(\mu)\underline{u}_N^{k-1}(\mu) + \underline{F}_N(\mu)\,g(t^k).$$

- LU-decomposition: $\underline{A}_N(\mu) + \frac{1}{\Delta t}\underline{M}_N(\mu)$
- Forward/Back Substitution: $\underline{u}_N^k(\mu),\ \forall k \in \mathbb{K}$

Arrays for $N \le N_{\max}$ are principal subarrays of arrays for $N = N_{\max}$.

Example: Concrete Delamination – Results



Input (parameter): $\mu \equiv (w_{\rm del}/2, \kappa \equiv \tilde{k}_{\rm FRP}/\tilde{k}_{\rm C}) \subset \mathcal{D}$,

where $\mathcal{D} \equiv [1, 10] \times [0.4, 1.8]$.

"Truth": $\mathcal{N} = 5601$, $K = 200$.

Example: Concrete Delamination – Results

N	$\epsilon^u_{\mathrm{max,rel}}$	$\epsilon^s_{\mathrm{max,rel}}$
20	8.09 E−02	6.76 E−01
40	2.71 E−02	1.44 E−02
60	1.02 E−02	3.34 E−03
80	5.02 E−03	1.43 E−03
120	7.40 E−04	9.81 E−05
160	2.13 E−04	2.34 E−05
200	9.55 E−05	6.02 E−06

- Maximum relative error:
$$\epsilon^u_{\mathrm{max,rel}} = \max_{\mu \in \Xi_{\mathrm{test}}} \frac{|||e^K|||_\mu}{|||u^K(\mu)|||}, \quad \mu_u = \arg \max_{\mu \in \Xi_{\mathrm{test}}} |||u^K(\mu)|||$$
- Maximum relative output error:
$$\epsilon^s_{\mathrm{max,rel}} = \max_{\mu \in \Xi_{\mathrm{test}}} \max_{k \in \mathbb{K}} \frac{|s^k(\mu) - s^k_N(\mu)|}{s_{\mathrm{max}}}, \quad s_{\mathrm{max}} = \max_{\mu \in \Xi_{\mathrm{test}}} \max_{k \in \mathbb{K}} |s^k(\mu)|$$

How do we choose N?

Example: Concrete Delamination – Results

N	$\epsilon^u_{\max,\mathrm{rel}}$	$\epsilon^s_{\max,\mathrm{rel}}$
20	8.09 E−02	6.76 E−01
40	2.71 E−02	1.44 E−02
60	1.02 E−02	3.34 E−03
80	5.02 E−03	1.43 E−03
120	7.40 E−04	9.81 E−05
160	2.13 E−04	2.34 E−05
200	9.55 E−05	6.02 E−06

- Maximum relative error:

$$\epsilon^u_{\max,\mathrm{rel}} = \max_{\mu\in\Xi_{\mathrm{test}}} \frac{|||e^K|||_\mu}{|||u^K(\mu)|||}, \quad \mu_u = \arg\max_{\mu\in\Xi_{\mathrm{test}}} |||u^K(\mu)|||$$

- Maximum relative output error:

$$\epsilon^s_{\max,\mathrm{rel}} = \max_{\mu\in\Xi_{\mathrm{test}}} \max_{k\in\mathbb{K}} \frac{|s^k(\mu)-s^k_N(\mu)|}{s_{\max}}, \quad s_{\max} = \max_{\mu\in\Xi_{\mathrm{test}}} \max_{k\in\mathbb{K}} |s^k(\mu)|$$

How do we choose N?

Motivation

How do we know that $u_N^k(\mu)$, $s_N^k(\mu)$ are accurate? ONLINE

$$|||u^k(\mu) - u_N^k(\mu)|||_\mu \le \epsilon_{\mathrm{tol,min}}, \quad \forall k \in \mathbb{K}, \ \forall \mu \in \mathcal{D}$$

$$|s^k(\mu) - s_N^k(\mu)| \le \epsilon^s_{\mathrm{tol,min}}, \quad \forall k \in \mathbb{K}, \ \forall \mu \in \mathcal{D}$$

How do we know what value of N to take? ONLINE/OFFLINE

N too large $\Rightarrow$ computational inefficiency
N too small $\Rightarrow$ unacceptable uncertainty

How do we choose the sample S_N optimally? OFFLINE

RB space has to approximate manifold $\mathcal{M}$ well, but
RB matrices need to be "well-conditioned."

Requirements

Our *a posteriori* error bounds, $\Delta_N^k(\mu)$ and $\Delta_N^{s\,k}(\mu)$, must be

- rigorous $\qquad 1 \le N \le N_{\max}$

$$\begin{aligned} |||u^k(\mu) - u_N^k(\mu)||| &\le \Delta_N(\mu), \quad \forall k \in \mathbb{K},\ \forall \mu \in \mathcal{D}, \\ |s^k(\mu) - s_N^k(\mu)| &\le \Delta_N^s(\mu), \quad \forall k \in \mathbb{K},\ \forall \mu \in \mathcal{D}. \end{aligned}$$

- reasonably sharp

$$\frac{\Delta_N^k(\mu)}{|||u^k(\mu) - u_N^k(\mu)|||} \le C, \quad \frac{\Delta_N^{s\,k}(\mu)}{|s^k(\mu) - s_N^k(\mu)|} \le C,$$

where $C \approx 1$.

- efficient

$\Rightarrow$ Online cost depends on N, Q, and K, but not on $\mathcal{N}$.

Inner Products and Norms

- X-inner product and induced norm (parameter-independent)

$$(w, v)_X \equiv a(w, v; \bar{\mu}), \quad \forall w, v \in X$$

$$\|w\|_X \equiv \sqrt{(w, w)_X}, \quad \forall w \in X$$

- L^2-inner product and induced norm (parameter-independent)

$$(w, v) \equiv m(w, v; \bar{\mu}), \quad \forall w, v \in X$$

$$\|w\| \equiv \sqrt{(w, w)}, \quad \forall w \in X$$

Inner Products and Norms

- "Spatio-temporal" energy norm (parameter-dependent)

$$
\begin{aligned}
(((w^k, v^k))) &= m(w^k, v^k; \mu) \\
&\qquad + \sum_{k'=1}^{k} \Delta t \, a(w^{k'}, v^{k'}; \mu), \\
|||w^k||| &= \Big(m(w^k, w^k; \mu) \\
&\qquad + \sum_{k'=1}^{k} \Delta t \, a(w^{k'}, w^{k'}; \mu) \Big)^{1/2}, \\
&\qquad\qquad 1 \le k \le K.
\end{aligned}
$$

Coercivity and Continuity constants

We also define

- Coercivity constants

$$\alpha(\mu) \equiv \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2}; \quad \sigma(\mu) \equiv \inf_{w \in X} \frac{m(w, w; \mu)}{\|w\|^2};$$

- Continuity constants

$$\gamma_a(\mu) \equiv \sup_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu)}{\|w\|_X \|v\|_X}.$$

$$\gamma_m(\mu) \equiv \sup_{w \in X} \sup_{v \in X} \frac{m(w, v; \mu)}{\|w\| \, \|v\|}.$$

Coercivity Lower Bound

We require a positive lower bound for the coercivity constant

- $\alpha_{\mathrm{LB}} : \mathcal{D} \to \mathbb{R}$
$$0 < \alpha_{\mathrm{LB}}(\mu) \le \alpha(\mu), \quad \forall \mu \in \mathcal{D}.$$
- $\sigma_{\mathrm{LB}} : \mathcal{D} \to \mathbb{R}$
$$0 < \sigma_{\mathrm{LB}}(\mu) \le \sigma(\mu), \quad \forall \mu \in \mathcal{D}.$$

This bound can be calculated using the

- "$\min \Theta$" Approach (if a is parametrically coercive), or
- Successive Constraint Method [HRSP]

exactly as in elliptic case.

Dual Norm of Residual

We define the residual, $\forall k \in \mathbb{K}$,

$$r^k(v;\mu) \equiv f(v;\mu)\,g(t^k) - m\left(\frac{u_N(t^k;\mu) - u_N(t^{k-1};\mu)}{\Delta t}, v; \mu\right) - a(u_N(t^k;\mu), v; \mu), \quad \forall\, v \in X$$

Dual Norm of Residual

Given $\mu \in \mathcal{D}$, the dual norm of $r^k(v;\mu)$ is defined as

$$\|r^k(\cdot;\mu)\|_{X'} \equiv \sup_{v \in X} \frac{r^k(v;\mu)}{\|v\|_X} = \|\hat{e}^k(\mu)\|_X,$$

where $\hat{e}^k(\mu) \in X$ satisfies

$$(\hat{e}^k(\mu), v)_X = r^k(v;\mu), \quad \forall v \in X.$$

Energy Error Bound

We define the error bound, $\Delta_N^k(\mu) = \Delta_N(t^k;\mu)$, $1 \le k \le K$, as

$$\Delta_N^k(\mu) = \alpha_{\mathrm{LB}}^{-1/2}(\mu) \left(\sum_{k'=1}^{k} \Delta t \, \|\hat{e}^{k'}(\mu)\|_X^2 \right)^{1/2} .$$

We can then prove

Proposition (Energy Error Bound)

For any $N = 1, \ldots, N_{\max}$, the error in the field variable, $e^k(\mu) = u^k(\mu) - u_N^k(\mu)$, is bounded by

$$|||e^k(\mu)||| \le \Delta_N^k(\mu), \quad \forall\, \mu \in \mathcal{D},\ \forall\, k \in \mathbb{K}.$$

Energy Error Bound

We define the error bound, $\Delta_N^k(\mu) = \Delta_N(t^k;\mu)$, $1 \le k \le K$, as

$$\Delta_N^k(\mu) = \alpha_{\mathrm{LB}}^{-1/2}(\mu) \left(\sum_{k'=1}^{k} \Delta t \, \|\hat{e}^{k'}(\mu)\|_X^2 \right)^{1/2} .$$

We can then prove

Proposition (Energy Error Bound)

For any $N = 1, \ldots, N_{\max}$, *the error in the field variable,* $e^k(\mu) = u^k(\mu) - u_N^k(\mu)$, *is bounded by*

$$|||e^k(\mu)||| \le \Delta_N^k(\mu), \quad \forall\, \mu \in \mathcal{D},\ \forall\, k \in \mathbb{K}.$$

Energy Error Bound

Proof.

Sketch: The error, $e^k(\mu) = u^k(\mu) - u_N^k(\mu)$, satisfies

$$m\left(\frac{e^k(\mu) - e^{k-1}(\mu)}{\Delta t}, v; \mu\right) + a(e^k(\mu), v; \mu) = r^k(v; \mu), \quad \forall\, v \in X,\ \forall\, k \in \mathbb{K}.$$

We now choose $v = e^k(\mu)$ and apply

- Cauchy-Schwarz to $m(e^{k-1}(\mu), e^k(\mu); \mu)$,
- the definition of the dual norm of the residual,
- Young's Inequality (twice): for $c \in \mathbb{R}$, $d \in \mathbb{R}$, $\rho \in \mathbb{R}_+$
$$2|c|\,|d| \le \frac{1}{\rho^2}c^2 + \rho^2 d^2$$
- and finally sum from $k' = 1$ to k.

□

Simple Output Error Bound

We define the output error bound, $\Delta_N^{s\,k}(\mu) = \Delta_N^{s}(t^k;\mu)$, $1 \le k \le K$, as

.

$$\Delta_N^{s\,k}(\mu) \equiv \sigma_{\mathrm{LB}}^{-1}(\mu) \left(\sup_{v \in X} \frac{\ell(v;\mu)}{\|v\|} \right) \Delta_N^{k}(\mu)$$

Proposition (Simple Output Error Bound)

For any $N = 1, \ldots, N_{\max}$, the error in the output is bounded by

$$|s^k(\mu) - s_N^k(\mu)| \le \Delta_N^{s\,k}(\mu), \quad \forall \mu \in \mathcal{D},\ \forall k \in \mathbb{K}.$$

Simple Output Error Bound

We define the output error bound, $\Delta_N^{s\,k}(\mu) = \Delta_N^s(t^k;\mu)$, $1 \leq k \leq K$, as

.

$$\Delta_N^{s\,k}(\mu) \equiv \sigma_{\rm LB}^{-1}(\mu) \left(\sup_{v \in X} \frac{\ell(v;\mu)}{\|v\|} \right) \Delta_N^k(\mu)$$

Proposition (Simple Output Error Bound)

For any $N = 1, \ldots, N_{\max}$, *the error in the output is bounded by*

$$|s^k(\mu) - s_N^k(\mu)| \leq \Delta_N^{s\,k}(\mu), \quad \forall \mu \in \mathcal{D},\ \forall k \in \mathbb{K}.$$

Error Bounds

Remarks:

- The error bounds are rigorous upper bounds for the reduced basis error for any $N = 1, \ldots, N_{\max}$, for all $\mu \in \mathcal{D}$, and for all $k \in \mathbb{K}$.
- Define: $s_N^{\pm}(t^k;\mu) = s_N(t^k;\mu) \pm \Delta^s(t^k;\mu)$, then
  $$\Rightarrow \; s_N^{-}(t^k;\mu) \leq s(t^k;\mu) \leq s_N^{+}(t^k;\mu)$$
- We may also consider other norms than $|||\cdot|||$, i.e., $L^2(\Omega)$ [HO].

Offline-Online Decomposition

Crucial ingredient: Dual norm of residual $\|\hat{e}^k(\mu)\|_X, \ \forall k \in \mathbb{K}$.

Computational procedure follows directly from the elliptic case with added complexity due to mass term and time dependence.

- Expand $u_N(\mu) = \sum_{j=1}^{N} u^k_{N\,j}(\mu)\, \zeta^j$
- Riesz representation:

$$(\hat{e}^k(\mu), v)_X = r^k(v; \mu)$$

- Affine decomposition
- Linear superposition

Offline-Online Decomposition

Summary of computational cost: $Q = Q_a + Q_m$

OFFLINE —

$$\underset{\text{solve Poisson problems}}{O(QN_{\max}\mathcal{N}^\bullet)} \quad + \quad \underset{\text{form } \mu\text{-independent inner products}}{O(Q^2N_{\max}^2\mathcal{N})} \quad ;$$

ONLINE —

$$\underset{\text{evaluate } \|\hat{e}^k(\mu)\|_X\text{-sum for } 1 \le k \le K}{O(KQ^2N^2)} \quad ;$$

Online cost is independent of $\mathcal{N}$.

Example: Concrete Delamination – Results

Convergence energy norm error and bound

N	$\epsilon^u_{\text{max,rel}}$	$\Delta^u_{\text{max,rel}}$	$\overline{\eta}^u$
20	8.09 E−02	3.18 E−01	2.74
40	2.71 E−02	8.01 E−02	2.77
60	1.02 E−02	2.01 E−02	2.58
80	5.02 E−03	8.40 E−03	2.83
120	7.40 E−04	1.71 E−03	2.45
160	2.13 E−04	4.84 E−04	2.21
200	9.55 E−05	2.70 E−04	2.20

- Maximum relative error bound:

$$\Delta^y_{\text{max,rel}} = \max_{\mu \in \Xi_{\text{test}}} \frac{\Delta^k_N(\mu)}{|||u^K(\mu)|||}, \qquad \mu_u = \arg \max_{\mu \in \Xi_{\text{test}}} |||u^K(\mu)|||$$

- Average effectivity:

$$\overline{\eta}^u = \frac{1}{n_{\text{train}} K} \sum_{\mu \in \Xi_{\text{test}}} \sum_{k \in \mathbb{K}} \frac{\Delta^k_N(\mu)}{|||e^k(\mu)|||}$$

Example: Concrete Delamination – Results

Convergence output error and bound

N	$\epsilon^s_{\max,\mathrm{rel}}$	$\Delta^s_{\max,\mathrm{rel}}$	$\overline{\eta}^s$
20	6.76 E−02	2.58 E+01	211
40	1.44 E−02	6.24 E+00	341
60	3.34 E−03	1.46 E+00	363
80	1.43 E−03	4.73 E−01	379
120	9.81 E−05	1.24 E−01	604
160	2.34 E−05	2.88 E−02	674
200	6.02 E−06	9.18 E−03	1117

- Maximum relative output bound:

$$\Delta^s_{\max,\mathrm{rel}} = \max_{\mu \in \Xi_{\mathrm{test}}} \frac{\Delta^{s\,K}_N(\mu)}{|s_{\max}|}$$

- Average output effectivity:

$$\overline{\eta}^s = \frac{1}{n_{\mathrm{train}}} \sum_{\mu \in \Xi_{\mathrm{test}}} \frac{\Delta^{s\,k_\eta(\mu)}_N(\mu)}{|s^{k_\eta(\mu)}(\mu) - s^{k_\eta(\mu)}_N(\mu)|}, \quad k_\eta(\mu) = \arg\max_{k \in \mathbb{K}} |s^k(\mu) - s^k_N(\mu)|$$

Motivation

The notion "compliance" does not exist in the parabolic context. Thus similar to the noncompliant elliptic problem, we consider a primal-dual formulation for the parabolic problem

Goal:

- Faster convergence of output error & bound.

$$\text{output error} = \text{primal error}(\boldsymbol{N}_{\mathbf{pr}}) \times \text{dual error}(\boldsymbol{N}_{\mathbf{du}})$$

- Improved effectivities for output error estimation.

Dual Problem

Introduce dual problem for output at time t':

Given $\mu \in \mathcal{D}$, the dual variable $\psi^{\mathrm{e}}(t;\mu)$, $0 < t \leq t'$, satisfies

$$m\left(v, \frac{\partial \psi^{\mathrm{e}}}{\partial t}(t;\mu);\mu\right) - a(v, \psi^{\mathrm{e}}(t;\mu);\mu) = 0, \quad \forall v \in X^{\mathrm{e}}$$

with final condition

$$m(v, \psi^{\mathrm{e}}(t';\mu);\mu) \equiv l(v;\mu), \quad \forall v \in X^{\mathrm{e}}.$$

Note that the dual problem evolves backward in time with final condition defined at the "time of interest."

Dual Problem – Truth Approximation

FD[t] – FE Galerkin[x] Truth Approximation:

- EB or CN: $\Delta t = t_f/K,\ t^k = k\,\Delta t,\ 0 \le k \le K$
- $\psi(t^k;\mu) = \psi^{\mathcal{N}}(t^k;\mu) \in X^{\mathcal{N}} \subset X^{\mathrm{e}}$, $\dim(X^{\mathcal{N}}) = \mathcal{N}$

$\Rightarrow$ inherited from primal problem.

Introduce truth dual problem for output at time $t^L,\ 1 \le L \le K$:

Given $\mu \in \mathcal{D}$, the dual variable $\psi^L(t^k;\mu),\ 1 \le k \le L$, satisfies

$$m\left(v, \frac{\psi^L(t^k;\mu) - \psi^L(t^{k+1};\mu)}{\Delta t};\mu\right) - a(v,\psi^L(t^k;\mu);\mu) = 0,\ \forall v \in X,$$

with final condition

$$m(v,\psi^L(t^L;\mu);\mu) \equiv l(v;\mu), \quad \forall v \in X.$$

Dual Problem – LTI Property

Invoking the LTI (linear time-invariance) property we can express the dual for the output at time t^L, $1 \le L \le K$, as

$$\psi^L(t^k;\mu) \equiv \Psi(t^{K-L+k};\mu),\ 1 \le k \le L,$$

where $\Psi(t^k;\mu),\ 1 \le k \le K$ evolves backward from the final time t^K.

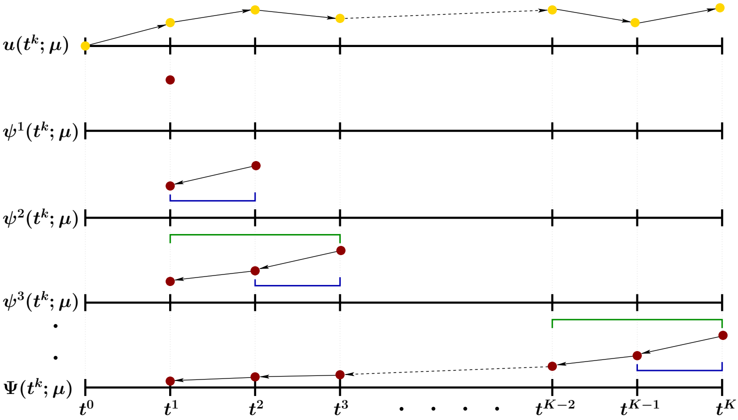
$\Rightarrow$ To obtain $\psi^L(t^k;\mu),\ 1 \le k \le L,\ 1 \le L \le K$, we

- solve once for $\Psi^k(t^k;\mu),\ 1 \le k \le K,$ and then
- appropriately shift the result

— we do not need to solve K dual problems.

Note: shifting property does not hold for LTV systems.

Dual Problem – LTI Property



Dual Problem – Truth Approximation

Given $\mu \in \mathcal{D}$, the dual variable $\Psi^k(\mu) = \Psi(t^k;\mu)$, $1 \le k \le K$, satisfies

$$m\left(v, \frac{\Psi(t^k;\mu) - \Psi(t^{k+1};\mu)}{\Delta t}; \mu\right) - a(v, \Psi(t^k;\mu);\mu) = 0, \quad \forall v \in X,$$

with final condition

$$m(v, \Psi(t^{K+1};\mu);\mu) \equiv l(v;\mu), \quad \forall v \in X.$$

- If either m or ℓ are parameter-dependent, we obtain an "elliptic subproblem" for the final condition.

Dual RB Space

Lagrangian RB space $\quad N_{\mathrm{du}} \neq N_{\mathrm{pr}}$ and $X^{\mathrm{du}}_{N_{\mathrm{du}}} \neq X^{\mathrm{pr}}_{N}$

$$X^{\mathrm{du}}_{N_{\mathrm{du}}} = \mathrm{span}\{\zeta^{\mathrm{du},n},\ 1 \le n \le N_{\mathrm{du}}\}, \quad 1 \le N_{\mathrm{du}} \le N_{\mathrm{du,max}},$$

with mutually $(\cdot,\cdot)_X$-orthonormal basis functions

$$\zeta^{\mathrm{du},n} \in X, \quad 1 \le n \le N_{\mathrm{du,max}}.$$

We thus obtain

$$X^{\mathrm{du}}_{N_{\mathrm{du}}} \subset X, \quad \dim(X^{\mathrm{du}}_{N_{\mathrm{du}}}) = N_{\mathrm{du}}, \quad 1 \le N_{\mathrm{du}} \le N_{\mathrm{du,max}},$$

and

$$X^{\mathrm{du}}_{1} \subset X^{\mathrm{du}}_{2} \subset \ldots \subset X^{\mathrm{du}}_{N_{\mathrm{du,max}}-1} \subset X^{\mathrm{du}}_{N_{\mathrm{du,max}}} (\subset X).$$

$\Rightarrow$ Constructed using POD(t)-Greedy(μ) algorithm.

Galerkin Projection – Dual

Given $\mu \in \mathcal{D}$, the dual variable $\Psi_N^k(\mu) \in X_{N_{\rm du}}^{\rm du}$, $1 \leq k \leq K$, satisfies

$$m\left(v, \frac{\Psi_N^k(\mu) - \Psi_N^{k+1}(\mu)}{\Delta t}; \mu\right) - a(v, \Psi_N^k(\mu); \mu) = 0, \quad \forall v \in X_{N_{\rm du}}^{\rm du},$$

with final condition

$$m(v, \Psi_N(t^{K+1}; \mu); \mu) \equiv l(v; \mu), \quad \forall v \in X_{N_{\rm du}}^{\rm du}.$$

$\Rightarrow$ RB inherits the fixed truth temporal discretization.

Galerkin Projection – Primal

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$ and $\Psi_N^k(\mu)$, evaluate $\quad \forall k \in \mathbb{K}$

$$s_N^k(\mu) = \ell(u_N^k(\mu);\mu) + \sum_{k'=1}^{k} r^{k'}(\Psi_N^{K-k+k'}(\mu);\mu)\Delta t$$

where $u_N^k(\mu) \in X_N^{(\mathrm{pr})}$ satisfies $\quad u_{N,0} = 0$

$$m\left(\frac{u_N(t^k;\mu) - u_N(t^{k-1};\mu)}{\Delta t}, v;\mu\right) + a(u_N(t^k;\mu), v;\mu) = f(v;\mu)\,g(t^k), \quad \forall\, v \in X_N^{(\mathrm{pr})}.$$

$\Rightarrow X_N = X_N^{\mathrm{pr}}$ and $r^k(v;\mu)$ is the primal residual.

Offline-Online Decomposition

- Similar to primal case
  - Exploit affine parameter dependence
- Evaluation of RB stiffness/mass matrix and RB output vector for dual problem similar to primal case (replace ζ by ζ^{du}).
- New ingredient: residual correction term

$$\sum_{k'=1}^{k} r^{k'}(\Psi_N^{K-k+k'}(\mu);\mu)\Delta t, \quad 1 \le k \le K,$$

where $r^k(v;\mu)$, $1 \le k \le K$, is given by

$$r^k(v;\mu) \equiv f(v;\mu)\,g(t^k) - m\left(\frac{u_N^k(\mu) - u_N^{k-1}(\mu)}{\Delta t}, v; \mu\right) - a(u_N^k(\mu), v; \mu), \quad \forall\, v \in X.$$

Algebraic Equations – Output Estimate

Evaluation of output with residual correction

$$s_N^k(\mu) = \underline{L}_N^T(\mu)\,\underline{u}_N^k(\mu) + \Delta t \sum_{k'=1}^{k} (\underline{\Psi}_N^{K-k+k'}(\mu))^T \Big(\underline{F}_N^{\mathrm{du}}(\mu)\, g(t^{k'}) - \underline{A}_N^{\mathrm{pr,du}}(\mu)\underline{u}_N^{k'}(\mu) - \frac{1}{\Delta t}\underline{M}_N^{\mathrm{pr,du}}(\mu)\big(\underline{u}_N^{k'}(\mu) - \underline{u}_N^{k'-1}(\mu)\big)\Big)$$

where $\underline{\Psi}_N^k(\mu) = [\Psi_{N\,1}^k(\mu) \ldots \Psi_{N\,N_{\mathrm{du}}}^k(\mu)] \in \mathbb{R}^{N_{\mathrm{du}}}$ is the solution of the dual problem.

Algebraic Equations – Example

Evaluation of RB Matrix $\underline{A}_N^{\text{pr,du}} \in \mathbb{R}^{N_{\text{pr}} \times N_{\text{du}}}$:

Parameter-independent matrices $\underline{\mathbb{A}}_N^{\text{pr,du},q} \in \mathbb{R}^{N_{\text{pr}} \times N_{\text{du}}}$, $1 \le q \le Q_a$:

$$\begin{aligned} \mathbb{A}^{\text{pr,du},q}_{N\,nm} &= a^q(\zeta^{\text{du},m}, \zeta^n) \\ &= \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \zeta_i^{\text{du},m}\, a^q(\varphi_i^{\mathcal{N}}, \varphi_j^{\mathcal{N}})\, \zeta_j^n, \quad \begin{aligned} &1 \le n \le N_{\text{pr}}, \\ &1 \le m \le N_{\text{du}}, \end{aligned} \end{aligned}$$

thus

$$\underline{\mathbb{A}}_N^{\text{pr,du},q} = (\mathbb{Z}_N^{\text{du}})^T\, \underline{\mathbb{A}}^{\mathcal{N}q}\, \mathbb{Z}_N.$$

We finally assemble

$$\underline{A}_N^{\text{pr,du}} = \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, \underline{\mathbb{A}}_N^{\text{pr,du},q}.$$

Here, $\mathbb{Z}_N^{\text{du}} = [\zeta^{\text{du},1}\, \zeta^{\text{du},2} \ldots \zeta^{\text{du},N_{\text{du}}}] \in \mathbb{R}^{\mathcal{N} \times N_{\text{du}}}$.

Offline-Online Decomposition

Summary computational cost: $(Q = Q_a + Q_m)$

OFFLINE — once, parameter *independent*

solve for ζ_n, ζ_n^{du}: $O(K(N_{\mathrm{pr,max}} + N_{\mathrm{du,max}})\mathcal{N}^{\bullet})$

μ-independ. quant.: $O(Q(N_{\mathrm{pr,max}}^2 + N_{\mathrm{du,max}}^2 + N_{\mathrm{pr,max}} N_{\mathrm{du,max}})\mathcal{N})$

ONLINE — many times, parameter *dependent*

form RB matrices: $O(Q(N_{\mathrm{pr}}^2 + N_{\mathrm{du}}^2 + N_{\mathrm{pr}} N_{\mathrm{du}}))$

solve for u_N^k, Ψ_N^k: $O(N_{\mathrm{pr}}^3 + N_{\mathrm{du}}^3 + K(N_{\mathrm{pr}}^2 + N_{\mathrm{du}}^2))$

evaluate output: $O(K(K+1)N_{\mathrm{pr}} N_{\mathrm{du}})$

Online cost is independent of $\mathcal{N}$.

Inner Products and Norms

- X-Norm and L^2-Norm already defined
- "Spatio-temporal" energy norm (parameter-dependent)

$$
\begin{aligned}
(((w^k, v^k)))^{\mathrm{du}} &= m(w^k, v^k; \mu) \\
&\quad + \sum_{k'=k}^{K} \Delta t \, a(w^{k'}, v^{k'}; \mu),
\end{aligned}
$$

$$
\begin{aligned}
|||w^k|||^{\mathrm{du}} &= \Big(m(w^k, w^k; \mu) \\
&\quad + \sum_{k'=k}^{K} \Delta t \, a(w^{k'}, w^{k'}; \mu) \Big)^{1/2}, \\
&\qquad 1 \le k \le K.
\end{aligned}
$$

Dual Final Condition

If m or ℓ are parameter-dependent, we define the residual

$$r^{\Psi_f}(v;\mu) \equiv \ell(v;\mu) - m(v, \Psi_N^{K+1};\mu), \quad \forall\, v \in X.$$

Lemma (Dual Error Bound – Final Condition)

Given $\mu \in \mathcal{D}$, the error $e^{\mathrm{du}}(t^{K+1};\mu) = \Psi^{K+1}(\mu) - \Psi_N^{K+1}(\mu)$ is bounded by

$$\|e^{\mathrm{du}}(t^{K+1};\mu)\| \le \Delta_N^{\Psi_f}(\mu) \equiv \frac{\varepsilon_N^{\Psi_f}(\mu)}{\sigma_{\mathrm{LB}}(\mu)}$$

where

$$\varepsilon_N^{\Psi_f}(\mu) \equiv \sup_{v \in X} \frac{r^{\Psi_f}(v;\mu)}{\|v\|}$$

Dual Norm of Dual Residual

We define the residual, $\forall k \in \mathbb{K}$,

$$r^{\mathrm{du},k}(v;\mu) \equiv -m\left(v, \frac{\Psi_N(t^k;\mu) - \Psi_N(t^{k+1};\mu)}{\Delta t}; \mu\right) - a(v, \Psi_N(t^k;\mu);\mu), \quad \forall\, v \in X$$

Dual Norm of Residual

Given $\mu \in \mathcal{D}$, the dual norm of $r^{\mathrm{du},k}(v;\mu)$ is defined as

$$\|r^{\mathrm{du},k}(\cdot;\mu)\|_{X'} \equiv \sup_{v \in X} \frac{r^{\mathrm{du},k}(v;\mu)}{\|v\|_X} = \|\hat{e}^{\mathrm{du},k}(\mu)\|_X,$$

where $\hat{e}^{\mathrm{du},k}(\mu) \in X$ satisfies

$$(\hat{e}^{\mathrm{du},k}(\mu), v)_X = r^{\mathrm{du},k}(v;\mu), \quad \forall v \in X.$$

Energy Error Bound – Dual

We define the error bound, $\Delta_N^{\mathrm{du},k}(\mu) = \Delta_N^{\mathrm{du}}(t^k;\mu)$, $1 \le k \le K$, as

$$\Delta_N^{\mathrm{du},k}(\mu) = \left(\frac{\Delta t}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|\hat{e}^{\mathrm{du},k'}(\mu)\|_X^2 + \sigma_{\mathrm{LB}}(\mu) \Delta_N^{\Psi_f}(\mu)^2 \right)^{1/2} .$$

We can then prove

Proposition (Energy Error Bound)

For any $N = 1, \ldots, N_{\mathrm{du,max}}$, the error in the dual variable, $e^{\mathrm{du},k}(\mu) = \Psi^k(\mu) - \Psi_N^k(\mu)$, is bounded by

$$|||e^{\mathrm{du},k}(\mu)|||^{\mathrm{du}} \le \Delta_N^{\mathrm{du},k}(\mu), \quad \forall\, \mu \in \mathcal{D},\ \forall\, k \in \mathbb{K}.$$

Energy Error Bound – Dual

We define the error bound, $\Delta_N^{\mathrm{du},k}(\mu) = \Delta_N^{\mathrm{du}}(t^k;\mu)$, $1 \le k \le K$, as

$$\Delta_N^{\mathrm{du},k}(\mu) = \left(\frac{\Delta t}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|\hat{e}^{\mathrm{du},k'}(\mu)\|_X^2 + \sigma_{\mathrm{LB}}(\mu) \Delta_N^{\Psi_f}(\mu)^2 \right)^{1/2} .$$

We can then prove

Proposition (Energy Error Bound)

For any $N = 1, \ldots, N_{\mathrm{du,max}}$, *the error in the dual variable,* $e^{\mathrm{du},k}(\mu) = \Psi^k(\mu) - \Psi_N^k(\mu)$, *is bounded by*

$$|||e^{\mathrm{du},k}(\mu)|||^{\mathrm{du}} \le \Delta_N^{\mathrm{du},k}(\mu), \quad \forall\, \mu \in \mathcal{D},\ \forall\, k \in \mathbb{K}.$$

Output Error Bound

We (re-)define the output error bound, $\Delta_N^{s\,k}(\mu) = \Delta_N^s(t^k;\mu)$, $1 \le k \le K$, as

.

$$\Delta_N^{s\,k}(\mu) \equiv \Delta_{N_{\text{pr}}}^{\text{pr},k}(\mu)\ \Delta_{N_{\text{du}}}^{\text{du},K-k+1}(\mu)$$

Proposition (Simple Output Error Bound)

For any $N = 1,\dots,N_{\max}$, the error in the output is bounded by

$$|s^k(\mu) - s_N^k(\mu)| \le \Delta_N^{s\,k}(\mu), \quad \forall \mu \in \mathcal{D},\ \forall k \in \mathbb{K}.$$

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We (re-)define the output error bound, $\Delta_N^{s\,k}(\mu) = \Delta_N^s(t^k;\mu)$, $1 \leq k \leq K$, as

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$$|s^k(\mu) - s_N^k(\mu)| \leq \Delta_N^{s\,k}(\mu), \quad \forall \mu \in \mathcal{D},\ \forall k \in \mathbb{K}.$$

Offline-Online Decomposition

Computational procedure to calculate $\|\hat{e}^{\mathrm{du},k}(\mu)\|_X, \ \forall k \in \mathbb{K}$, follows directly from the primal problem

- Expand $\Psi_N(\mu) = \sum_{j=1}^{N_{\mathrm{du}}} \Psi^k_{N\,j}(\mu)\, \zeta^{\mathrm{du},j}$
- Riesz representation:
$$(\hat{e}^{\mathrm{du},k}(\mu), v)_X = r^{\mathrm{du},k}(v;\mu)$$
- Affine decomposition
- Linear superposition

Offline-Online Decomposition

Summary of computational cost: $Q = Q_a + Q_m$

OFFLINE —

$$O(Q(N_{\mathrm{pr,max}} + N_{\mathrm{du,max}})\mathcal{N}^{\bullet}) \quad + \quad O(Q^2(N^2_{\mathrm{pr,max}} + N^2_{\mathrm{du,max}})\mathcal{N}) \;;$$

solve Poisson problems — form μ-independent inner products

ONLINE —

$$O(KQ^2(N^2_{\mathrm{pr}} + N^2_{\mathrm{du}})) \;;$$

evaluate $\|\hat{e}^{\mathrm{pr/du},k}(\mu)\|_X$-sum for $1 \le k \le K$

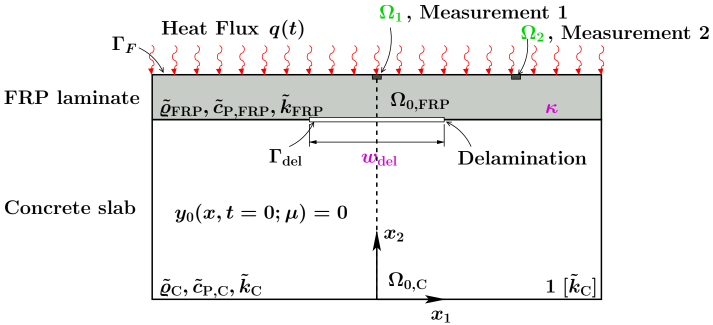
Online cost is independent of $\mathcal{N}$.

Summary

Remarks:

- We require a separate dual problem for each output
  $\Rightarrow$ Primal-dual formulation becomes expensive.
- Shifting property for dual only holds for LTI systems
  $\Rightarrow$ Bounds are valid also for linear time-varying systems,
  but we require K dual problems (for each output).
- Computational cost: two smaller problems are "better" than one big problem, e.g., consider $N_{\text{pr}} = N_{\text{du}} = 1/2N$.
- Residual correction term: $O(K(K+1)N_{\text{pr}}N_{\text{du}})$
  $\Rightarrow$ Reduce cost by considering only every (say) tenth timestep.

Example: Concrete Delamination – Results



Input (parameter): $\mu \equiv (w_{\mathrm{del}}/2, \kappa \equiv \tilde{k}_{\mathrm{FRP}}/\tilde{k}_{\mathrm{C}}) \subset \mathcal{D}$,

where $\mathcal{D} \equiv [1, 10] \times [0.4, 1.8]$.

"Truth": $\mathcal{N} = 5601$, $K = 200$.

Example: Concrete Delamination – Results

Dual problem: convergence energy norm error & bound output 1

N_{du}	$\epsilon^{\mathrm{du}}_{\mathrm{max,rel}}$	$\Delta^{\mathrm{du}}_{\mathrm{max,rel}}$	$\overline{\eta}^{\mathrm{du}}$
20	2.04 E–01	7.46 E–01	2.62
40	5.23 E–02	9.69 E–02	2.41
60	1.36 E–02	2.23 E–02	2.56
80	3.30 E–03	5.39 E–03	2.61
100	1.74 E–03	2.27 E–03	2.29
120	6.45 E–04	9.00 E–04	2.25
140	1.51 E–04	3.77 E–04	2.13
160	8.16 E–05	1.41 E–04	2.09

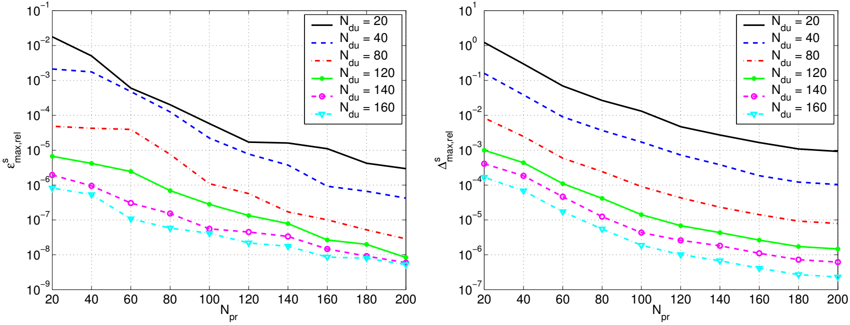
Example: Concrete Delamination – Results

Primal-dual formulation: convergence output bound ($N_{\text{pr}} = N_{\text{du}}$)

N	$\epsilon^s_{\text{max,rel}}$	$\Delta^s_{\text{max,rel}}$	$\overline{\eta}^s$	$\epsilon^{s,\text{simple}}_{\text{max,rel}}$	$\Delta^{s,\text{simple}}_{\text{max,rel}}$
20	1.78 E−02	1.23 E+00	174	6.76 E−02	2.58 E+01
40	1.75 E−03	3.85 E−02	260	1.44 E−02	6.24 E+00
60	1.67 E−04	2.24 E−03	189	3.34 E−03	1.46 E+00
80	7.57 E−06	2.43 E−04	268	1.43 E−03	4.73 E−01
100	6.21 E−07	3.21 E−05	222	3.71 E−04	2.77 E−01
120	1.34 E−07	6.84 E−06	212	9.81 E−05	1.24 E−01
140	3.36 E−08	1.82 E−06	210	4.59 E−05	6.33 E−02
160	8.64 E−09	4.14 E−07	384	2.34 E−05	2.88 E−02

Example: Concrete Delamination – Results

Primal-dual formulation: convergence output error and bound



Example: Concrete Delamination – Results

Primal-dual formulation: online compuational times

$N_{\mathrm{pr}} = N_{\mathrm{du}}$	$s_N(\mu, t^k)$	$\Delta_N^s(\mu, t^k)$	$s(\mu, t^k)$
20	3.11 E–03	9.78 E–04	1
40	5.22 E–03	1.54 E–03	1
60	7.90 E–03	2.34 E–03	1
80	9.49 E–03	3.88 E–03	1
100	1.48 E–02	9.98 E–03	1
120	2.01 E–02	1.74 E–02	1
140	2.55 E–02	3.21 E–02	1
160	3.10 E–02	4.36 E–02	1

Output & Bound for $1 \leq k \leq K$

Savings with respect to truth: ≈ 150

Example: Concrete Delamination – Results

Primal-dual formulation: online compuational times

$N_{pr} = N_{du}$	$s_N(\mu, t^k)$	$\Delta^s_N(\mu, t^k)$	$s(\mu, t^k)$
20	6.90 E–04	9.78 E–04	1
40	9.70 E–04	1.54 E–03	1
60	1.31 E–03	2.34 E–03	1
80	1.82 E–03	3.88 E–03	1
100	2.97 E–03	9.98 E–03	1
120	5.59 E–03	1.74 E–02	1
140	9.28 E–03	3.21 E–02	1
160	1.23 E–02	4.36 E–02	1

Output & Bound for every tenth timestep $k = [10, 20, \ldots, K]$

Savings with respect to truth: ≈ 400

Example: Concrete Delamination – Results

Primal formulation: online compuational times

N_{pr}	$\hat{s}_N(\mu, t^k)$	$\hat{\Delta}_N^s(\mu, t^k)$	$s(\mu, t^k)$
20	2.10 E–04	4.52 E–04	1
40	3.97 E–04	6.36 E–04	1
60	6.73 E–04	8.75 E–04	1
80	1.08 E–03	1.33 E–03	1
100	2.05 E–03	3.70 E–03	1
120	4.37 E–03	6.20 E–03	1
140	6.44 E–03	1.20 E–02	1
160	8.24 E–03	1.65 E–02	1

Output & Bound for every timestep $1 \leq k \leq K$

Savings with respect to truth: ≈ 40

Summary

- Choice primal-dual vs. primal-only formulation is problem specific and depends on
  - convergence rate of primal problem.
  - convergence rate of dual problem.
  - number of outputs.
- Same argument holds for choice of $N_{\mathbf{pr}}$ vs. $N_{\mathbf{du}}$.
- Primal-only formulation advantageous if
  - K is large, i.e., $K \gg N$; complexity for residual correction is $O(K(K+1)N_{\mathbf{pr}}N_{\mathbf{du}})$.
  - we have many outputs are of interest (separate dual for each output).
  - the system is time-varying.

Sampling Strategy

We extend the Greedy Algorithm to a POD(t)-Greedy(μ) sampling procedure [HO], combining a

- small POD in time, with
  $\Rightarrow$ optimally captures causality of time variation
- (exhaustive) Greedy search in parameter space $\mathcal{D}$.
  $\Rightarrow$ (sub-)optimal selection for high-dimensional $\mathcal{D}$ (large n_{train}).

We define

- Desired error tolerance $\varepsilon_{\text{tol,min}}$.
- Train sample $\Xi_{\text{train}} \equiv \{\mu^1_{\text{train}}, \ldots, \mu^{n_{\text{train}}}_{\text{train}}\} \subset \mathcal{D}$, with
- Cardinality (size) $|\Xi_{\text{train}}| = n_{\text{train}}$.
  $\Rightarrow$ Ξ_{train} serves as our (finite) surrogate for $\mathcal{D}$.

POD(t)-Greedy(μ)

Proper Orthogonal Decomposition (POD) in time:

- Let
$$\mathbf{POD}_X(\{u^k(\mu), 1 \le k \le K\}, R)$$
return the R largest POD modes, $\{\Psi^{\mathrm{POD},i}, 1 \le i \le R\}$, with respect to the $(\cdot,\cdot)_X$ inner product.
- The set $\mathcal{P}_R = \{\Psi^{\mathrm{POD},i}, 1 \le i \le R\}$ is $(\cdot,\cdot)_X$ orthogonal and satisfies the optimality property

$$\mathcal{P}_R = \arg \inf_{X_R \subset \mathrm{span}\{u^k(\mu), 1 \le k \le K\}} \left(\frac{1}{K} \sum_{k=1}^{K} \inf_{v \in X_R} \|u^k(\mu) - v\|_X^2 \right)^{1/2}$$

POD(t)-Greedy(μ)

Evaluation of $\Psi^{\text{POD},1} = \text{POD}_X(\{u^k(\mu), 1 \le k \le K\}, 1)$:

1. Form correlation matrix $\underline{C}^{\text{POD}} \in \mathbb{R}^{K \times K}$ given by
$$C_{ij}^{\text{POD}} = \frac{1}{K}(u^i(\mu), u^j(\mu))_X, \quad 1 \le i, j \le K.$$

2. Solve for eigenpair $(\underline{\psi}^{\text{POD,max}} \in \mathbb{R}^K, \lambda^{\text{POD,max}} \in \mathbb{R}_{+0})$, corresponding to largest eigenvalue $\lambda^{\text{POD,max}}$ from
$$\underline{C}^{\text{POD}}\, \underline{\psi}^{\text{POD},k} = \lambda^{\text{POD},k} \underline{\psi}^{\text{POD},k}.$$

3. Compute largest POD mode
$$\Psi^{\text{POD},1} \equiv \sum_{k=1}^{K} \psi_k^{\text{POD,max}}\, u^k(\mu).$$

POD(t)-Greedy(μ)

We require a rigorous, sharp, inexpensive error bound:

$$|||u^k(\mu) - u_N^k(\mu)||| \leq \Delta_N^k(\mu), \quad \forall \mu \in \mathcal{D}.$$

Recall

- Effectivities $\bar{\eta}^u$ are $O(1)$.
- Computational cost to evaluate $\Delta_N^k(\mu)$ is $O(KQ^2N^2)$.

Greedy(μ) Idea:

- $\Delta_N^k(\mu)$ is monotonically increasing in time.
- Find parameter value such that

$$\mu^* = \arg \max_{\mu \in \Xi_{\text{train}}} \Delta_N^K(\mu)$$

$\Rightarrow$ Largest error bound at final time.

POD(t)-Greedy(μ)

Greedy, $L^\infty(\Xi_{\text{train}}, |||\cdot|||)$, space "economization"

$$K n_{\text{train}} \text{ contestants} \;\Rightarrow\; N_{\max} \ll K n_{\text{train}} \text{ winners}$$

$$\in \Xi_{\text{train}} \times \mathbb{I} \qquad\qquad \mu_1^*, \ldots, \mu_{N_{\max}}^*$$

in which we *never form* most snapshots:

$$|||u^k(\mu) - u_N^k(\mu)||| \quad \text{replaced} \quad \Delta_N^k(\mu)$$

$$n_{\text{train}} \cdot O(K\mathcal{N}^\bullet) \quad \text{by} \quad n_{\text{train}} \cdot O(KQ^2N^2)^{\dagger}$$

note good *effectivity* of estimator is crucial.

---

† *In addition* to the offline effort that is required in any event for online rigorous/sharp certification.

POD(t)-Greedy(μ) Algorithm

POD(t)-Greedy(μ) Algorithm

Set $X_N = \{0\}$, $S_N = \{0\}$, $N = 0$, $\mu^* = \mu_0^*$

while $\Delta_N^{\max} \geq \varepsilon_{\mathrm{tol,min}}$

$$e^k_{N,\mathrm{proj}}(\mu^*) = u^k(\mu^*) - \mathrm{proj}_{X,X_N} u^k(\mu^*),\ 1 \leq k \leq K$$

$$S_{N+1} = S_N \cup \mu^*;$$

$$X_{N+1} = X_N + \mathrm{POD}_X(\{e^k_{N,\mathrm{proj}}(\mu^*), 1 \leq k \leq K\}, 1);$$

$$N = N + 1;$$

$$\mu^* = \arg \max_{\mu \in \Xi_{\mathrm{train}}} \Delta_N^K(\mu)/|||y_N^K(\mu)|||;$$

$$\Delta_N^{\max} = \Delta_N^K(\mu^*)/|||y_N^K(\mu^*)|||;$$

end

POD(t)-Greedy(μ)

Remarks

- Spaces X_N are hierarchical.
- Algorithm guarantees that

$$|||u^k(\mu) - u_N^k(\mu)||| \le \Delta_N^k(\mu) \le \varepsilon_{\mathrm{tol,min}}, \quad \forall \mu \in \Xi_{\mathrm{train}}.$$

- We can replace condition on $\Delta_N^{\max}$ by a condition on $N_{\max}$ (hp-Reduced Basis).
- No additional Gram-Schmidt orthogonalization required, basis functions are "by construction" X-orthogonal.
- Computational complexity remains $O(K\mathcal{N}^{\bullet}) + O(n_{\mathrm{train}})$ – not $O(K\mathcal{N}^{\bullet} n_{\mathrm{train}})$.

Extensions

- Nonzero initial conditions, $u_0(\mu) \neq 0$.
  - Nonzero (but constant) initial condition
  $$\Rightarrow \ \zeta^1 = u_0(\mu) \neq 0.$$
  - Affinely parameter dependent initial condition
  $$u_0(\mu) = \sum_{q=1}^{Q_{u_0}} \Theta^q_{u_0}(\mu) u_0^q$$
  where $u_0^q \in X$, μ-independent and known, and
  $\Theta^q_{u_0} : \mathcal{D} \to \mathbb{R}$, μ-dependent functions.
  We then initialize
  $$\Rightarrow \ X_N = \text{span}\{u_0^q, \ 1 \leq q \leq Q_{u_0}\}.$$
  - No *a priori* knowledge
    - Series representation of u_0;
    - Projection of u_0 onto X_N ($\mathcal{N}$-dependent cost);
    - Contribution to error & bound.

Extensions

- Unknown "control" input, $g(t^k)$ (e.g. optimal control).
  Duhamel's Principle: given any control input $g(t^k)$, we can obtain $u^k(\mu)$ from
  $$u^k(\mu) = \sum_{j=1}^{K} h(t^{k-j+1}; \mu)\, g(t^j), \quad \forall k \in \mathbb{K},$$
  where $h(t^k; \mu)$ is the impulse response. We thus train the RB approximation on an impulse input
  $$\Rightarrow \; g(t^k) = \delta_{1k}, \; \forall k \in \mathbb{K}.$$
  only valid for LTI systems
- Multiple "control" inputs, $g(t^k) \in \mathbb{R}^m$.
  $\Rightarrow$ recursive training on each input (LTI).

Extensions & Outlook

Straightforward:

- Non-symmetric Problems (convection-diffusion)
  - Define norms appropriately (replace a by symmetric part of a)
  - Adjust time discretization (Crank-Nicolson instead of EB)
  - Expect much larger N (need for hpRB)
- Dynamic systems (parametric or non-parametric).

Not Straightforward:

- Non-affine Problems
  - Empirical Interpolation Method
- Non-parabolic (hyperbolic) Problems
  - a non-coercive: $L^2(\Omega)$ error bound.
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    - Online cost for Δ_N is $O(N^4)$
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