Reduced Basis Methods

Nonaffine and (some) Nonlinear Problems

Summerschool “Reduced Basis Methods”
TU München, September 16-19, 2013

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Outline

1. **Linear Parabolic Problems** (yesterday)
   - RB Approximation
   - *A Posteriori* Error Estimation
   - Sampling Procedure
2. **Nonaffine and (some) Nonlinear Problems** (this lecture)
   - Motivation
   - Empirical Interpolation Method
   - Nonaffine Problems
   - Nonlinear Problems
3. **Parametrized Optimal Control Problems** (this lecture)
   - RB Approximation
   - *A Posteriori* Error Estimation

"Truth" Problem Statement

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

$$\boldsymbol{s}(\boldsymbol{\mu}) = \boldsymbol{\ell}(\boldsymbol{u}(\boldsymbol{\mu}); \boldsymbol{\mu})$$

where $\boldsymbol{u}(\boldsymbol{x}; \boldsymbol{\mu}) \in \boldsymbol{X}$ satisfies

$$\boldsymbol{a}(\boldsymbol{u}(\boldsymbol{\mu}), \boldsymbol{v}; \boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{v}; \boldsymbol{\mu}), \quad \forall\, \boldsymbol{v} \in \boldsymbol{X}(\boldsymbol{\Omega}).$$

Assumptions:

- linearity, coercivity, continuity;
- affine parameter dependence.

Reduced Basis Sample and Space

Parameter samples:

$$S_N = \{\mu^1 \in \mathcal{D}, \ldots, \mu^N \in \mathcal{D}\}, \quad 1 \le N \le N_{\max},$$

with

$$S_1 \subset S_2 \subset \ldots \subset S_{N_{\max}-1} \subset S_{N_{\max}} \subset \mathcal{D}.$$

Lagrangian reduced basis spaces:

$$X_N = \text{span}\{\underbrace{u(\mu^n)}_{\text{“snapshots”}}, 1 \le n \le N\}, \quad 1 \le N \le N_{\max},$$

with

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

Reduced Basis Method

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

$$s_N(\mu) = \ell(u_N(\mu); \mu)$$

where $u_N(x; \mu) \in X_N \subset X$ satisfies

$$a(u_N(\mu), v; \mu) = f(v; \mu), \quad \forall\, v \in X_N.$$

Furthermore, we can bound the reduced basis error by

$$\|u(\mu) - u_N(\mu)\|_X = \frac{\|r(\cdot; \mu)\|_{X'}}{\alpha_{\mathrm{LB}}(\mu)}, \quad \forall \mu \in \mathcal{D},$$

where $r(v; \mu) = f(v; \mu) - a(u_N(\mu, v; \mu), \forall v \in X$, is the residual.

Affine parameter dependence

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

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

where for $q = 1,\ldots,Q_a$

$\Theta_a^q : \mathcal{D} \to \mathbb{R}$, μ-dependent functions;

$a^q : X^{\mathrm{e}} \times X^{\mathrm{e}} \to \mathbb{R}$, μ-independent forms.

This assumption is crucial for

- the offline-online decomposition, and thus for
- the computational efficiency of the reduced basis method . . .

Offline-Online Decomposition

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

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

$$a(u_N(\mu), v; \mu) = f(v; \mu)$$

$$\sum_{j=1}^{N} u_{N\,j}(\mu) a(\zeta^j, \zeta^i; \mu) = f(\zeta^i; \mu)$$

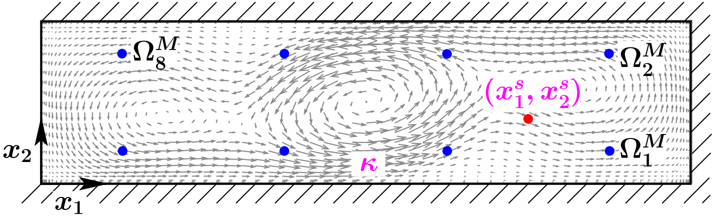
$$\underbrace{\sum_{j=1}^{N} u_{N\,j}(\mu) \underbrace{\sum_{q=1}^{Q_a} \Theta_a^q(\mu) \underbrace{a^q(\zeta^j, \zeta^i)}_{\text{OFFLINE: } \mathcal{O}(\mathcal{N})}}_{\text{ONLINE: } \mathcal{O}(Q_a N^2)} = \underbrace{\sum_{q=1}^{Q_f} \Theta_f^q(\mu) \underbrace{f^q(\zeta^i)}_{\text{OFFLINE: } \mathcal{O}(\mathcal{N})}}_{\text{ONLINE: } \mathcal{O}(Q_f N)}}_{\text{ONLINE: } \mathcal{O}(N^3)}$$

Affine parameter dependence

. . . **but**

- not all problems satisfy affine-parameter dependence, so
- where and how does our approach fail in the “nonaffine” case?
- how do we deal with “nonaffine” problems?

Contaminant Transport [Gre05]



Concentration $u(t;\mu)$ of pollutant in Ω governed by scalar convection-diffusion equation $u(x, t = 0; \mu) = 0$

$$\frac{\partial}{\partial t} u(t;\mu) + \mathrm{U} \cdot \nabla u(t;\mu) = \kappa \, \nabla^2 u(t;\mu) + g^{\mathrm{PS}}(x;\mu) \, g(t),$$

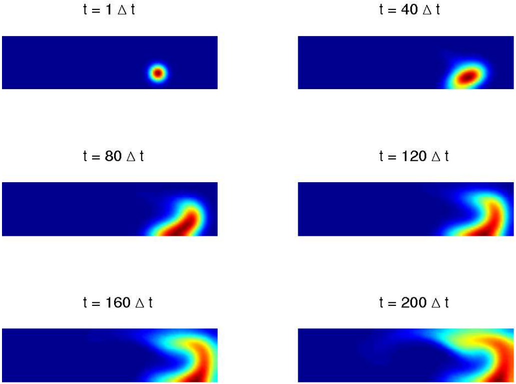
with source term modeled by

$$g^{\mathrm{PS}}(x;\mu) = \frac{50}{\pi} \, e^{-50((x_1 - x_1^s)^2 + (x_2 - x_2^s)^2)}.$$

Goal: Identify source location $\Rightarrow$ parameter $\mu \equiv (\kappa, x_1^s, x_2^s)$.

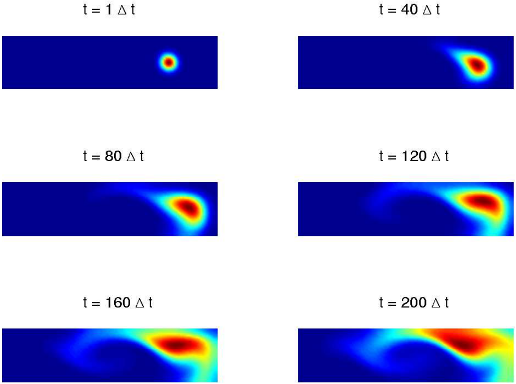
Contaminant Transport – Sample Solutions

Field variable: $\boldsymbol{\mu = (0.05, 2.9, 0.3)}$ $\qquad$ $\boldsymbol{(\mathbb{N} = 3720)}$



Contaminant Transport – Sample Solutions

Field variable: $\boldsymbol{\mu} = (\mathbf{0.05}, \mathbf{3.1}, \mathbf{0.5})$ $(\mathbb{N} = \mathbf{3720})$



Contaminant Transport – Truth Problem Statement

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

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

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

$$m\left(\frac{u(t^k;\mu) - u(t^{k-1};\mu)}{\Delta t}, v; \mu\right) + \frac{1}{2}\, a(u(t^k;\mu) + u(t^{k-1};\mu), v; \mu)$$

$$= b(v;\mu)\, \frac{1}{2}\,(g(t^k) + g(t^{k-1})),\ \forall v \in X,$$

for $b(v;\mu) = \int_\Omega g^{\mathrm{PS}}(x;\mu)\, v$ with g^{PS} nonaffine.

Nonaffine Source Term

Evaluation of RB quantities $(v = \zeta_i,\ 1 \leq i \leq N_{\max})$:

$$\begin{aligned} b(\zeta_i; \mu) &= \int_\Omega g^{\mathrm{PS}}(x; \mu)\, \zeta_i \\ &= \frac{50}{\pi} \int_\Omega e^{-50((x_1-\mu_2)^2+(x_2-\mu_3)^2)}\, \zeta_i \end{aligned}$$

requires even in the online stage

$\mathcal{O}(\mathcal{N} N)$ operations.

Difficulty

There is no ($\mathcal{N}$-independent) affine representation of $g^{\mathrm{PS}}(x; \mu)$.

Empirical Interpolation Method [BMNP04, GMNP07]

Main Idea

$$g^{\mathrm{PS}}(x;\mu) \approx g_M^{\mathrm{PS}}(x;\mu) = \sum_{m=1}^{M} \underbrace{\varphi_{Mm}(\mu)}_{\text{EIM}} \quad \underbrace{q_m(x)}_{\text{Collateral RB}}$$

Recall:
$$b(\zeta_i;\mu) = \int_\Omega g^{\mathrm{PS}}(x;\mu)\,\zeta_i \approx \int_\Omega g_M^{\mathrm{PS}}(x;\mu)\,\zeta_i$$
$$= \sum_{m=1}^{M} \varphi_{Mm}(\mu) \int_\Omega q_m(x)\,\zeta_i\ ,$$

If we can calculate the $\varphi_{Mm}(\mu)$ efficiently, we can again follow an offline-online computational procedure, but

- how do we calculate the $q_m(x)$ and the $\varphi_{Mm}(\mu)$?
- what is the interpolation error introduced?

Greedy Approach [MNPP07]

Empirical Interpolation: Greedy approach for constructing both

- interpolation points $T_M = \{x_1^T \in \Omega, \ldots, x_M^T \in \Omega\}$, and
- sample set $S_M^g \equiv \{\mu_1^g \in \mathcal{D}, \ldots, \mu_M^g \in \mathcal{D}\}$ and associated discrete spaces $W_M^g = \text{span}\{q_1, \ldots, q_M\}$.

Greedy Procedure:

We first choose $\mu_1^g \in \mathcal{D}$ and compute

$$\xi_1 \equiv g(x; \mu_1^g).$$

The first interpolation point is

$$x_1 = \arg\ \max_{x \in \Omega} |\xi_1(x)|,$$

and we set $q_1 = \xi_1(x)/\xi_1(x_1)$ and $B_{11}^1 = 1$.

Greedy Approach [MNPP07]

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Greedy Approach

We then proceed by induction to generate S_M^g, W_M^g, and T_M:

For $1 \leq M \leq M_{\max}$, we first solve the interpolation problem

$$g_M(x_i;\mu) = \sum_{j=1}^{M} B_{ij}^M \varphi_{M\,j}(\mu) = g(x_i;\mu), \quad 1 \leq i \leq M,$$

where $B_{ij}^M = q_j(x_i)$, $1 \leq i, j \leq M$, then compute

$$g_M(x;\mu) \equiv \sum_{m=1}^{M} \varphi_{M\,m}(\mu) q_m(x),$$

and evaluate the interpolation error

$$\varepsilon_M(\mu) = \|g(\cdot;\mu) - g_M(\cdot;\mu)\|_{L^\infty(\Omega)}$$

for all $\mu \in \Xi_{\mathrm{train}}^g$.

Greedy Approach

We then determine

$$\mu^g_{M+1} \equiv \arg \max_{\mu \in \Xi^g_{\mathrm{train}}} \varepsilon_M(\mu)$$

and compute $\xi_{M+1} \equiv g(x; \mu^g_{M+1})$.

To generate the interpolation points we solve the linear system

$$\sum_{j=1}^{M} \sigma^M_j \, q_j(x_i) = \xi_{M+1}(x_i), \quad 1 \le i \le M$$

and we set $r_{M+1}(x) = \xi_{M+1}(x) - \sum_{j=1}^{M} \sigma^M_j \, q_j(x)$.

The next interpolation point is

$$x_{M+1} = \arg \max_{x \in \Omega} |r_{M+1}(x)|,$$

and $q_{M+1}(x) = r_{M+1}(x)/r_{M+1}(x_{M+1})$.

Greedy Approach

We then determine

$$\mu^g_{M+1} \equiv \arg \max_{\mu \in \Xi^g_{\text{train}}} \varepsilon_M(\mu)$$

and compute $\xi_{M+1} \equiv g(x; \mu^g_{M+1})$.

To generate the interpolation points we solve the linear system

$$\sum_{j=1}^{M} \sigma_j^M \, q_j(x_i) = \xi_{M+1}(x_i), \quad 1 \leq i \leq M$$

and we set $r_{M+1}(x) = \xi_{M+1}(x) - \sum_{j=1}^{M} \sigma_j^M \, q_j(x)$.

The next interpolation point is

$$x_{M+1} = \arg \max_{x \in \Omega} |r_{M+1}(x)|,$$

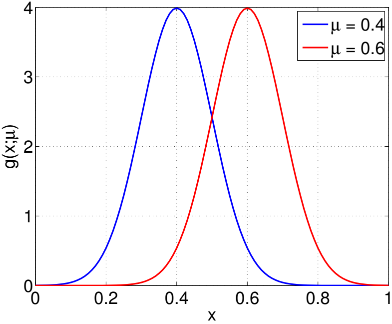
and $q_{M+1}(x) = r_{M+1}(x)/r_{M+1}(x_{M+1})$.

Example/Demo

We consider the nonaffine function

$$g(x;\mu) \equiv \frac{10}{\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{0.1}\right)^2}$$

for $x \in \Omega \equiv [0,1]$ and $\mu \in \mathcal{D} \equiv [0.4, 0.6]$.



Properties

If $M_{\max}$ is smaller than the dimension of $\mathrm{span}\ \mathcal{M}^g$, where $\mathcal{M}^g \equiv \{g(\cdot;\mu) | \mu \in \mathcal{D}\}$, for any $M \le M_{\max}$ we have

- the space W_M^g is of dimension M and coincides with $\mathrm{span}\{\xi_1, \dots, \xi_M\}$
- the matrix B^M lower triangular with unity diagonal (and hence invertible)
- the interpolation is well-defined

It follows that for any $g(x;\mu) \in W_M^g$ we have

$$g_M(x;\mu) = g(x;\mu)$$

i.e., the interpolation is exact for all $g(x;\mu) \in W_M^g$.

A Priori Stability: Lebesgue constant

We define a Lebesgue constant

$$\Lambda_M \equiv \sup_{x\in\Omega} \sum_{m=1}^{M} |V_m^M(x)|,$$

where the $V_m^M(x) \in W_M^g$ is the associated Lagrange basis,

$$V_m^M(x_n) \equiv \delta_{mn},\ 1 \le m, n \le M.$$

We can prove

Proposition

The Lebesgue constant Λ_M satisfies $\Lambda_M \le 2^M - 1$.

and

Proposition

The interpolation error $\varepsilon_M(\mu)$ satisfies

$$\varepsilon_M(\mu) \le (1 + \Lambda_M) \inf_{z\in W_M^g} \|g(\cdot;\mu) - z\|_{L^\infty(\Omega)}.$$

A Posteriori Error Estimation

We have two options:

- Method 1: "Next Point" Estimator [BMNP04, GMNP07]
  - Very inexpensive to evaluate
    $\Rightarrow$ one additional evaluation of $g(x; \mu)$ at a single point in Ω.
  - In general not a rigorous upper bound for the error
    $\Rightarrow$ requires the saturation hypothesis.
- Method 2: Rigorous Estimator [EGP10]
  - Higher offline cost, since we require
    $\Rightarrow$ analytical upper bounds for parametric derivatives
    $\Rightarrow$ EIM approximation error at finite set of points in $\mathcal{D}$.
  - Provides rigorous upper bound for the error

A Posteriori Error Estimation

Given an approximation $g_M(x;\mu)$ for $M \le M_{\max} - 1$, we define

$$\hat{\varepsilon}_M(\mu) \equiv |g(x_{M+1};\mu) - g_M(x_{M+1};\mu)|$$

and obtain

Proposition

If $g(\,\cdot\,;\mu) \in W^g_{M+1}$, then

$$\|g(\,\cdot\,;\mu) - g_M(\,\cdot\,;\mu)\|_{L^\infty(\Omega)} = \hat{\varepsilon}_M(\mu).$$

Note

- in general $g(\,\cdot\,;\mu) \notin W^g_{M+1}$, and hence our estimator $\hat{\varepsilon}_M(\mu)$ is indeed a lower bound; however,
- if $\varepsilon_M(\mu) \to 0$ very fast, we expect (and check) that the effectivity, $\eta_M(\mu) \equiv \hat{\varepsilon}_M(\mu)/\varepsilon_M(\mu) \approx 1$.

Numerical Example

We consider the nonaffine function

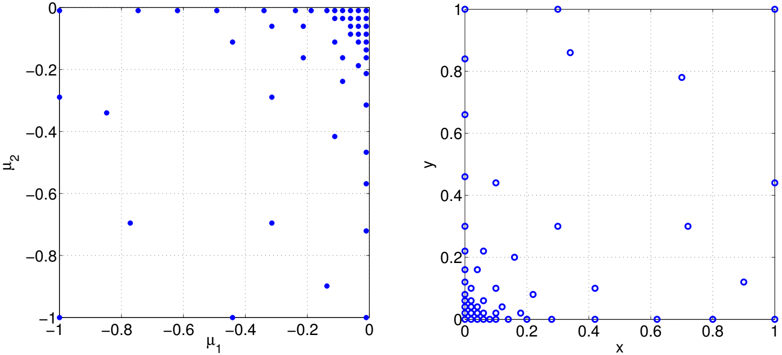
$$G(x;\mu) \equiv \frac{1}{\sqrt{(x_1-\mu_{(1)})^2+(x_2-\mu_{(2)})^2}}$$

for $x \in \Omega \equiv]0,1[^{\,2}$ and $\mu \in \mathcal{D} \equiv [-1,-0.01]^2$.

M	$\varepsilon^*_{M,\max}$	$\overline{\rho}_M$	Λ_M	$\overline{\eta}_M$	κ_M
8	8.30 E–02	0.68	1.76	0.17	3.65
16	4.22 E–03	0.67	2.63	0.10	6.08
24	2.68 E–04	0.49	4.42	0.28	9.19
32	5.64 E–05	0.48	5.15	0.20	12.86
40	3.66 E–06	0.54	4.98	0.60	18.37
48	6.08 E–07	0.37	7.43	0.29	20.41

Table: NE 1: $\varepsilon^*_{M,\max}$ is the best fit error, $\overline{\rho}_M$ is the averaged ratio $\frac{\varepsilon_M(\mu)}{\varepsilon^*_M(\mu)(1+\Lambda_M)}$, $\overline{\eta}_M$ is the average effectivity, and $\varkappa_M$ is the condition number of B^M.

Numerical Example



Parameter sample set S_M^g, $M_{\max} = 51$, and interpolation points $x_m,\ 1 \le m \le M_{\max}$.

Nonaffine "Truth" Problem Statement

Given $\boldsymbol{\mu} \in \boldsymbol{\mathcal{D}} \subset \mathbb{R}^{\boldsymbol{P}}$, evaluate $\qquad (\cdot) = (\cdot)^{\mathcal{N}}$

$$s(\boldsymbol{\mu}) = \ell(\boldsymbol{u}(\boldsymbol{\mu}); \boldsymbol{\mu})$$

where $\boldsymbol{u}(\boldsymbol{x}; \boldsymbol{\mu}) \in \boldsymbol{X}$ satisfies

$$\boldsymbol{a}(\boldsymbol{u}(\boldsymbol{\mu}), \boldsymbol{v}; \boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{v}; \boldsymbol{g}(\boldsymbol{x}; \boldsymbol{\mu})), \quad \forall\, \boldsymbol{v} \in \boldsymbol{X}.$$

We consider the particular form

$$\boldsymbol{a}(\boldsymbol{w}, \boldsymbol{v}; \boldsymbol{\mu}) = \boldsymbol{a}_0(\boldsymbol{w}, \boldsymbol{v}) + \boldsymbol{a}_1(\boldsymbol{w}, \boldsymbol{v}; \boldsymbol{g}(\boldsymbol{x}; \boldsymbol{\mu})), \quad \forall \boldsymbol{w}, \boldsymbol{v} \in \boldsymbol{X}.$$

where $\boldsymbol{g}(\boldsymbol{x}; \boldsymbol{\mu}) \in \boldsymbol{L}^{\infty}(\boldsymbol{\Omega})$ is nonaffine.

Hypotheses

We assume

- $a_0 : X \times X \to \mathbb{R}$ is bilinear and parameter independent
$$a_0(w,v) = \int_\Omega \nabla w \, \nabla v, \quad \forall w, v \in X$$
- $a_1 : X \times X \times L^\infty(\Omega) \to \mathbb{R}$ is trilinear
$$a_1(w,v,z) = \int_\Omega w \, v \, z, \quad \forall w, v \in X, \; z \in L^\infty(\Omega)$$
- and $f(v; g(x;\mu)) = \int_\Omega v \, g(x;\mu)$ is a linear form.

Coercivity & Continuity

We also assume that $a : X \times X \times \mathcal{D} \to \mathbb{R}$ is

- coercive

$$(0 <)\ \alpha(\mu) \equiv \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2};$$

- and continuous

$$\gamma(\mu) \equiv \sup_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu)}{\|w\|_X \|v\|_X}\ (< \infty),$$

and that a_1 satisfies

$$a_1(w, v, z) \leq \gamma_{a_1} \|w\|_X \, \|v\|_X \, \|z\|_{L^\infty(\Omega)}, \qquad \forall w, v \in X,\ z \in L^\infty(\Omega).$$

Reduced Basis Sample and Space

Parameter samples:

$$S_N = \{\mu^1 \in \mathcal{D}, \ldots, \mu^N \in \mathcal{D}\}, \quad 1 \leq N \leq N_{\max},$$

with

$$S_1 \subset S_2 \subset \ldots \subset S_{N_{\max}-1} \subset S_{N_{\max}} \subset \mathcal{D}.$$

Lagrangian reduced basis spaces:

$$X_N = \mathrm{span}\{ \underbrace{u(\mu^n)}_{\text{“snapshots”}}, 1 \leq n \leq N\}, \quad 1 \leq N \leq N_{\max},$$

with

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

Reduced Basis Approximation

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

$$s_{N,M}(\mu) = \ell(u_{N,M}(\mu); \mu)$$

where $u_{N,M}(x; \mu) \in X_N \subset X$ satisfies

$$a_0(u_{N,M}(\mu), v) + a_1(u_{N,M}(\mu), v; g_M(x; \mu)) = f(v; g_M(x; \mu)), \quad \forall\, v \in X_N.$$

where

$$g_M(x; \mu) \equiv \sum_{m=1}^{M} \varphi_{M\,m}(\mu) q_m(x),$$

and $$\sum_{j=1}^{M} B_{ij}^M \varphi_{M\,j}(\mu) = g(x_i; \mu), \quad 1 \le i \le M.$$

Admits *offline-online* treatment: online cost $\mathcal{O}(M^2 + MN^2 + N^3)$

Error Residual Equation

The error, $e(\mu) \equiv u(\mu) - u_N(\mu) \in X$, satisfies

$$\begin{aligned} a_0(e(\mu), v) + a_1(e(\mu), v; g(x;\mu)) = \\ r(v;\mu) + f(v; g(x;\mu) - g_M(x;\mu)) \\ - a_1(u_{N,M}(\mu), v; g(x;\mu) - g_M(x;\mu)), \\ \forall\, v \in X, \end{aligned}$$

where the residual is defined as

$$\begin{aligned} r(v;\mu) \equiv f(v; g_M(x;\mu)) \\ - a_0(u_N(\mu), v) - a_1(u_N(\mu), v; g_M(x;\mu)), \\ \forall\, v \in X. \end{aligned}$$

Energy Norm & Output Bound

Energy norm bound [Ngu07]

$$\Delta^u_{N,M}(\mu) = \frac{1}{\alpha_{\mathrm{LB}}(\mu)}\Big(\underbrace{\|r(\cdot;\mu)\|_{X'}}_{\text{affine}} + \underbrace{\hat{\varepsilon}_M(\mu)\Phi^{\mathrm{na}}_M(\mu)}_{\text{nonaffine}} \Big),$$

contribution to error bound

where

$\alpha_{\mathrm{LB}}(\mu)$	...	Lower bound of coercivity constant,
$\|r(\cdot;\mu)\|_{X'}$	...	dual norm of residual,
$\hat{\varepsilon}_M(\mu)$	...	interpolation induced error.

and

$$\Phi^{\mathrm{na}}_M(\mu) = \sup_{v\in X} \frac{f(v;q_{M+1}) - a_1(u_{N,M},v;q_{M+1})}{\|v\|_X}$$

Energy Error Bound

Proposition (Energy Error Bound)

If $g(x;\mu) \in W^g_{M+1}$, *the error,* $e(\mu) = u(\mu) - u_{N,M}(\mu)$, *satisfies*

$$\|e(\mu)\|_X \leq \Delta^u_{N,M}(\mu), \quad \forall \mu \in \mathcal{D},$$

and for any $N = 1, \ldots, N_{\max}$ *and any* $M = 1, \ldots, M_{\max}$.

Note:

- In general $g(x;\mu) \notin W^g_{M+1}$, thus

$$\|e(\mu)\|_X \lessapprox \Delta^u_{N,M}(\mu), \quad \forall \mu \in \mathcal{D}.$$

- Admits offline-online treatment: online cost $\mathcal{O}(M^2 N^2)$.

Output Error Bound

We define

- the output error bound:

$$\Delta^s_{N,M}(\mu) \equiv \|\ell(\cdot;\mu)\|_{X'} \, \Delta_{N,M}(\mu)$$

- and the output effectivity: $\eta^s_N(\mu) \equiv \dfrac{\Delta^s_N(\mu)}{|s(\mu) - s_N(\mu)|}$

Proposition (Output Error Bound)

For any $N = 1, \ldots, N_{\max}$ and any $M = 1, \ldots, M_{\max}$, the error, $|s(\mu) - s_N(\mu)|$, satisfies

$$|s(\mu) - s_N(\mu)| \leq \Delta^s_{N,M}(\mu), \qquad \forall \mu \in \mathcal{D}.$$

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$$|s(\mu) - s_N(\mu)| \leq \Delta^s_{N,M}(\mu), \qquad \forall \mu \in \mathcal{D}.$$

Error Bounds – Remarks

Remarks:

- The *a posteriori* error bounds are
  - rigorous only for $g(x; \mu) \in W^g_{M+1}$, but
  - are very cheap to evaluate – one additional evaluation of $g(x; \mu)$ at one point in Ω.
- We can replace the "next point" estimator with the rigorous *a posteriori* error estimator, but they require more extensive offline computations [KGV12].
- The dual formulation can be extended to the nonaffine case [KGV12]

Model Problem

We consider the model problem with

$$g(x;\mu) \equiv \frac{1}{\sqrt{(x_1-\mu_{(1)})^2+(x_2-\mu_{(2)})^2}}$$

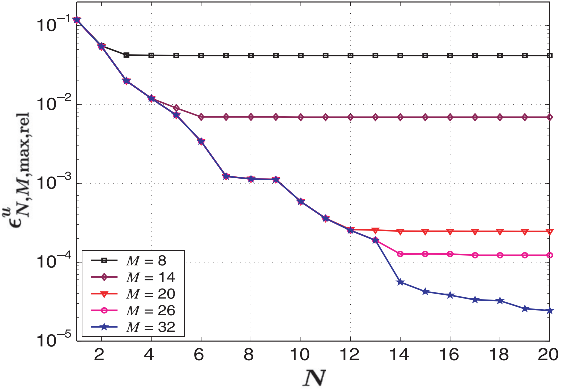
for $x \in \Omega \equiv]0,1[^2$ and $\mu \in \mathcal{D} \equiv [-1,-0.01]^2$.

Maximum relative error and bounds in field variable and output [N]

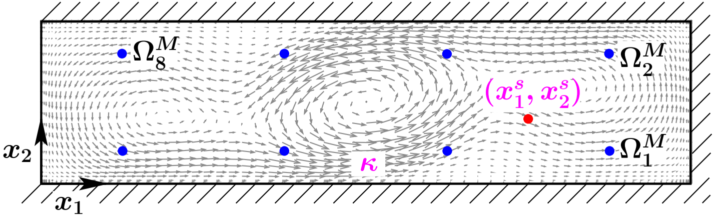
N	M	$\epsilon^u_{\max,\mathrm{rel}}$	$\Delta^u_{\max,\mathrm{rel}}$	$\bar{\eta}^u$	$\epsilon^s_{\max,\mathrm{rel}}$	$\Delta^s_{\max,\mathrm{rel}}$	$\bar{\eta}^s$
4	15	1.20 E−02	1.35 E−02	1.16	5.96 E−03	1.43 E−02	11.32
8	20	1.14 E−03	1.23 E−03	1.01	2.42 E−04	1.30 E−03	13.41
12	25	2.54 E−04	2.77 E−04	1.08	1.76 E−04	2.92 E−04	17.28
16	30	3.82 E−05	3.93 E−05	1.00	7.92 E−06	4.15 E−05	20.40

Model Problem

Maximum relative error in the field variable



Contaminant Transport



Concentration $u(t;\mu)$ of pollutant in Ω governed by scalar convection-diffusion equation $\quad u(x, t=0;\mu) = 0$

$$\frac{\partial}{\partial t} u(t;\mu) + \mathrm{U} \cdot \nabla u(t;\mu) = \kappa \, \nabla^2 u(t;\mu) + g^{\mathrm{PS}}(x;\mu)\, g(t),$$

with source term modeled by

$$g^{\mathrm{PS}}(x;\mu) = \frac{50}{\pi}\, e^{-50((x_1 - x_1^s)^2 + (x_2 - x_2^s)^2)}.$$

Goal: Identify source location $\Rightarrow$ parameter $\mu \equiv (\kappa, x_1^s, x_2^s)$.

Energy Norm & Output Bound

Energy norm bound [Gre05]

$$\Delta^{u\,k}_{N,M}(\mu) = \left\{ \frac{2\Delta t}{\alpha_{\mathrm{LB}}(\mu)} \Bigg(\underbrace{\sum_{k'=1}^{k} \|r^{k'}_{N,M}(\cdot;\mu)\|^2_{X'}}_{\text{affine}} + \underbrace{\hat{\varepsilon}^2_M(\mu) \sum_{k'=1}^{k} \Phi^{\mathrm{na}}_M(t^{k'};\mu)^2}_{\text{nonaffine}} \Bigg) \right\}^{\frac{1}{2}},$$

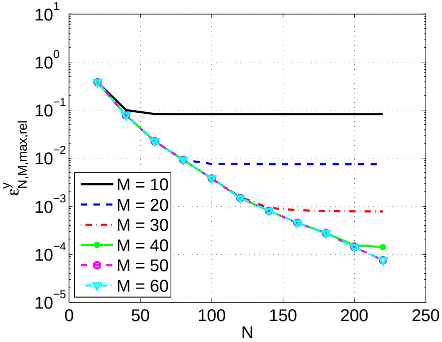
contribution to error bound

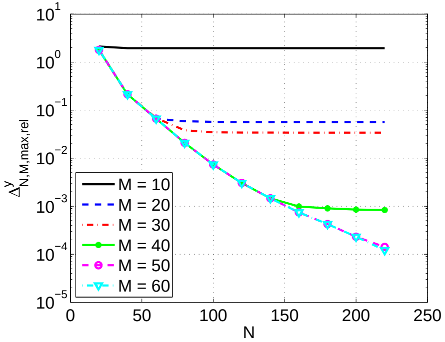
where
$\alpha_{\mathrm{LB}}(\mu)$ ... lower bound of coercivity constant,
$\|r^k_{N,M}(\cdot;\mu)\|_{X'}$ ... dual norm of residual,
$\hat{\varepsilon}_M(\mu)$ ... interpolation induced error.

Output bound

$$\Delta^{s\,k}_{N,M}(\mu) \equiv \left(\sup_{v \in Y} \frac{\ell(v)}{\|v\|_{L^2(\Omega)}} \right) \Delta^{u\,k}_{N,M}(\mu).$$

Contaminant Dispersion – Convergence: Energy Norm





Results for random sample $\Xi_{\mathbf{Test}} \in \boldsymbol{\mathcal{D}}$ of size $\mathbf{2000}$.

Contaminant Dispersion – Convergence: Energy Norm

N	M	$\epsilon^y_{N,M,\max,\mathrm{rel}}$	$\Delta^y_{N,M,\max,\mathrm{rel}}$	$\bar{\eta}^y_{N,M}$
40	20	7.79 E−02	2.13 E−01	3.62
80	30	9.25 E−03	3.80 E−02	3.20
120	40	1.49 E−03	3.05 E−03	2.29
160	50	4.52 E−04	7.43 E−04	2.09
200	60	1.41 E−04	2.32 E−04	2.00

Results for random sample $\Xi_{\mathrm{Test}} \in \mathcal{D}$ of size 2000.

Contaminant Dispersion – Convergence: Output

N	M	$\epsilon^s_{N,M,\max,\mathrm{rel}}$	$\Delta^s_{N,M,\max,\mathrm{rel}}$	$\bar{\eta}^s_{N,M}$
40	20	3.82 E−02	1.86 E+00	61.2
80	30	7.25 E−03	3.32 E−01	64.0
120	40	6.71 E−04	2.65 E−02	66.9
160	50	1.13 E−04	6.47 E−03	78.4
200	60	4.42 E−05	2.02 E−03	74.1

Results for random sample $\Xi_{\mathrm{Test}} \in \mathcal{D}$ of size 2000.

Contaminant Dispersion – Online Computational Times

N	M	$s_{N,M}(t^k;\mu)$	$\Delta^s_{N,M}(t^k;\mu)$	$s(t^k;\mu)$
40	20	4.36 E–03	8.85 E–03	1
80	30	1.09 E–02	1.24 E–02	1
120	40	2.07 E–02	1.73 E–02	1
160	50	3.39 E–02	2.36 E–02	1
200	60	5.11 E–02	3.16 E–02	1

Output & Bound $\forall\, k \in \mathbb{K}$

Truth Problem Statement

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

$$s^k(\mu) = \ell(u^k(\mu))$$

where $u^k(\mu) \in X$, $1 \leq k \leq K$, satisfies $\qquad u^0(\mu) = 0$

$$\frac{1}{\Delta t} m(u^k(\mu) - u^{k-1}(\mu), v) + a(u^k(\mu), v; \mu)$$
$$+ \int_\Omega g^{\mathrm{nl}}(u^k(\mu); x; \mu)\, v = b(v)u(t^k), \ \forall v \in X.$$

Assumptions:

- $g^{\mathrm{nl}} : \mathbb{R} \times \Omega \times \mathcal{D} \to \mathbb{R}$ continuous;
- $g^{\mathrm{nl}}(u_1; x; \mu) \leq g^{\mathrm{nl}}(u_2; x; \mu), \ \forall u_1 \leq u_2$;
- $\forall u \in \mathbb{R}, \ u\, g^{\mathrm{nl}}(u; x; \mu) \geq 0$, for any $x \in \Omega, \ \mu \in \mathcal{D}$.

Standard RB Approach

Sample Computation:

We expand $u_N(t^k;\mu) = \sum_{j=1}^{N} u_{Nj}(t^k;\mu)\,\zeta_j$,

and obtain $\qquad (v = \zeta_i,\ \ i,j \in \mathcal{N})$

$$\int_\Omega g(u_N(t^k;\mu);x;\mu)\zeta_i = \int_\Omega g\left(\sum_{j=1}^{N} u_{Nj}(t^k;\mu)\,\zeta_j;x;\mu\right)\zeta_i$$

$\Rightarrow \mathcal{N}$-dependent online cost.

Note:

- Standard RB-Galerkin recipe suffices for (at most) quadratic nonlinearities: $\mathcal{O}(N^4)$ online cost ([VPP03, VP05, NVP05]...)
- Higher order or nonpolynomial nonlinearities $\Rightarrow$ EIM.

Empirical Interpolation Method

Interpolation Points and Spaces:

$$\begin{aligned} T_M^g &= \{x_1^T \in \Omega, \ldots, x_M^T \in \Omega\} \quad \text{and} \\ W_M^g &= \operatorname{span}\{\xi_m,\ 1 \le m \le M\} \\ &= \operatorname{span}\{q_1, \ldots, q_M\}, \quad 1 \le M \le M_{\max}, \end{aligned}$$

ξ_m are chosen by POD_t-Greedy_μ procedure.

Approximation : for given $w^k(\mu) \in Y$

$$g^{\mathrm{nl}}(w^k(\mu); x; \mu) \approx g_M^{\mathrm{nl}, w^k}(x; \mu) = \sum_{m=1}^{M} \varphi_{Mm}^k(\mu)\, q_m(x),$$

where

$$\sum_{m=1}^{M} q_m(x_n^T)\, \varphi_{Mm}^k(\mu) = g^{\mathrm{nl}}(w(x_n^T, t^k; \mu); x_n^T; \mu),\ 1 \le n \le M.$$

Note: $\varphi_{Mm}^k(\mu) = \varphi_{Mm}(t^k; \mu)$, function of (discrete) time t^k.

Sampling Procedure

POD_t-Greedy_μ Algorithm for EIM [Gre12a]

Set $\mu^* = \mu_0^*,\ W_0^g = \{0\},\ S_0^g = \{0\},\ M = 0$

while $M \le M_{\max}$

$e_{M,\text{EIM}}^k(\mu^*) = g^{\text{nl}}(u^k(\mu^*); x; \mu^*) - g_M^{\text{nl},u^k}(x;\mu^*),\ 1 \le k \le K$

$S_M^g = S_{M-1}^g \cup \mu^*;$

$W_M^g = W_{M-1}^g + \text{POD}_{L^2(\Omega)}(\{e_{M,\text{EIM}}^k(\mu^*), 1 \le k \le K\}, 1);$

$M = M + 1;$

Calculate $x_M,\ q_M;$

$\mu^* = \arg\max_{\mu\in\Xi_{\text{train}}} \sum_{k=1}^K \varepsilon_M^k(\mu);$

end

Galerkin Projection

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

$$s^k_{N,M}(\mu) = \ell(u^k_{N,M}(\mu))$$

where $u^k_{N,M}(\mu) \in W^u_N$, $1 \leq k \leq K$, satisfies $u^0_{N,M}(\mu) = 0$

$$\frac{1}{\Delta t} m(u^k_{N,M}(\mu) - u^{k-1}_{N,M}(\mu), v) + a(u^k_{N,M}(\mu), v; \mu)$$
$$+ \int_\Omega g_M^{\mathrm{nl}, u^k_{N,M}}(x; \mu)\, v = b(v)\, u(t^k), \quad \forall\, v \in W^u_N.$$

Computational Procedure:

- Admits an *offline-online* treatment
- *Online cost*† is $\mathcal{O}(MN^2 + N^3)$ and thus independent of $\mathcal{N}$.

† Cost per Newton iteration per timestep.

Energy Norm & Output Bound

Energy norm bound [Gre12a]

$$\Delta^{u\,k}_{N,M}(\mu) = \left\{ \frac{2\Delta t}{\alpha_{\rm LB}(\mu)} \left(\underbrace{\sum_{k'=1}^{k} \varepsilon^{k'}_{N,M}(\mu)^2}_{\text{linear}} + \underbrace{{\vartheta^q_M}^2 \sum_{k'=1}^{k} \hat{\varepsilon}^{k'}_M(\mu)^2}_{\text{nonlinear}} \right) \right\}^{\frac{1}{2}},$$

contribution to error bound

where $\alpha_{\rm LB}(\mu)$ ... Lower bound of "a"-coercivity constant,
$\varepsilon^{k}_{N,M}(\mu)$ ... dual norm of residual,
$\hat{\varepsilon}^{k}_{M}(\mu)$ ... interpolation induced error.

Output bound

$$\Delta^{s}_{N,M}(t^k;\mu) \equiv \left(\sup_{v \in Y} \frac{\ell(v)}{\|v\|_{L^2(\Omega)}} \right) \Delta^{u\,k}_{N,M}(\mu).$$

Bound Theorem

Proposition

If $g(u^k_{N,M}(\mu); x; \mu) \in W^g_{M+1}$, $1 \le k \le K$, then

$$|||u^k(\mu) - u^k_{N,M}(\mu)||| \le \Delta^{u\,k}_{N,M}(\mu), \quad \forall \mu \in \mathcal{D},\ 1 \le k \le K.$$

and

$$|s^k(\mu) - s^k_{N,M}(\mu)| \le \Delta^{s\,k}_{N,M}(\mu), \quad \forall \mu \in \mathcal{D},\ 1 \le k \le K.$$

for all $1 \le N \le N_{\max}$, $1 \le M \le M_{\max}$.

Note

- In general $g(u^k_{N,M}(\mu); x; \mu) \notin W^g_{M+1}$, thus
$$|||u^k(\mu) - u^k_{N,M}(\mu)||| \lessapprox \Delta^{u\,k}_{N,M}(\mu).$$
- Admits *offline-online* treatment:*online cost* $\mathcal{O}(K(N+M)^2)$.

Model Problem

Given $\mu = (\mu_1, \mu_2) \in \mathcal{D} \equiv [0.01, 10]^2$, evaluate $\qquad \Omega =]0,1[^2$

$$s^k(\mu) = \int_\Omega u^k_{N,M}(\mu)$$

where $u^k_{N,M}(\mu) \in Y$, $1 \le k \le K$, satisfies $\qquad u^0(\mu) = 0$

$$\frac{1}{\Delta t} m(u^k_{N,M}(\mu) - u^{k-1}_{N,M}(\mu), v) + a(u^k_{N,M}(\mu), v) + \int_\Omega g^{\mathrm{nl}}(u^k(\mu); x; \mu)\, v = b(v)\, \sin(2\pi t^k), \quad \forall\, v \in Y,$$

with $g^{\mathrm{nl}}(u^k(\mu); x; \mu) = \mu_1 \dfrac{e^{\mu_2\, y^k(\mu)} - 1}{\mu_2}$.

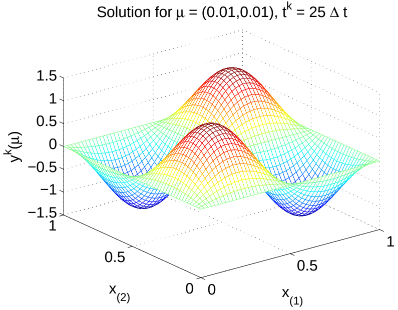
Truth Approximation

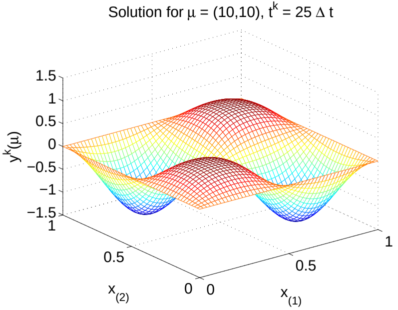
- Space: $Y \subset Y^{\mathrm{e}} \equiv H^1_0(\Omega)$ with dimension $\mathcal{N} = 2601$;
- Time: $\bar{I} = (0, 2]$, $\Delta t = 0.01$, and thus $K = 200$.

Sample Results

Truth solution $y(t^k;\mu)$ at time $t^k = 25\Delta t$ and

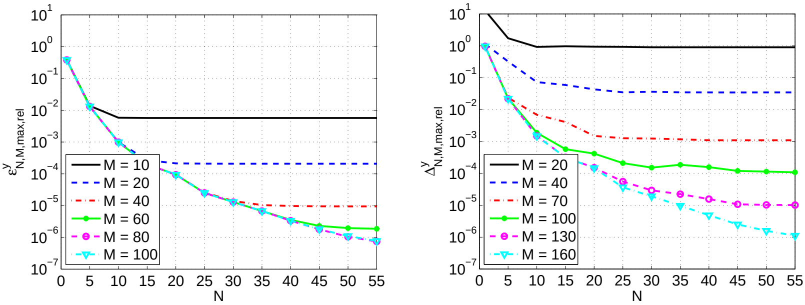
$\mu = (0.01, 0.01)$ $\mu = (10, 10)$





$$b(v) = 100 \int_\Omega v \; \sin(2\pi x_1) \cos(2\pi x_2)$$

Convergence: Energy Norm



Results for sample $\Xi_{\mathbf{test}} \in \mathcal{D}$ of size $\mathbf{225}$.

- "Plateau" in curves for M fixed.
- "Knees" reflect balanced contribution of both error terms.
- Sharp bounds require conservative choice of M.

Convergence: Energy Norm

N	M	$\epsilon^y_{N,M,\max,\mathrm{rel}}$	$\Delta^y_{N,M,\max,\mathrm{rel}}$	$\bar{\eta}^y_{N,M}$
1	40	3.83 E−01	1.15 E+00	2.44
5	60	1.32 E−02	4.59 E−02	2.43
10	80	9.90 E−04	3.41 E−03	2.10
20	100	9.40 E−05	4.16 E−04	2.77
30	120	1.30 E−05	7.34 E−05	2.48
40	140	3.36 E−06	8.75 E−06	1.64

Results for sample $\Xi_{\mathrm{test}} \in \mathcal{D}$ of size $\mathbf{225}$.

- Choose N vs. M such that

$$\text{error}(EIM) \ll \text{error}(RB)$$

to obtain sharp bounds.

Convergence: Output

N	M	$\epsilon^s_{N,M,\max,\mathrm{rel}}$	$\Delta^s_{N,M,\max,\mathrm{rel}}$	$\bar{\eta}^s_{N,M}$
1	40	9.99 E−01	2.49 E+01	14.1
5	60	5.35 E−03	1.00 E+00	130
10	80	2.57 E−04	7.42 E−02	146
20	100	1.43 E−05	9.06 E−03	436
30	120	5.34 E−06	1.60 E−03	307
40	140	2.85 E−06	1.90 E−04	205

Results for sample $\Xi_{\mathrm{test}} \in \mathcal{D}$ of size 225.

- Accuracy of output bound $< 1\%$ for $(N, M) = (20, 100)$.
- Use adjoint techniques for faster convergence.

Online Computational Times

N	M	$s_{N,M}(\mu, t^k)$	$\Delta^s_{N,M}(\mu, t^k)$	$s(\mu, t^k)$
1	40	5.42 E–05	9.29 E–05	1
5	60	9.67 E–05	8.58 E–05	1
10	80	1.19 E–04	9.37 E–05	1
20	100	1.71 E–04	1.05 E–04	1
30	120	2.42 E–04	1.18 E–04	1
40	140	3.15 E–04	1.35 E–04	1

Average CPU times for sample $\Xi_{\text{test}} \in \mathcal{D}$ of size 225.

- Computational savings $\mathcal{O}(10^3)$ for $\Delta^s_{N,M,\text{max,rel}} < 1\%$.
- But offline stage much more expensive than for linear case.

Problem Statement [Gre12b]

Reaction-diffusion equation

$$\frac{\partial \mathrm{y}(\mathrm{x},\mathrm{t};\mu)}{\partial t} = \nabla(D(\mu)\mathrm{y}(x,t;\mu)) + \mathrm{f}(\mathrm{y}(x,t;\mu);\mu)$$

Specific Example: self-ignition of coal stockpile

$$\begin{aligned}\frac{\partial T(x,t)}{\partial t} &= \nabla^2 T(x,t) + \beta\,\Phi^2\,(c(x,t)+1)\,e^{-\gamma/(T(x,t)+1)},\\ \frac{\partial c(x,t)}{\partial t} &= \mathrm{Le}\,\nabla^2 c(x,t) - \Phi^2\,(c(x,t)+1)\,e^{-\gamma/(T(x,t)+1)},\end{aligned}$$

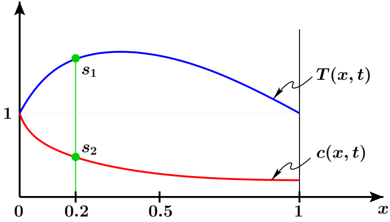
where

γ : Arrhenius number,

β : Prater temperature,

Le : Lewis number,

Φ : Thiele modulus.



Problem Statement

We consider

- $\boldsymbol{\beta = 4.287}$,
- $\mathbf{Le = 0.233}$,
- $\boldsymbol{\Phi^2 = 70000}$ fixed, and
- $\boldsymbol{\mu \equiv \gamma \in [12, 12.6]}$;

$\Rightarrow$ exhibits very rich dynamic behavior for this parameter range.

Truth Approximation:

- FE in space with $\boldsymbol{\mathcal{N} = 800}$,
- FD in time with $\boldsymbol{\Delta t = 0.001}$, $\boldsymbol{K = 6000}$.

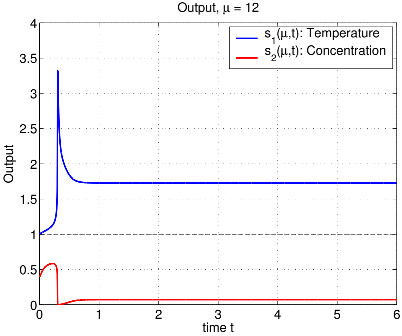
Note

- Nonlinearity not monotonic: *a posterior* error bounds not valid.

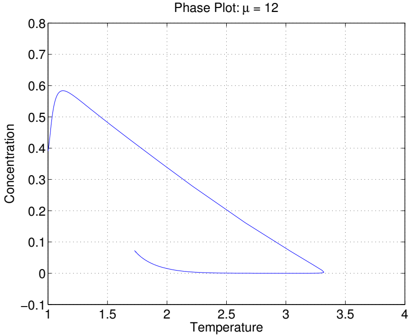
Sample Results

Temperature and Concentration for $\mu = 12.0$

as a function of time



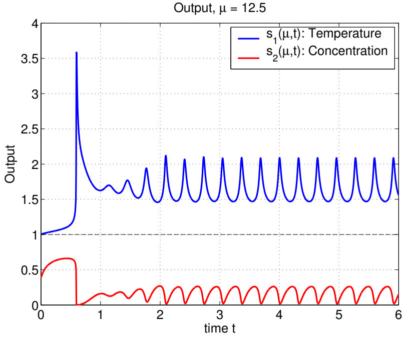
as a phase plane plot

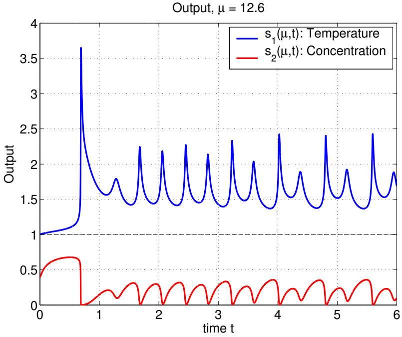


Sample Results

Outputs as a function of time for

$\mu = 12.5$ $\mu = 12.6$

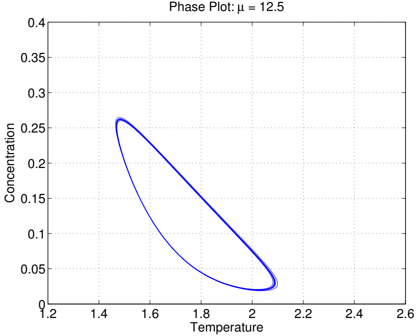




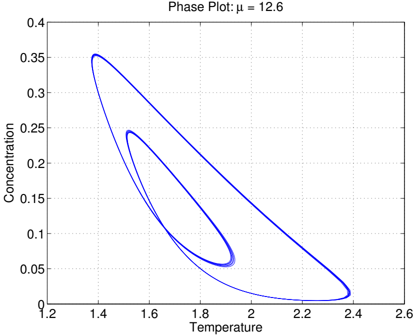
Sample Results

Phase Plane plot for

$\boldsymbol{\mu = 12.5}$



$\boldsymbol{\mu = 12.6}$

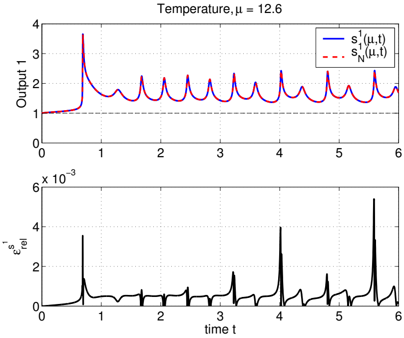


Reduced Basis Approximation

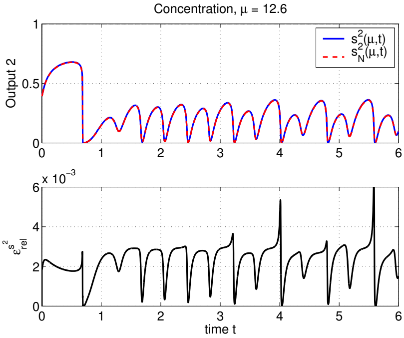
RB: $N_T = 20, N_c = 22,\ M = 44$.

Truth and RB Approximation for $\mu = 12.6$

Temperature



Concentration



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