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Figu

Extension to time dependent problems

Christophe Prud'homme

prudhomme@unistra.fr

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CeMosis - http://www.cemosis.fr
IRMA
Université de Strasbourg

Linear Parabolic Problems

Model order reduction: time-dependent problems

Figu

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

Figu

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

$$s^{\mathrm{e}}(t;\mu) = \ell\left(u^{\mathrm{e}}(x;t;\mu);\mu\right) \tag{1}$$

where $u^{\mathrm{e}}(x;t;\mu) \in L^2\left(0, t_f; X^{\mathrm{e}}(\Omega)\right) \cup C^0\left([0,t_f]; L^2(\Omega)\right)$ satisfies

$$m\left(\frac{\partial u^{\mathrm{e}}}{\partial t}(x;t;\mu), v; \mu\right) + a\left(u^{\mathrm{e}}(x;t;\mu), v; \mu\right) = \underline{f(v;\mu)g(t)}, \quad \forall v \in X^{\mathrm{e}} \tag{2}$$

contrôle

with initial condition $\boldsymbol{u}_0 = 0$. (Note: extension to nonzero initial conditions are briefly discussed below).

$$u^e(t=0) = \underline{u}_0 = 0$$

Definitions

Figu

- μ : input parameter $-\mu = (\mu_1, \mu_2, \dots, \mu_P)$; P-tuple
- $\mathcal{D}$: parameter domain in $\mathbb{R}^P$;
- $\boldsymbol{\Omega}$: spatial domain in $\mathbb{R}^d$;
- s^{e} : output;
- ℓ : output functional;
- $\boldsymbol{u}^{\mathrm{e}}$: field variable;
- X^{e} : function space $\left(\boldsymbol{H}_0^1(\Omega)\right)^\nu \subset \boldsymbol{X}^{\mathrm{e}} \subset \left(\boldsymbol{H}^1(\Omega)\right)^\nu$ we assume here $\nu = 1$, with inner product $(\boldsymbol{w}, \boldsymbol{v})_{X^{\mathrm{e}}}, \forall \boldsymbol{w}, \boldsymbol{v} \in \boldsymbol{X}^{\mathrm{e}}$, and induced norm $\|\boldsymbol{w}\|_{X^{\mathrm{e}}} = \sqrt{(\boldsymbol{w}, \boldsymbol{w})_{X^{\mathrm{e}}}}, \quad \forall \boldsymbol{w} \in \boldsymbol{X}^{\mathrm{e}}$.

$\nu = 1$

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 $\mathcal{T}(\cdot;\mu) : \Omega \to \Omega_o(\mu)$

$$a_o(w_o, v_o; \mu) \text{ over } \Omega_o(\mu)$$

$$\Downarrow$$

$$\mathcal{T}(\cdot;\mu)^{-1} : \Omega_o(\mu) \to \Omega_{\text{ref}} \equiv \Omega \quad (\Omega_{\text{ref}} = \Omega_o(\mu_{\text{ref}}))$$

$$\Downarrow$$

$$a(w, v; \mu) \text{ over } \Omega$$

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

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

Hypotheses i

Figu

Linear forms and functions

$$
\begin{aligned}
f(\cdot;\mu) &: \text{ linear, affine in } \mu, \\
&: \boldsymbol{X}^{\mathrm{e}}\text{-bounded}, \quad \forall \mu \in \mathcal{D} \\
g(\cdot) &: L^2(0, t_f) \qquad \text{"control" input} \\
\ell(\cdot;\mu) &: \text{linear, affine in } \mu, \\
&: L^2(\Omega)\text{-bounded}, \quad \forall \mu \in \mathcal{D}
\end{aligned}
$$

Hypotheses ii

Figu

$$
\begin{aligned}
a(\cdot,\cdot;\mu) : &\ \text{bilinear, affine in } \mu,\\
&\ (\text{symmetric,})\\
&\ X^{\mathrm{e}}\text{-continuous,}\\
&\ X^{\mathrm{e}}\text{-coercive form,} \quad \forall \mu \in \mathcal{D};\\
m(\cdot,\cdot;\mu) : &\ \text{bilinear, affine in } \mu,\\
&\ \text{symmetric,}\\
&\ L^2(\Omega)\text{-continuous,}\\
&\ L^2(\Omega)\text{-coercive form,} \quad \forall \mu \in \mathcal{D};
\end{aligned}
\tag{3}
$$

Note: *a* may satisfy a weak coercivity condition.

Hypotheses iii

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

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

where

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

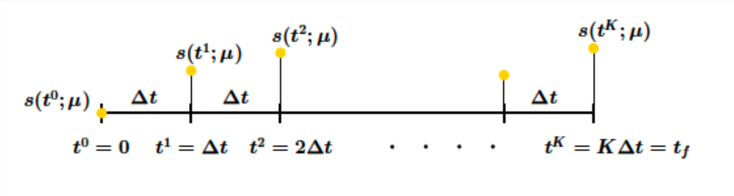
Note: affine assumption may be relaxed.

Figu

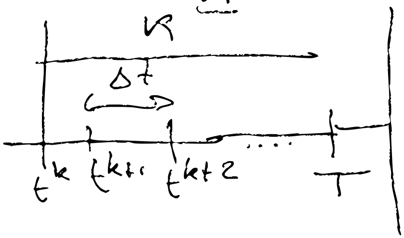
Temporal Discretization: Finite Difference

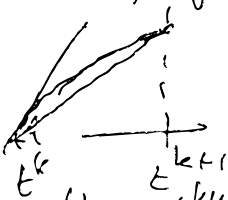
$$\frac{\partial u}{\partial t}\left(t^k;\mu\right) \approx \frac{u\left(t^k;\mu\right) - u\left(t^{k-1};\mu\right)}{\Delta t}$$

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



$$m\left(\frac{\partial u}{\partial t}, v; \mu\right) + a(u, v; \mu) = f(v;\mu)\, g(t) \quad (1)$$





$$\frac{\partial u}{\partial t}(t^k)$$

$$\frac{\partial u(t^k)}{\partial t} \simeq \frac{u(t^{k+1}) - u(t^k)}{\Delta t}$$

en $t = t^k$ avec DF progressive

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

Problem Statement

Figu

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

$$\forall k \in \mathbb{K}$$

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

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

$$m\left(\frac{u\left(t^k;\mu\right) - u\left(t^{k-1};\mu\right)}{\Delta t}, v;\mu\right) + a\left(u\left(t^k;\mu\right), v;\mu\right)$$

$$= f(v;\mu) g\left(t^k\right), \quad \forall v \in X$$

Note: We directly drop the superscript $\mathcal{N}$, i.e., $\boldsymbol{X} = \boldsymbol{X}^{\mathcal{N}}$,

$$u\left(t^k;\mu\right) = u^{\mathcal{N}}\left(t^k;\mu\right), s\left(t^k;\mu\right) = s^{\mathcal{N}}\left(t^k;\mu\right)$$

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

$$\left(\frac{1}{\Delta t}\mathbb{M} + \mathbb{A}\right) U^k = F g(t^k) + \frac{1}{\Delta t}\mathbb{M} U^{k-1} \quad (*)$$

$$U^k = \underbrace{\begin{pmatrix} u_1(t^k) \\ \vdots \\ u_{\mathcal{N}}(t^k) \end{pmatrix}}_{\mathcal{N}} \qquad u(t^k) = \sum_{i=1}^{\mathcal{N}} u_i(t^k)\,\varphi_i(x)$$

$(*)$ $k = 1, \dots, K$

Role

Figu

We shall

- build our reduced basis approximation upon "truth" solutions $u\left(t^k;\mu\right) \in X$
- measure the error in the reduced basis approximation relative to the "truth" solution $u\left(t^k;\mu\right) \in X$ (and $s\left(t^k;\mu\right)$);

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

Reduced Basis Approximation

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

Figu

We assume

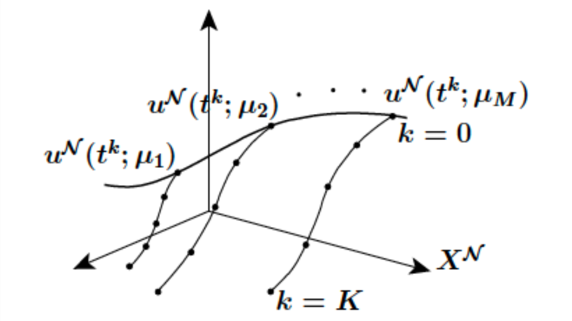
- the form a is continuous and coercive (or inf-sup stable); and
- the form m is continuous and coercive;
- and the $\Theta^q_{m,a}(\mu), 1 \leq q \leq Q_{m,a}$, are smooth; then

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

lies on a smooth $\boldsymbol{P}+$ 1-dimensional manifold in $\boldsymbol{X}$.

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

we need not represent every possible function in $\boldsymbol{X}^{\mathcal{N}}$.

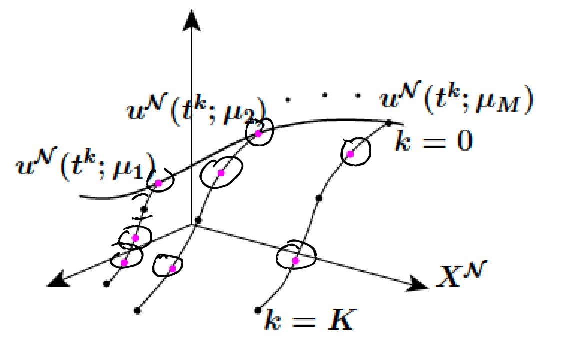


$$X_N \subset \operatorname{span}\left\{u\left(t^k;\mu^m\right), 1 \leq k \leq K, 1 \leq m \leq M\right\} \tag{4}$$

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

Figu

we need not represent every possible function in $\boldsymbol{X}^{\mathcal{N}}$.



○ solutions EF utilisées pour construire la base réduite

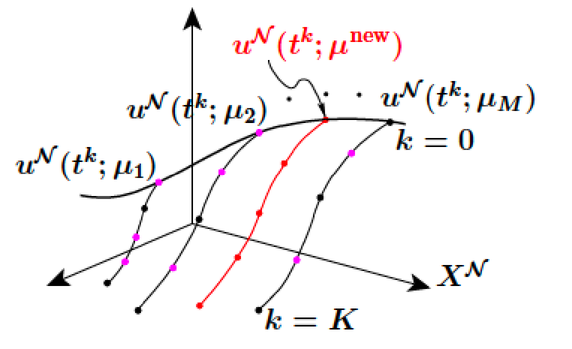
LOCALIZATION

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

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

we need not represent every possible function in $\boldsymbol{X}^{\mathcal{N}}$.

Figu



SMOOTHNESS

We define the Lagrangian RB space

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

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

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

We thus obtain

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

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.

Figu

Galerkin Projection

Figu

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

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

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

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

$$= f(v;\mu)g\left(t^k\right), \quad \forall v \in X_N.$$

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

$$\underbrace{\left(\frac{1}{\Delta t} M^N + A^N\right)}_{N \times N} \underbrace{u_N^k}_{N} = \underbrace{F_N\, g(t^k)}_{N} + \underbrace{\underbrace{\frac{1}{\Delta t} \mathbb{M}_N}_{N \times N} u_N^{k-1}}_{N}$$

Introduction

Figu

- Similar to elliptic case
  - Additional terms due to m
  - Time-dependence: LU-decomposition
- Affine parameter dependence of (bi)linear forms
- Hierarchical RB space
  - Arrays for $N \leq N_{\max}$ are principal subarrays of arrays for $N = N_{\max}$.

Figu

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

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

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

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

and $v = \zeta^i, 1 \leq i \leq N$ Figu

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

$$\ldots = \sum_{j=1}^{N} \frac{1}{\Delta t} m\left(\zeta^j, \zeta^i; \mu\right) u_{Nj}^{k-1}(\mu) + f\left(\zeta^i; \mu\right) g\left(t^k\right)$$

$$\ldots = \sum_{j=1}^{N} \frac{1}{\Delta t} \underbrace{\sum_{m}^{Q_m} \Theta_m^q(\mu) \underbrace{m^q\left(\zeta^j, \zeta^i\right)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_m N^2)} u_{Nj}^{k-1}(\mu) + \underbrace{\sum_{q=1}^{Q_f} \Theta_f^q(\mu) \underbrace{f^q\left(\zeta^i\right)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_f N)} g\left(t^k\right)$$

K

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

$O\left(N^3 + KN^2\right)$ → resolution

factorisation

Output Evaluation

Figu

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

$$
\begin{aligned}
s_N^k(\mu) = \ell\left(u_N^k(\mu);\mu\right) &= \sum_{j=1}^{N} u_{Nj}^k(\mu)\ell\left(\zeta^j;\mu\right) \\
&= \underbrace{\sum_{j=1}^{N} u_{Nj}^k(\mu) \underbrace{\sum_{q=1}^{Q_\ell} \Theta_\ell^q(\mu) \quad \underbrace{\ell^q\left(\zeta^j\right)}_{\text{OFFLINE: } O(\mathcal{N})}}_{\text{ONLINE: } O(Q_\ell N)}}_{\text{ONLINE: } O(N)}
\end{aligned}
$$

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

Computational cost

Figu

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

- OFFLINE - once, parameter independent

$$\underbrace{O\left(KN_{\max}\mathcal{N}^{\bullet}\right)}_{\text{solve for } \zeta_n} + \underbrace{O\left(QN_{\max}^2\mathcal{N}\right)}_{\text{form } \mu\text{-independent quantities}}$$

- ONLINE - many times, parameter dependent $\boldsymbol{\mu}^{\text{new}}$

$$\underbrace{O\left(QN^2\right)}_{\text{form RB matrices}} + \underbrace{O\left(N^3 + KN^2\right)}_{\text{solve for } u_{Nj}^k(\mu)} + \underbrace{O(KN)}_{\text{evaluate output}}$$

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

Stiffness Matrix

Figu

Evaluation of RB Stiffness Matrix $\underline{A}_N \in \mathbb{R}^{N\times N}$: Parameter-independent matrices $\mathbb{A}_N^q \in \mathbb{R}^{N\times N}, 1 \leq q \leq Q_a$:

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

thus

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

We finally assemble

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

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

Mass Matrix

Figu

Evaluation of RB Mass Matrix $\underline{M}_N \in \mathbb{R}^{N\times N}$: Parameter-independent matrices $\mathbb{M}_N^q \in \mathbb{R}^{N\times N}, 1 \leq q \leq Q_m$:

$$\begin{aligned}\mathbb{M}_{Nnm}^q &= m^q\left(\zeta^m, \zeta^n\right)\\ &= \sum_{i=1}^{\mathcal{N}}\sum_{j=1}^{\mathcal{N}} \zeta_i^m m^q\left(\varphi_i^{\mathcal{N}}, \varphi_j^{\mathcal{N}}\right)\zeta_j^n, \quad 1 \leq n, m \leq N\end{aligned}$$

thus

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

We finally assemble

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

Evaluation of RB Load/Source Vector $\underline{F}_N \in \mathbb{R}^N$: Parameter-independent vectors $\mathbb{F}_N^q \in \mathbb{R}^N, 1 \leq q \leq Q_f$:

$$\mathbb{F}_{Nn}^q = f^q\left(\zeta^n\right) = \sum_{i=1}^{\mathcal{N}} \zeta_i^m f^q\left(\varphi_i^{\mathcal{N}}\right), \quad 1 \leq n \leq N$$

thus

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

We finally assemble

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

Output Vector

Figu

Evaluation of RB Output Vector $\underline{L}_N \in \mathbb{R}^N$: Parameter-independent vectors $\mathbb{L}_N^q \in \mathbb{R}^N, 1 \leq q \leq Q_\ell$:

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

thus

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

We finally assemble

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

Summary

Figu

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

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

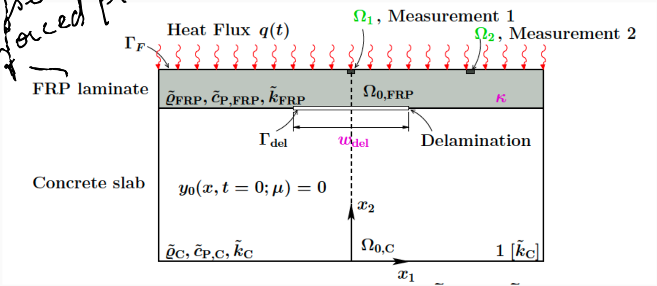
where $\underline{u}_N^k(\mu) \in \mathbb{R}^N$ satisfies $\quad u_{N,0}(\mu) = 0$

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

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

Example: Concrete Delamination - Results i

Fibre unforced plastic



Figu

- Input (parameter) : $\mu \equiv \left(w_{\mathrm{del}}\ /2, \kappa \equiv \tilde{k}_{\mathrm{FRP}}/\tilde{k}_{\mathrm{C}} \right) \subset \mathcal{D}$ where $\mathcal{D} \equiv [1, 10] \times [0.4, 1.8]$.
- "Truth": $\mathcal{N} = 5601, K = 200.$

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

Figu

- Maximum relative error:

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

- Maximum relative output error:

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

How do we choose N?

A posteriori error estimation

Motivation

Figu

- How do we know that $\boldsymbol{u}_{\boldsymbol{N}}^k(\boldsymbol{\mu}), s_N^k(\boldsymbol{\mu})$ are accurate? ONLINE

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

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

- How do we know what value of $\boldsymbol{N}$ to take? ONLINE/OFFLINE
  - N too large $\Rightarrow$ computational inefficiency
  - N too small $\Rightarrow$ unacceptable uncertainty

$\Rightarrow$ norme d'erreur

- How do we choose the sample $\boldsymbol{S_N}$ optimally? OFFLINE
  - RB space has to approximate manifold $\mathcal{M}$ well, but
  - RB matrices need to be "well-conditioned."

Requirements

Figu

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

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

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

- reasonably sharp

$$
\frac{\Delta_N^k(\mu)}{\left\| u^k(\mu) - u_N^k(\mu) \right\| |} \le C, \quad \frac{\Delta_N^{sk}(\mu)}{\left|s^k(\mu) - s_N^k(\mu)\right|} \le C \tag{5}
$$

where $C \approx 1$

- efficient

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

Preliminaries: Inner Products and Norms i

Figu

- $\boldsymbol{X}$-inner product and induced norm (parameter-independent)

$$
\begin{aligned}
(w, v)_X &\equiv a(w, v; \bar{\mu}), \quad \forall w, v \in X \\
\|w\|_X &\equiv \sqrt{(w, w)_X}, \quad \forall w \in X
\end{aligned}
$$

- $\boldsymbol{L}^2$-inner product and induced norm (parameter-independent)

$$
\begin{aligned}
(w, v) &\equiv m(w, v; \bar{\mu}), \quad \forall w, v \in X \\
\|w\| &\equiv \sqrt{(w, w)}, \quad \forall w \in X
\end{aligned}
$$

Masse

Figu

- "Spatio-temporal" energy norm (parameter-dependent) $\quad 1 \leq k \leq K$

$$\begin{aligned}\left(\left(\left(w^k, v^k\right)\right)\right) =& m\left(w^k, v^k; \mu\right) \\ &+ \sum_{k'=1}^{k} \Delta t a\left(w^{k'}, v^{k'}; \mu\right)\end{aligned}$$

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

Figu

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

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

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

Preliminaries: Coercivity lower bound

Figu

We require a positive lower bound for the coercivity constant

$$\alpha_{\mathrm{LB}} : \mathcal{D} \rightarrow \mathbb{R}$$

$$0 < \alpha_{\mathrm{LB}}(\mu) \leq \boldsymbol{\mu}(\mu), \quad \forall \mu \in \mathcal{D}$$

$$\sigma_{\mathrm{LB}} : \mathcal{D} \rightarrow \mathbb{R}$$

$$0 < \sigma_{\mathrm{LB}}(\mu) \leq \boldsymbol{\mu}(\mu), \quad \forall \mu \in \mathcal{D}$$

$\Theta^q > 0$

This bound can be calculated using the

- "min Θ" Approach (if *a* is parametrically coercive), or $a^q(v,v) \geq 0$
- Successive Constraint Method

$m^q(v,v) \geq 0$

exactly as in elliptic case.

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

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

Figu

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

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

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

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

Energy error bound

Figu

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

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

We can then prove

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

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

Simple Output Error Bound

Figu

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

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

Proposition (Simple Output Error Bound)
For any $N = 1,\ldots,N_{\max}$, the error in the output is bounded by

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

Figu

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: $s_N^{\pm}\left(t^k;\mu\right) = s_N\left(t^k;\mu\right) \pm \Delta^s\left(t^k;\mu\right)$, then

$$\Rightarrow s_N^{-}\left(t^k;\mu\right) \leq s\left(t^k;\mu\right) \leq s_N^{+}\left(t^k;\mu\right)$$

- We may also consider other norms than $|||\cdot\cdot|||_\mu$, i.e., $L^2(\Omega)$
- Results for energy norm and output bound directly extend to nonsymmetric problems
  - if we choose an appropriate definition for the energy norm

Offline/Online Decomposition i

Figu

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

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

- Expand $u_N(\mu) = \sum_{j=1}^{N} u_{Nj}^k(\mu)\zeta^j$
- Riesz representation:

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

$|||r^k||| = \|\hat{e}^k\|_X$

- Affine decomposition
- Linear superposition

Figu

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

OFFLINE -

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

ONLINE -

$$\underbrace{O\left(KQ^2N^2\right)}_{\text{evaluate } \left\|\hat{e}^k(\mu)\right\|_X \text{-sum for } 1 \leq k \leq K}$$

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

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

Table 1: Convergence energy norm error and bound

Figu

- Maximum relative error bound:

$$\Delta^y_{\textbf{max,rel}} = \max_{\mu \in \Xi_{\textbf{test}}} \frac{\Delta^\alpha_N(\mu)}{\|u^K(\mu)\|}, \quad \mu_u = \arg \max_{\mu \in \Xi_{\textbf{test}}} \left\| u^K(\mu) \right\|$$

- Average effectivity:

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

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

Table 2: Convergence output error and bound

Figu

- Maximum relative output bound:

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

- Average output effectivity:

$$\bar{\eta}^s = \frac{1}{n_{\mathbf{train}}} \sum_{\mu \in \Xi_{\mathbf{test}}} \frac{\Delta_N^{sk_\eta(\mu)}(\mu)}{\left| s_\eta^{k_\eta(\mu)}(\mu) - s_N^{k_\eta(\mu)}(\mu) \right|}, \quad k_\eta(\mu) = \arg\max_{k \in \mathbb{K}} \left| s^k(\mu) - s^k_N(\mu) \right|$$

Primal Dual Formulation

Figu

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.
$$\text{output error} = \text{primal error } (N_{\mathrm{pr}}) \times \text{ dual error } (N_{\mathrm{du}})$$
- Improved effectivities for output error estimation.

Sampling Strategy

Sampling Strategy

Greedy $(t+\mu)$

We extend the Greedy Algorithm to a POD(t)-Greedy (μ) sampling procedure, 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 $\boldsymbol{n}_{\text{train}}$).

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) $|\Xi_{\text{train}}| = n_{\text{train.}}$. $\Rightarrow$ $\boldsymbol{\Xi}_{\text{train}}$ serves as our (finite) surrogate for $\mathcal{D}$.

Figu

Figu

Proper Orthogonal Decomposition (POD) in time:

- Let

$$\mathrm{POD}_X\left(\underline{\left\{u^k(\mu), 1 \leq k \leq K\right\}}, R\right)$$

RIC ε_{tol}

$(\cdot,\cdot)_X$

orthonormale

  return the R largest POD modes, $\left\{\Psi^{\mathrm{POD},i}, 1 \leq i \leq R\right\}$, with respect to the $(\cdot,\cdot)_X$ inner product.

- The set $\mathcal{P}_R = \left\{\Psi^{\mathrm{POD},i}, 1 \leq i \leq R\right\}$ is $(\cdot,\cdot)_X$ orthogonal and satisfies the optimality property

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

POD(t) -Greedy (μ) ii

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

1. Form correlation matrix $\underline{C}^{\mathrm{POD}} \in \mathbb{R}^{K\times K}$ given by

   POD

$$C_{ij}^{\mathrm{POD}} = \frac{1}{K}\left(u^i(\mu), u^j(\mu)\right)_X, \quad 1 \le i,j \le K.$$

2. Solve for eigenpair $\left(\underline{\psi}^{\mathrm{POD,max}} \in \mathbb{R}^K, \lambda^{\mathrm{POD,max}} \in \mathbb{R}_{+0}\right)$,

$$\underline{C}^{\mathrm{POD}}\underline{\psi}^{\mathrm{POD},k} = \lambda^{\mathrm{POD},k}\underline{\psi}^{\mathrm{POD},k}.$$

3. Compute largest POD mode

$$\Psi^{\mathrm{POD},1} \equiv \sum_{k=1}^{K} \psi_k^{\mathrm{POD,max}} u^k(\mu)$$

Figu

Figu

Remarks

- Perform POD on projection error instead of data, i.e.

$$\mathrm{POD}_X\left(\left\{e^k_{N,\mathrm{proj}}(\mu), 1 \leq k \leq K\right\}, 1\right)$$

  where $e^k_{N,\mathrm{proj}}(\mu) = u^k(\mu) - \mathrm{proj}_{X,X_N}\, u^k(\mu)$, and $\mathrm{proj}_{X,X_N}\, u^k(\mu)$ is the X-orthogonal projection of $u^k(\mu)$ onto $\boldsymbol{X}_N$.

- Algebraic notation

$$\underline{e}^k_{N,\mathrm{proj}}(\mu) = \underline{u}^k(\mu) - \mathbb{Z}_N\left(\mathbb{Z}_N^T \mathbb{X}^{\mathcal{N}}\, \underline{u}^k(\mu)\right)$$

- In general, we set $R = 1$ and add only one mode at each iteration (offline vs. online effort).

POD(t) -Greedy (μ) iv

We require a rigorous, sharp, inexpensive error bound:

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

Figu

Note (see below)

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

Use Greedy ($\boldsymbol{\mu}$) Idea:

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

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

$\Rightarrow$ Largest error bound at final time.

POD(t) -Greedy (μ) v

Figu

Greedy, L^∞ (Ξ_{train} , $\|\cdot\|\|\ |$), space "economization"

$$\underbrace{\boxed{Kn_{\text{train}}}}_{\in\, \Xi_{\text{train}} \times \mathbb{I}} \text{ contestants } \Rightarrow \underbrace{N_{\max}}_{}(\ll Kn_{\text{train}}) \text{ winners } \underset{\mu_1^*, \ldots, \mu_{N_{\max}}^*}{}$$

in which we never form most snapshots:

$$\begin{array}{ccc} \|\|\|u^k(\mu) - u_N^k(\mu)\| & \text{replaced} & \Delta_N^k(\mu) \\ n_{\text{train}} \cdot O\left(K\mathcal{N}^\bullet\right) & \text{by} & n_{\text{train}} \cdot O\left(KQ^2N^2\right)^1 \end{array}$$

note good effectivity of estimator is crucial.

Figu

$\mathrm{POD}(t)$-**Greedy** (μ) **Algorithm**

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

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

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

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

$$X_{N+1} = X_N + \text{POD}_X\left(\left\{e_{N,\text{proj}}^k(\mu^*), 1 \leq k \leq K\right\}, 1\right)$$

$$N = N + 1;$$

$$\mu^* = \arg\max_{\mu \in \Xi_{\text{train}}} \Delta_N^K(\mu) / \left\| u_N^K(\mu) \right\|;$$

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

end while

Figu

Remarks

- Spaces X_N are hierarchical.
- Algorithm guarantees that $\left\| u^k(\mu) - u_N^k(\mu) \right\| | \leq \Delta_N^k(\mu) \leq \varepsilon_{\text{tol,min}}$, $\forall \mu \in \Xi_{\text{train}}$.
- 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" $\boldsymbol{X}$-orthogonal.
- Computational complexity remains $O\left(K\mathcal{N}^{\bullet}\right) + O\left(n_{\text{train}}\right)$ not $O\left(K\mathcal{N}^{\bullet} n_{\text{train}}\right)$

[1] In addition to the offline effort that is required in any event for online rigorous/sharp certification.

Extensions i

à $t = 0$

$u(t=0) = u_0$

u_0^N

- 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

$$u_0(\mu) = \sum_{q=1}^{Q_{u_0}} \Theta^q_{u_0}(\mu) u_0^q \in X$$

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

$$\Rightarrow X_N = \text{span}\left\{u_0^q, 1 \leq q \leq Q_{u_0}\right\}.$$

  - No a priori knowledge
    - Series representation of u_0;
    - Projection of u_0 onto X_N($\mathcal{N}$-dependent cost);
    - Contribution to error & bound.

Figu

Extensions ii

- Unknown "control" input, $g\left(t^k\right)$ (e.g. optimal control). Duhamel's Principle: given any control input $g\left(t^k\right)$, we can obtain $u^k(\mu)$ from

$$u^k(\mu) = \sum_{j=1}^{K} h\left(t^{k-j+1};\mu\right) g\left(t^j\right), \quad \forall k \in \mathbb{K},$$

  where $h\left(t^k;\mu\right)$ is the impulse response. We thus train the RB approximation on an impulse input

$$\Rightarrow g\left(t^k\right) = \delta_{1k}, \forall k \in \mathbb{K}.$$

  linear time invariant

  only valid for LTI systems

- Multiple "control" inputs, $g\left(t^k\right) \in \mathbb{R}^m$

  $\Rightarrow$ recursive training on each input (LTI).

Figu

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