Model Reduction Methods

Application to Parameter Estimation and Optimal Control

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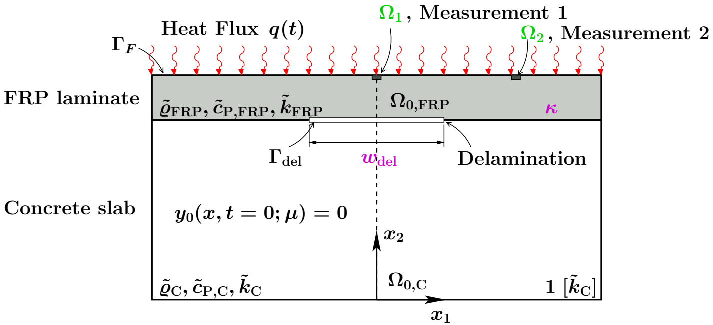
Concrete Delamination [HJN], [S]



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

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

Problem Statement

Given $(\mu_1, \mu_2) \in \mathcal{D} \equiv [1, 5] \times [0.5, 2.0]$, 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, $X_0 \equiv \{v \in H^1(\Omega_0(\mu_1)) | \; v|_{\Gamma_{\text{bottom}}} = 0\}$; $y_0(t^0; \mu) = 0$.

Problem Statement

$$\frac{1}{\Delta t}\int_{\Omega_0(\mu_1)} (y_0(t^k;\mu) - y_0(t^{k-1};\mu))\, v_0$$

$$+ \quad \mu_2 \int_{\Omega_{0,\mathrm{FRP}}(\mu_1)} \nabla y_0(t^k;\mu)\cdot\nabla v_0$$

$$+ \int_{\Omega_{0,\mathrm{C}}(\mu_1)} \nabla y_0(t^k;\mu)\cdot\nabla v_0 = u(t^k)\int_{\Gamma_{\mathrm{F}}} v_0 \ ,$$

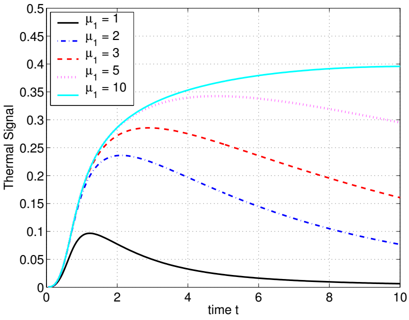
$$\forall v_0 \in X_0,$$

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

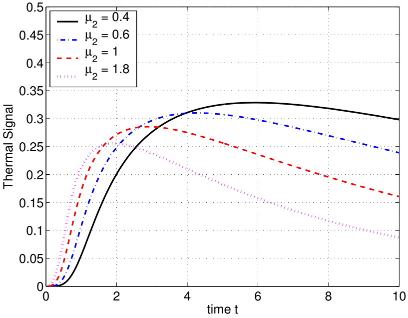
Numerical Results

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

$\kappa = 1$



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



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?

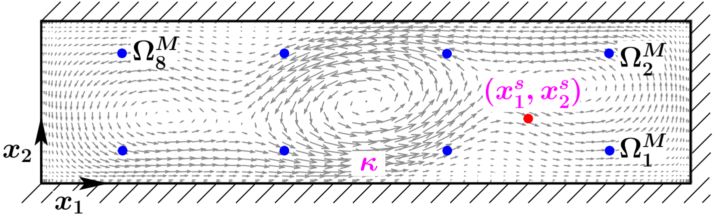
Contexts: Real-time & Many Query

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

Contaminant Transport

- Application: Identification of Sources

Dispersion of a pollutant $\Omega = [0,4] \times [0,1]$



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

(say, $\mu \equiv (\kappa, x_1^s, x_2^s)$)

† Thanks to K Veroy for providing the velocity field.

Contaminant Transport – Problem Statement

Scalar Convection-Diffusion $y(x, t = 0; \mu) = 0$

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

INPUTS: $\mu \equiv (\kappa, x_1^s, x_2^s) \in \mathcal{D} \subset \mathbb{R}^{P=3}$, where

$$\mathcal{D} = [0.05, 0.5] \times [2.9, 3.1] \times [0.3, 0.5];$$

$\mathrm{U}(\mathrm{Gr} = 10^5)$ from $\mathrm{Pr} = 0$

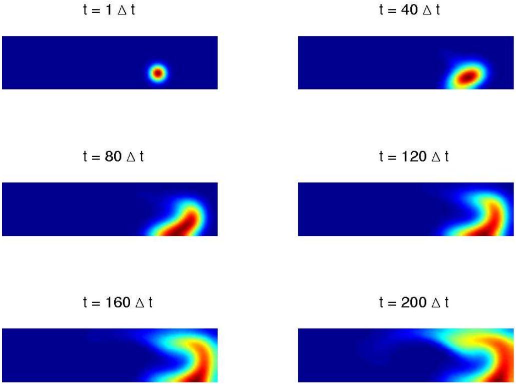
Natural Convection (Navier-Stokes);

$u(t)$ “control” input (source strength).

OUTPUTS: Measurements $s_q(t;\mu)$, $1 \le q \le 8$.

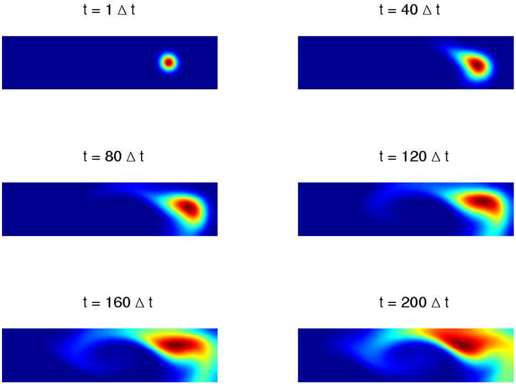
Contaminant Transport – Sample Solutions

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



Contaminant Transport – Sample Solutions

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



Parameter Estimation

In the "field," can we deduce

- the source location (x_1^s, x_2^s), and
- the release time,

from noisy measurements of

- the contaminant concentrations?

Contexts: Real-time & Many Query

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

RB Relevance

Real-Time Context (control, . . .):

$$\begin{array}{ccc} \mu & \rightarrow & s_N(\mu),\ \Delta^s_N(\mu). \\ t_0 \ (\text{“need”}) & & t_0 + \partial t_{\text{comp}} \ (\text{“response”}) \end{array}$$

Many-Query Context (design, . . .):

$$\begin{array}{ccc} \mu_j & \rightarrow & (s_N(\mu_j),\ \Delta^s_N(\mu_j)),\ j = 1,\ldots,J. \\ t_0 & & t_0 + \partial t_{\text{comp}}\, J \text{ as } J \rightarrow \infty \end{array}$$

$\Rightarrow$ Low marginal (real-time) and/or low average (many-query) cost.

Problem Statement

Determine: $\mu^* \in \mathcal{D}$ (actual value)

Given experimental data

measurements : $s_{\rm exp}(t^k) = s^{\mathcal{N}}(t^k;\mu^*) + \epsilon^k_{\rm exp},\ \forall k \in \mathbb{K}_{\rm exp}$,

observations : $\mathbb{K}_{\rm exp} \subset \mathbb{K} \equiv \{1,\dots,K\},\ n_{\rm exp} \equiv |\mathbb{K}_{\rm exp}|$,

error : $\epsilon^k_{\rm exp} \sim \mathcal{N}(0,\sigma^2_{\rm exp}),\ \sigma_{\rm exp} \in \mathbb{R}$ (Gaussian, white),

input : $u(t^k) = \delta_{1k},\ \forall k \in \mathbb{K}$ or specified "online"

Classical Results [MT]

We define the

- likelihood function

$$\Pi_{\exp}(s_{\exp}|\mu) = (2\pi\sigma_{\exp}^2)^{-\frac{n_{\exp}}{2}}\, e^{-\frac{\|s_{\exp}-s_{\mathrm{pre}}(\mu)\|^2}{2\sigma_{\exp}^2}},$$

  for $s_{\mathrm{pre}}^k(\mu) = s^{\mathcal{N}}(t^k;\mu),\ \forall k \in \mathbb{K}_{\exp}$;

- prior distribution on μ

$$\Pi_0(\mu) = (2\pi\sigma_0^2)^{-\frac{P}{2}}\, e^{-\frac{\|\mu-\mu_0\|^2}{2\sigma_0^2}},$$

  where μ_0 . . . prior mean;
  σ_0^2 . . . associated variance.

Classical Results

We then obtain the expected value

$$\mathbf{E}[\mu^*|s_{\rm exp}] = \frac{\int_{\mathcal{D}} \mu\, \Pi_{\rm exp}(s_{\rm exp}|\mu)\, \Pi_0(\mu)\, d\mu}{\int_{\mathcal{D}} \Pi_{\rm exp}(s_{\rm exp}|\mu)\, \Pi_0(\mu)\, d\mu}$$

$$\text{“}=\text{”} \quad \frac{\sum_{j=1}^{n_{\rm quad}} \omega_j\, \mu_j\, \Pi_{\rm exp}(s_{\rm exp}|\mu_j)\, \Pi_0(\mu_j)\, d\mu}{\sum_{j=1}^{n_{\rm quad}} \omega_j\, \Pi_{\rm exp}(s_{\rm exp}|\mu_j)\, \Pi_0(\mu)\, d\mu}$$

$\Rightarrow$ requires $n_{\rm quad}$ evaluations $\{\mu \rightarrow s^{\mathcal{N}}(t^k;\mu),\ \forall k \in \mathbb{K}_{\rm exp}\}$

Reduce cost of forward evaluations by

- POD-based model reduction [WZ]
- RB approach & *a posteriori* error estimation [NRHP]

Certified Reduced Basis

Let $s_N^{k\pm} = s_N^k \pm \Delta_N^{s\,k}$, then define

$$B_N^k(\mu) = \max\{|s_{\exp}^k - s_N^{k-}|, |s_{\exp}^k - s_N^{k+}|\}$$

$\Rightarrow B_N^k(\mu) \geq s_{\exp}^k - s_{\mathrm{pre}}^k(\mu), \;\forall k \in \mathbb{K}_{\exp}$

$\Rightarrow$ overestimation of diff(experimental data, model prediction)

and

$$D_N^k(\mu) = \begin{cases} 0, & \text{if } s_{\exp}^k \in [s_N^{k-}, s_N^{k+}] \\ \min\{|s_{\exp}^k - s_N^{k-}|, |s_{\exp}^k - s_N^{k+}|\}, & \text{otherwise} \end{cases}$$

$\Rightarrow D_N^k(\mu) \leq s_{\exp}^k - s_{\mathrm{pre}}^k(\mu), \;\forall k \in \mathbb{K}_{\exp}$

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$\Rightarrow D_N^k(\mu) \leq s_{\exp}^k - s_{\mathrm{pre}}^k(\mu), \; \forall k \in \mathbb{K}_{\exp}$

$\Rightarrow$ underestimation of diff(experimental data, model prediction)

Certified Reduced Basis

We introduce

$$\Pi^B_{\exp N}(s_{\exp}|\mu) = (2\pi\sigma^2_{\exp})^{-\frac{n_{\exp}}{2}}\, e^{-\frac{\|B(\mu)\|^2}{2\sigma^2_{\exp}}},$$

$$\Pi^D_{\exp N}(s_{\exp}|\mu) = (2\pi\sigma^2_{\exp})^{-\frac{n_{\exp}}{2}}\, e^{-\frac{\|D(\mu)\|^2}{2\sigma^2_{\exp}}},$$

and note that

$$\Pi^B_{\exp N}(s_{\exp}|\mu) \le \Pi_{\exp}(s_{\exp}|\mu) \le \Pi^D_{\exp N}(s_{\exp}|\mu),$$

Define

$$E^{LB}_N[\mu^*|s_{\exp}] = \frac{\sum_{j=1}^{n_{\text{quad}}} \omega_j\, \mu_j\, \Pi^B_{\exp N}(s_{\exp}|\mu_j)\, \Pi_0(\mu_j)\, d\mu}{\sum_{j=1}^{n_{\text{quad}}} \omega_j\, \Pi^D_{\exp N}(s_{\exp}|\mu_j)\, \Pi_0(\mu)\, d\mu}$$

$$E^{UB}_N[\mu^*|s_{\exp}] = \frac{\sum_{j=1}^{n_{\text{quad}}} \omega_j\, \mu_j\, \Pi^D_{\exp N}(s_{\exp}|\mu_j)\, \Pi_0(\mu_j)\, d\mu}{\sum_{j=1}^{n_{\text{quad}}} \omega_j\, \Pi^B_{\exp N}(s_{\exp}|\mu_j)\, \Pi_0(\mu)\, d\mu}$$

Certified Reduced Basis

We introduce

$$\Pi^B_{\exp N}(s_{\exp}|\mu) = (2\pi\sigma^2_{\exp})^{-\frac{n_{\exp}}{2}} \, e^{-\frac{\|B(\mu)\|^2}{2\sigma^2_{\exp}}},$$

$$\Pi^D_{\exp N}(s_{\exp}|\mu) = (2\pi\sigma^2_{\exp})^{-\frac{n_{\exp}}{2}} \, e^{-\frac{\|D(\mu)\|^2}{2\sigma^2_{\exp}}},$$

and note that

$$\Pi^B_{\exp N}(s_{\exp}|\mu) \leq \Pi_{\exp}(s_{\exp}|\mu) \leq \Pi^D_{\exp N}(s_{\exp}|\mu),$$

Define

$$\mathrm{E}^{\mathrm{LB}}_N[\mu^*|s_{\exp}] = \frac{\sum_{j=1}^{n_{\mathrm{quad}}} \omega_j \, \mu_j \, \Pi^B_{\exp N}(s_{\exp}|\mu_j) \, \Pi_0(\mu_j) \, d\mu}{\sum_{j=1}^{n_{\mathrm{quad}}} \omega_j \, \Pi^D_{\exp N}(s_{\exp}|\mu_j) \, \Pi_0(\mu) \, d\mu}$$

$$\mathrm{E}^{\mathrm{UB}}_N[\mu^*|s_{\exp}] = \frac{\sum_{j=1}^{n_{\mathrm{quad}}} \omega_j \, \mu_j \, \Pi^D_{\exp N}(s_{\exp}|\mu_j) \, \Pi_0(\mu_j) \, d\mu}{\sum_{j=1}^{n_{\mathrm{quad}}} \omega_j \, \Pi^B_{\exp N}(s_{\exp}|\mu_j) \, \Pi_0(\mu) \, d\mu}$$

Certified Reduced Basis

- Certainty

$$\mathbf{E}_N^{\mathbf{LB}}[\mu^*|s_{\exp}] \leq \mathbf{E}[\mu^*|s_{\exp}] \leq \mathbf{E}_N^{\mathbf{UB}}[\mu^*|s_{\exp}]$$

- Accuracy

$$\mathbf{E}_N^{\mathbf{UB}}[\mu^*|s_{\exp}] - \mathbf{E}_N^{\mathbf{LB}}[\mu^*|s_{\exp}] \approx \mathcal{F}_P(\Delta_N^s(\cdot))$$

- Efficiency

Online cost $s_{\exp} \longrightarrow \mathbf{E}_N^{\mathbf{LB}}[\mu^*|s_{\exp}],\ \mathbf{E}_N^{\mathbf{UB}}[\mu^*|s_{\exp}]$
is $n_{\text{quad}}\, \partial t_{\text{comp}}$ independent of $\mathcal{N}$

In fact, Offline + Online cost is $\approx n_{\text{quad}}\, \partial t_{\text{comp}}$
as $n_{\text{quad}} \longrightarrow \infty$ (many-query).

Concrete Delamination – Numerical Results

	Delamination half-width			Conductivity ratio		
N	$\mathsf{E}_N^{\mathrm{LB}}[\mu_{1\star}]$	$\mathsf{E}_N^{\mathrm{UB}}[\mu_{1\star}]$	$\Delta\mathsf{E}_N[\mu_{1\star}]$	$\mathsf{E}_N^{\mathrm{LB}}[\mu_{2\star}]$	$\mathsf{E}_N^{\mathrm{UB}}[\mu_{2\star}]$	$\Delta\mathsf{E}_N[\mu_{2\star}]$
10	1.0527	7.5175	6.4648	0.3427	2.4468	2.1041
20	2.3896	3.3120	0.9224	0.7764	1.0759	0.2996
30	2.7417	2.8836	0.1419	0.8917	0.9378	0.0461
40	2.8008	2.8236	0.0228	0.9111	0.9185	0.0074
50	2.8096	2.8192	0.0096	0.9136	0.9171	0.0035

Table: Lower bound, upper bound, and bound gap for expected value of delamination half-width $\boldsymbol{\mu_1}$ and conductivity ratio $\boldsymbol{\mu_2}$ as a function of $\boldsymbol{N}$. The true parameter value is $\boldsymbol{\mu_1^* = 2.8}$ and $\boldsymbol{\mu_2^* = 0.9}$. Source: [NRHP].

Problem Statement

Determine: $\mu^* \in \mathcal{D}$ (actual value)

Given experimental data

measurements : $z(t^k) \in \mathcal{Z}^k_{\text{exp}}, \ \forall k \in \mathbb{K}_{\text{exp}}$, where

$$\mathcal{Z}^k_{\text{exp}} \equiv [s^{\mathcal{N}}(t^k;\mu^*) - \epsilon_{\text{exp}}, s^{\mathcal{N}}(t^k;\mu^*) + \epsilon_{\text{exp}}]$$

observations : $\mathbb{K}_{\text{exp}} \subset \mathbb{K} \equiv \{1, \ldots, K\}$

error : $\epsilon_{\text{exp}} \in \mathbb{R}$ (bounded, “white”)

input : $u(t^k) = \delta_{1k}, \ \forall k \in \mathbb{K}$

Parameter Estimation – (Regularized) Solution

Given noisy measurements, $z(t^k)$, $k \in \mathbb{K}_{\text{exp}}$, solve

- Output least squares problem

$$\hat{\mu} = \arg\min_{\mu \in \mathcal{D}} \frac{1}{2} \sum_{k=1}^{\mathbb{K}_{\text{exp}}} \| s_{\mathcal{N}}(t^k;\mu) - z(t^k) \|_W^2$$

s.t. $\text{PDE}_{\mathcal{N}}(\mu)$ being satisfied; or

- Regularized problem

$$\hat{\mu} = \arg\min_{\mu \in \mathcal{D}} \frac{1}{2} \sum_{k=1}^{\mathbb{K}_{\text{exp}}} \| s_{\mathcal{N}}(t^k;\mu) - z(t^k) \|_W^2 + \frac{1}{2}\delta_R R(\mu)$$

s.t. $\text{PDE}_{\mathcal{N}}(\mu)$ being satisfied.

Parameter Estimation – (Regularized) Solution

Given noisy measurements, $z(t^k)$, $k \in \mathbb{K}_{\text{exp}}$, solve

- Output least squares problem

$$\hat{\mu} = \arg\min_{\mu \in \mathcal{D}} \frac{1}{2} \sum_{k=1}^{\mathbb{K}_{\text{exp}}} \| s_{\mathcal{N}}(t^k; \mu) - z(t^k) \|_W^2$$

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s.t. $\text{PDE}_{\mathcal{N}}(\mu)$ being satisfied.

$\Rightarrow$ Solution expensive: $\mathcal{N}$-dependent cost

Parameter Estimation – (Regularized) Solution

Given noisy measurements, $z(t^k)$, $k \in \mathbb{K}_{\text{exp}}$, solve

- Output least squares problem

$$\hat{\mu} = \arg\min_{\mu \in \mathcal{D}} \frac{1}{2} \sum_{k=1}^{\mathbb{K}_{\text{exp}}} \| s_N(t^k; \mu) - z(t^k) \|_W^2$$

s.t. $\text{PDE}_N(\mu)$ being satisfied; or

- Regularized problem

$$\hat{\mu} = \arg\min_{\mu \in \mathcal{D}} \frac{1}{2} \sum_{k=1}^{\mathbb{K}_{\text{exp}}} \| s_N(t^k; \mu) - z(t^k) \|_W^2 + \frac{1}{2} \delta_R R(\mu)$$

s.t. $\text{PDE}_N(\mu)$ being satisfied.

$\Rightarrow$ Surrogate model approach: N-dependent cost

Uncertainty Region – Truth Approximation

$\Rightarrow$ "Classic" solution neglects measurement errors $\epsilon_{\mathbf{exp}}$

(Truth) "Uncertainty Region" Approach

$$\mathcal{U}_{\mathcal{N}} \equiv \{\mu \in \mathcal{D} \,|\, s^{\mathcal{N}}(t^k;\mu) \in \mathcal{Z}^k_{\mathbf{exp}}, \ \forall k \in \mathbb{K}_{\mathbf{exp}}\}$$

$$\Big(\text{OR} \quad \mathcal{B}_{\mathcal{N}} \equiv [\mu^{\min} = \min_{\mu \in \mathcal{U}_{\mathcal{N}}} \mu, \mu^{\max} = \max_{\mu \in \mathcal{U}_{\mathcal{N}}} \mu] \ \Big)$$

. . . all parameter values in $\mathcal{D}$ consistent with experimental data

$$\longrightarrow \mu^* \in \mathcal{U}_{\mathcal{N}} \subset \mathcal{B}_{\mathcal{N}}$$

but expensive to construct.

Goal: Approximation $\mathcal{U}_N$ to $\mathcal{U}_{\mathcal{N}}$, such that

- $\mathcal{U}_{\mathcal{N}} \subset \mathcal{U}_N$, and hence $\mu^* \in \mathcal{U}_N$ — *RELIABILITY*
- $\mathcal{U}_N$ is inexpensive to construct — *EFFICIENCY*

Uncertainty Region – RB Approach

Define

$$\mathcal{I}_N^k(\mu) \equiv [s_N(t^k;\mu) - \Delta_N^s(t^k;\mu), s_N(t^k;\mu) + \Delta_N^s(t^k;\mu)], \quad \forall k \in \mathbb{K}_{\mathrm{exp}}$$

and

$$\mathcal{U}_N \equiv \left\{\mu \in \mathcal{D} \mid \mathcal{I}_N^k(\mu) \cap \mathcal{Z}_{\mathrm{exp}}^k \neq \emptyset, \ \forall k \in \mathbb{K}_{\mathrm{exp}}\right\}.$$

We then obtain: $\mathcal{U}_{\mathcal{N}} \subset \mathcal{U}_N \rightarrow \mu^* \in \mathcal{U}_N$

$\mathcal{U}_N$ reflects uncertainty in

- experimental data through $\mathcal{Z}_{\mathrm{exp}}^k$
- RB approximation through $\mathcal{I}_N^k(\mu)$

$\mathcal{U}_N \rightarrow \mathcal{U}_{\mathcal{N}}$ as $\Delta_N^s(t^k;\mu) \rightarrow 0$ *ACCURACY*

Construction of $\tilde{\mathcal{U}}_N$

1. Find μ_{IC}[†]:

$$\mu_{\text{IC}} = \arg\min_{\mu \in \mathcal{D}} \sum_{k \in \mathbb{K}_{\text{exp}}} \frac{1}{2} \| s_N(t^k; \mu) - \overline{\mathcal{Z}}^k_{\text{exp}} \|^2 .$$

2. Find boundary points $\hat{\mu}_j$:

   binary chop along J directions d_j, $1 \leq j \leq J$, from μ_{IC}.

3. Smallest Enclosing Ellipsoid (Box) for $\hat{\mu}_j$, $1 \leq j \leq J$.

NOTE[‡]: In general, $\mathcal{U}_N \not\subset \tilde{\mathcal{U}}_N$ not guaranteed,

but $\tilde{\mathcal{U}}_N \to \mathcal{U}_N$ for $J \to \infty$ and $\mathcal{U}_N$ convex.

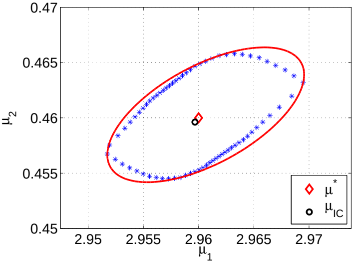
† $\overline{\mathcal{Z}}^k_{\text{exp}} = \frac{1}{2}(\mathcal{Z}^{k,\text{LB}}_{\text{exp}} + \mathcal{Z}^{k,\text{UB}}_{\text{exp}})$

‡ See [NGPL] for a $\tilde{\mathcal{U}}_N$ such that $\mathcal{U}_N \subset \tilde{\mathcal{U}}_N$ provable under certain conditions.

Contaminant Transport – Sample Solution

Solve for μ_{IC} & $\tilde{\mathcal{U}}_N$: $T_{\mathrm{CPU}} = 1.35 + 70.0$ sec †

(892 forward solutions, $J = 72$)

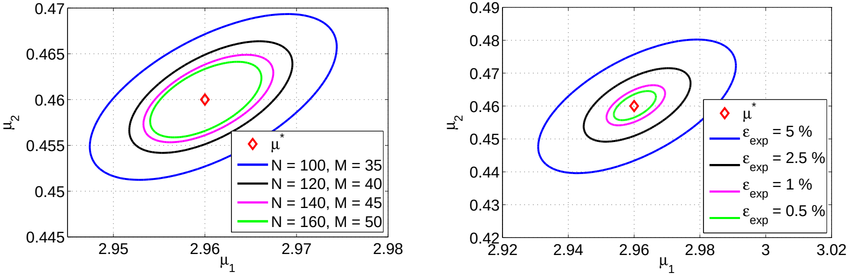


Here, $\epsilon_{\mathrm{exp}} = 1.0\%$, $N = 120$, $M = 40$,

$\mathbb{K}_{\mathrm{exp}} = \{10, 20, \ldots, 200\}$, $\mathcal{S}_{\mathrm{exp}} = \{1, 2, 3, 4\}$

† MATLAB 7.5 on Intel DualCore 1.8GHz

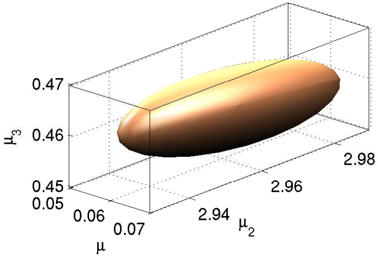
Contaminant Transport – Sensitivity: $\Delta^s_{N,M}$ and ϵ_{exp}

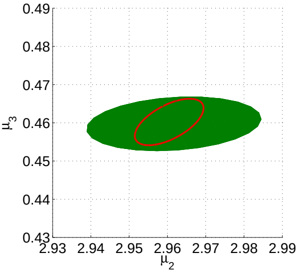


Here, $\mathbb{K}_{\mathrm{exp}} = \{10, 20, \ldots, 100\}$, $\mathcal{S}_{\mathrm{exp}} = \{1, 2, 3, 4\}$

Contaminant Transport – Sensitivity: uncertainty in κ

Increased uncertainty in (μ_2, μ_3) due to unknown κ





Here, $\mu^* = (0.06, 2.96, 0.46)$, $\epsilon_{\text{exp}} = 1.0\%$, $N = 120$, $M = 40$, $\mathbb{K}_{\text{exp}} = \{10, 20, \ldots, 200\}$, $\mathcal{S}_{\text{exp}} = \{1, 2, 3, 4\}$

Contaminant Transport – Sensitivity: release time

So far: time of release, $t^{k_{rel}}$, assumed known

$$\longrightarrow \ u(t^k) = \delta_{1k}, \ \forall k \in \mathbb{K}$$

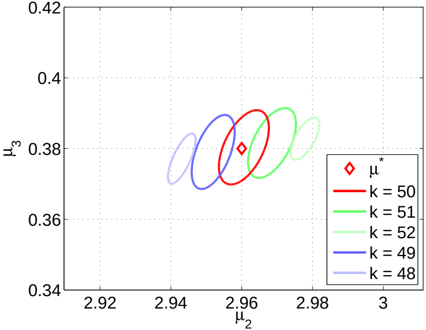
Extension: consider $t^{k_{rel}}$ unknown, then

$$\tilde{\mu}_{\mathrm{IC}} = \arg\min_{\tilde{\mu} \in \tilde{\mathcal{D}}} \sum_{k' \in \mathbb{K}_{\mathrm{exp}}} \frac{1}{2} \| s_N^{\delta}(t^{k'} - t^{k-1}; \mu) - \mathcal{Z}_{\mathrm{exp}}^{k'} \|^2 .$$

where $\tilde{\mu} \equiv (t^k; \mu) \in \tilde{\mathcal{D}} \equiv \{t^1, \ldots, t^K\} \times \mathcal{D}$, and
$s_N^{\delta}(t^k; \mu)$ impulse response for $u(t^k) = \delta_{1k}, \forall k \in \mathbb{K}$.

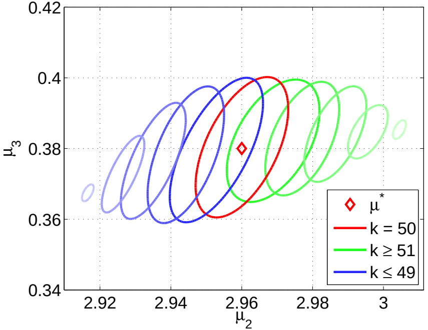
Approach:
1. Solve for $\tilde{\mu}_{\mathrm{IC}}$ (and thus $t^{k_{rel}}$)
2. Given $t^{k_{rel}}$, construct $\tilde{\mathcal{U}}_N$ in $\mu_2 - \mu_3$ space

Contaminant Transport – Sensitivity: release time



Here, $\epsilon_{\mathbf{exp}} = 1.0\%, \mu^* = (0.06, 2.96, 0.38),\ t^{k_{rel}} = 50,$
$N = 120,\ M = 40,\ \mathbb{K}_{\mathbf{exp}} = \{10, 20, \ldots, 200\},$
$\mathcal{S}_{\mathbf{exp}} = \{1, 2, 3, 4\}$

Contaminant Transport – Sensitivity: release time



Here, $\epsilon_{\mathbf{exp}} = \mathbf{2.5\%}, \boldsymbol{\mu}^* = (\mathbf{0.06}, \mathbf{2.96}, \mathbf{0.38}),\ \boldsymbol{t}^{\boldsymbol{k_{rel}}} = \mathbf{50}$, $\boldsymbol{N} = \mathbf{120}$, $\boldsymbol{M} = \mathbf{40}$, $\mathbb{K}_{\mathbf{exp}} = \{\mathbf{10}, \mathbf{20}, \ldots, \mathbf{200}\}$, $\boldsymbol{\mathcal{S}}_{\mathbf{exp}} = \{\mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{4}\}$

Problem Statement[†]

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

$$J(y^{\mathrm{e}}(t;\mu), u(t;\mu); \mu) =$$

$$\frac{1}{2}\int_0^{t_f} \|y^{\mathrm{e}}(t;\mu) - y_d(t)\|_Z^2 \, dt + \frac{\gamma}{2}\int_0^{t_f} (u(t;\mu) - u_d(t))^2 \, dt$$

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

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

with initial condition $y_0 = 0$.

[†] Luca Dedè, *Reduced Basis Method and A Posteriori Error Estimation for Parametrized Linear-Quadratic Optimal Control Problems.*

Truth Approximation

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, evaluate $\qquad t^k = k\Delta t,\ 1 \le k \le K$

$$J(y(\mu), u(\mu); \mu) =$$

$$\frac{\Delta t}{2}\left(\frac{1}{2}\|y^K(\mu) - y_d^K\|_Z^2 + \sum_{k=1}^{K-1}\|y^k(\mu) - y_d^k\|_Z^2\right) + \frac{\gamma}{2}\left(\frac{1}{2}(u^K(\mu) - u_d^K)^2 + \sum_{k=1}^{K-1}(u^k(\mu) - u_d^k)^2\right)$$

where $y^k(\mu) \equiv y(t^k; \mu) \in X$ satisfies $\qquad \forall k \in \mathbb{K}$

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

with initial condition $y_0 = 0$.

First Order Necessary Conditions – Truth

- State Equation $\quad 1 \le k \le K, \ \forall\, v \in X$
  $$m\left(\frac{y^k(\mu)-y^{k-1}(\mu)}{\Delta t}, v; \mu\right) + a(y^k(\mu), v; \mu) = b(v;\mu)\, u^k.$$
  with initial condition $y_0 = 0$.

- Adjoint $\quad 1 \le k \le K-1, \ \forall\, v \in X$
  $$m\left(v, \frac{p^k(\mu)-p^{k+1}(\mu)}{\Delta t}; \mu\right) + a(v, p^k(\mu); \mu) = (y^k(\mu) - y_d^k, v)_Z.$$
  with final condition $\quad \forall\, v \in X$
  $$m\left(v, p^K(\mu); \mu\right) + a(v, p^K(\mu); \mu) = \tfrac{1}{2}(y^K(\mu) - y_d^K, v)_Z.$$

- Optimality Condition $\quad 1 \le k \le K,$
  $$b(p^k(\mu);\mu) + \gamma(u^k(\mu) - u_d^k) = 0,$$
  and
  $$b(p^K(\mu);\mu) + \tfrac{1}{2}\gamma(u^K(\mu) - u_d^K) = 0.$$

First Order Necessary Conditions – RB

- State Equation $\quad 1 \le k \le K, \ \forall\, v \in X_N$

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

with initial condition $y_{N,0} = 0$.

- Adjoint $\quad 1 \le k \le K-1, \ \forall\, v \in X_N$

$$m\left(v, \frac{p_N^k(\mu) - p_N^{k+1}(\mu)}{\Delta t}; \mu\right) + a(v, p_N^k(\mu); \mu) = (y_N^k(\mu) - y_d^k, v)_Z.$$

with final condition $\quad \forall\, v \in X_N$

$$m\left(v, p_N^K(\mu); \mu\right) + a(v, p_N^K(\mu); \mu) = \tfrac{1}{2}(y_N^K(\mu) - y_d^K, v)_Z.$$

- Optimality Condition $\quad 1 \le k \le K,$

$$b(p_N^k(\mu); \mu) + \gamma(u_N^k(\mu) - u_d^k) = 0,$$

and

$$b(p_N^K(\mu); \mu) + \tfrac{1}{2}\gamma(u_N^K(\mu) - u_d^K) = 0.$$

A Posteriori Error Bound

Proposition (L. Dedè)

Given $\boldsymbol{\mu} \in \mathcal{D}$, the reduced basis error in the cost functional is bounded by

$$|J^*(\boldsymbol{\mu}) - J_N^*(\boldsymbol{\mu})| \lessapprox \Delta_N^J(\boldsymbol{\mu}), \quad \forall \boldsymbol{\mu} \in \mathcal{D},$$

and for all $1 \leq N \leq N_{\max}$.

Here, the error bound is defined as

$$\Delta_N^J(\boldsymbol{\mu}) \equiv \Delta_N^K(\boldsymbol{\mu})\, \Delta_N^{\mathrm{du},1}(\boldsymbol{\mu}),$$

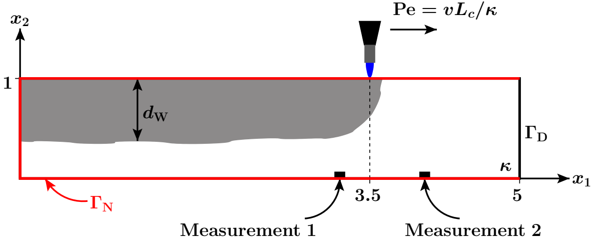
where $\Delta_N^K(\boldsymbol{\mu})$ and $\Delta_N^{\mathrm{du},1}(\boldsymbol{\mu})$ are the energy norm error bounds for the primal and adjoint problem, respectively.

Note: Extension to the control constraint case also possible.

GMA Welding Process [SH93],[SH94]

- Application: Real-time parameter estimation and control

Welding Process $\Omega = [0,5] \times [0,1]$



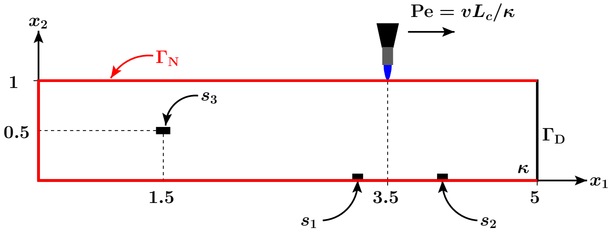
Torch: $q_{\mathrm{w}}(x;\mu) = \frac{\eta_{\mathrm{w}}}{2\pi\sigma_{\mathrm{w}}^2}\, e^{-((x_1-3.5)^2+(x_2-1)^2)/(2\sigma_{\mathrm{w}}^2)}$,

$$\mu \equiv (\eta_{\mathrm{w}}, \sigma_{\mathrm{w}})$$

GMA Welding Process [SH93],[SH94]

- Application: Real-time parameter estimation and control

Introduce "fictitious" output s_3 $\qquad \Omega = [0,5] \times [0,1]$



Torch: $q_\mathrm{w}(x;\mu) = \frac{\eta_\mathrm{w}}{2\pi\sigma_\mathrm{w}^2}\, e^{-((x_1-3.5)^2+(x_2-1)^2)/(2\sigma_\mathrm{w}^2)}$,

$$\mu \equiv (\eta_\mathrm{w}, \sigma_\mathrm{w})$$

GMA Welding Process – Problem Statement

Scalar Convection-Diffusion $y(x, t = 0; \mu) = 0$

$$\frac{\partial}{\partial t} y(t;\mu) + \mathrm{Pe} \cdot \frac{\partial}{\partial x} y(t;\mu) = \kappa \nabla^2 y(t;\mu) + q_{\mathrm{w}}(x;\mu)\, u(t),$$

INPUTS: $\mu \equiv (\eta_{\mathrm{w}}, \sigma_{\mathrm{w}}) \in \mathcal{D} \subset \mathbb{R}^{P=2}$, where

$$\mathcal{D} = [0.1, 0.4] \times [0.15, 0.65];$$

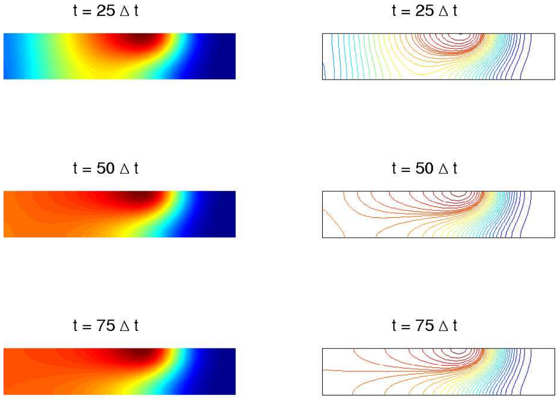
Torch velocity Pe;

$u(t)$ “control” input (source strength).

OUTPUTS: Measurements 1 & 2.

GMA Welding Process – Sample Solution

Field variable: $\mu = (0.3, 0.4)$ $(\mathcal{N} = 3720)$



GMA Welding Process – Results

Approach to real-time parameter estimation and control:

1. Start welding with nominal control $u_{\mathrm{n}}(t)$
2. Take temperature measurements $z_{1,2}(t)$ of outputs $s_{1,2}(t;\mu)$
3. Solve parameter estimation problem for μ^*
   $\Rightarrow$ PDE$_{(N)}(\mu)$-constrained optimization problem
4. Given μ^*, solve optimal control problem for $u^*(t)$
   $\Rightarrow$ PDE$_{(N)}(\mu)$-constrained optimization problem
5. Apply optimal control law $u^*(t)$

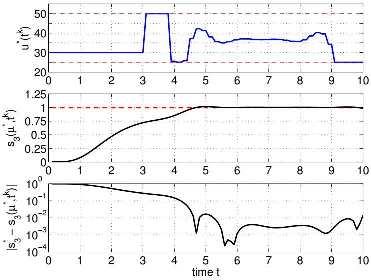
(6. Go to 2. - Model Predictive Control)

GMA Welding Process – Results

Parameter estimation & control: $\mu^* = (0.34, 0.46)$, $s_{d,3}(t) = 1$

$\mu_{\rm IC} = (0.339, 0.463)$

$\epsilon_{\rm exp} = 1\%$, $f_s = 5$ Hz



$\mu_{\rm IC} = (0.334, 0.473)$

$\epsilon_{\rm exp} = 5\%$, $f_s = 5$ Hz