Parametric Manifold Models for Validation;

Verification for Parametric Manifold Models

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(F Fahroo)

Multi-Scale Fusion of Information Uncertainty Quantification and Management in Large-Scale Simulations

Brown: K Karniadakis, J Hesthaven, B Rozovsky
Caltech: T Hou
Cornell: N Zabaras
MIT: A Patera, K Willcox

Frequentist

Validation Framework

with

“Exact”† Model

† Exact in the sense of verification, not validation.

“Exact” Model

Given $\boldsymbol{\mu} \in \boldsymbol{\mathcal{D}} \subset \mathbb{R}^{\boldsymbol{P}}$, $\boldsymbol{\mu}$: parameter $\boldsymbol{P}$-vector

$$\boldsymbol{u}^{\mathbf{model}}(\,\cdot\,;\boldsymbol{\mu}) \in \boldsymbol{X}(\boldsymbol{\Omega})\ ,$$

for $\boldsymbol{\Omega}$ a domain in $\mathbb{R}^{\boldsymbol{d}}$.

Note the field $\boldsymbol{u}^{\mathbf{model}}(\boldsymbol{x};\boldsymbol{\mu})$ may derive from a *parametrized* partial differential equation.†

† In an example we also consider time-dependent fields.

Measurements of Physical System

Given measurement functionals,

$$\ell_i^{\text{meas}}\colon X \to \mathbb{R},\ 1 \le i \le m\ ,$$

assume experiments yield outputs

$$Y_i^{\text{exp}} = \underbrace{\ell_i^{\text{meas}}(u^{\text{phy}})}_{Y_i^{\text{phy}}} + \epsilon(\omega_i),\ 1 \le i \le m\ ,$$

for $\epsilon(\omega)$ a zero-mean Gaussian process.

Note $u^{\text{phy}}(x)$ serves to “interpret” Y_i^{phy}.

Validation Hypothesis

For given $\mu \in \mathcal{D}$, $\delta \geq 0$

$$\mathcal{H}(\mu): \begin{cases} \text{For all } \mu' \in \mathcal{N}_\delta(\mu) \ , \\ \qquad \| Y^{\text{phy}} - Y^{\text{model}}(\mu') \| \leq \delta \ . \end{cases}$$

Here $Y_i^{\text{model}}(\mu') = \ell_i^{\text{meas}}(u^{\text{model}}(\,\cdot\,;\mu'))$, $1 \leq i \leq m$;
$\mathcal{N}_\delta(\mu)$ a neighborhood in $\mathcal{D}$ about μ.

Note: $\mathcal{H}(\mu)$ FALSE, $\forall\, \mu \in \mathcal{D} \Rightarrow$ "unmodeled physics."

Statistical Test

For any $\mu \in \mathcal{D}$,

REJECT $\mathcal{H}(\mu)$ vs. ACCEPT $\mathcal{H}(\mu)$

if and only if

$$\mathcal{F}_{\epsilon}(Y^{\text{exp}}, Y^{\text{model}}(\mu)) > B_{\delta}(\mu) \; ;$$

require $\mathbf{Pr}\{\mathbf{Error}_{\mathbf{Type\,I}}\} \leq 1 - \gamma$.†

† $\mathcal{H}(\mu)$ TRUE: $\mathbf{Pr}\{$REJECT $\mathcal{H}(\mu)\} \leq 1 - \gamma$.

Frequentist Validation Framework

with

Approximate Model

Approximate Model

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, μ: parameter P-vector

$$\tilde{u}^{\text{model}}(\,\cdot\,;\mu) \in \tilde{X}(\Omega) \subset X(\Omega)\ ,$$

where $\tilde{u}(\mu) \approx u^{\text{model}}(\mu)$.

Introduce $\tilde{Y}_i^{\text{model}}(\mu) = \ell_i^{\text{meas}}(\tilde{u}(\,\cdot\,;\mu))$, $1 \le i \le m$.

Measurements of Physical System

Given measurement functionals,

$$\ell_i^{\text{meas}}\colon X \to \mathbb{R},\ 1 \le i \le m\ ,$$

assume experiments yield outputs

$$Y_i^{\text{exp}} = \underbrace{\ell_i^{\text{meas}}(u^{\text{phy}})}_{Y_i^{\text{phy}}} + \epsilon(\omega_i),\ 1 \le i \le m\ ,$$

for $\epsilon(\omega)$ a zero-mean Gaussian process.

Note $u^{\text{phy}}(x)$ is an "interpretation" of Y_i^{phy}.

Validation Hypothesis

For given $\mu \in \mathcal{D}$, $\delta \geq 0$

$$\mathcal{H}(\mu)\text{:}\ \left\{ \begin{array}{l} \text{For all } \mu' \in \mathcal{N}_\delta(\mu)\ , \\ \qquad \|Y^{\text{phy}} - Y^{\text{model}}(\mu')\| \leq \delta\ . \end{array} \right.$$

Here $Y_i^{\text{model}}(\mu') = \ell_i^{\text{meas}}(u^{\text{model}}(\,\cdot\,;\mu'))$, $1 \leq i \leq m$;
$\mathcal{N}_\delta(\mu)$ a neighborhood in $\mathcal{D}$ about μ.

Note: $\mathcal{H}(\mu)$ FALSE, $\forall\, \mu \in \mathcal{D} \Rightarrow$ "unmodeled physics."

Statistical Test

For any $\mu \in \mathcal{D}$,

REJECT $\mathcal{H}(\mu)$ vs. ACCEPT $\mathcal{H}(\mu)$

if and only if

$$\mathcal{F}_\epsilon(Y^{\text{exp}}, \tilde{Y}^{\text{model}}(\mu)) > \underbrace{\tilde{B}_\delta(\mu)}_{\text{Verification}} \quad ; \quad (\geq B_\delta(\mu))$$

require $\mathbf{Pr}\{\mathbf{Error}_{\mathbf{Type\,I}}\} \leq 1 - \gamma$.†

† $\mathcal{H}(\mu)$ TRUE: $\mathbf{Pr}\{\text{REJECT } \mathcal{H}(\mu)\} \leq 1 - \gamma$.

Statistical Test

For many $\mu \in \mathcal{D}$,

REJECT $\mathcal{H}(\mu)$ vs. ACCEPT $\mathcal{H}(\mu)$

if and only if

$$\mathcal{F}_\epsilon(Y^{\rm exp}, \tilde{Y}^{\rm model}(\mu)) > \tilde{B}_\delta(\mu) \quad ; \quad (\geq B_\delta(\mu))$$

Verification

require $\mathbf{Pr}\{\mathbf{Error}_{\mathbf{Type\,I}}\} \leq 1 - \gamma$.†

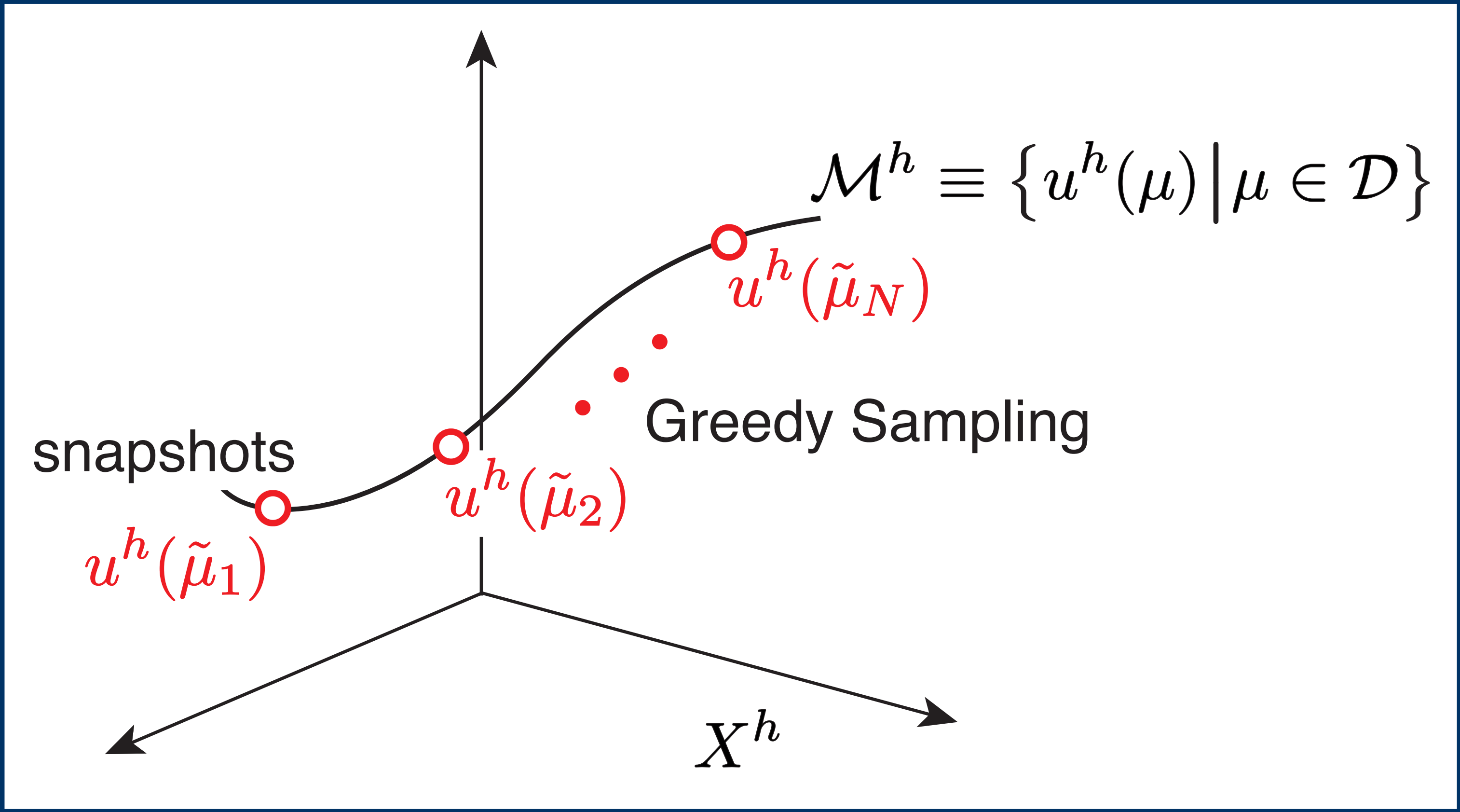
† $\mathcal{H}(\mu)$ TRUE: $\mathbf{Pr}\{$REJECT $\mathcal{H}(\mu)\} \leq 1 - \gamma$.

Parametric Manifold Models

Approximation Space

Parametric Manifold $\mathcal{M}^h$

Introduce $u^h(\mu) \in X^h \subset X$: a highly accurate finite element (FE) surrogate for $u^{\mathrm{model}}(\mu)$.



Approximation Space: $\tilde{X}_{\mathcal{D}} = \mathrm{span}\{u^h(\tilde{\mu}_n), 1 \le n \le N\}$.

Parametric Manifold Models

Approximation Space

Reduced Basis (RB)

Galerkin Projection

Given weak form (parametrized PDE),

$$\mu \in \mathcal{D} \rightarrow \mathcal{A}(w, v; \mu),\ \forall\, w, v \text{ in } X(\Omega)\ ,^{\dagger}$$

$\tilde{u}_{\mathrm{RB}} \in \tilde{X}_{\mathcal{D}}$ satisfies

$$\mathcal{A}(\tilde{u}_{\mathrm{RB}}, v; \mu) = 0,\ \forall\, v \in \tilde{X}_{\mathcal{D}}\ .$$

Advantage: $N = \dim(\tilde{X}_{\mathcal{D}}) \ll \dim(X^h)$.

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†Note $u^{\mathrm{model}}(\mu) \in X$: $\mathcal{A}(u^{\mathrm{model}}(\mu), v; \mu) = 0,\ \forall\, v \in X$;

$u^h(\mu) \in X^h$: $\mathcal{A}(u^h(\mu), v; \mu) = 0,\ \forall\, v \in X^h$.

A Posteriori Error Estimation

For any $\mu \in \mathcal{D}$,

$$
\begin{aligned}
&\|\tilde{u}_{\mathrm{RB}}(\mu) - u^{\mathrm{model}}(\mu)\|_X \\
&\quad \le \|\tilde{u}_{\mathrm{RB}}(\mu) - u^h(\mu)\|_X + \|u^h(\mu) - u^{\mathrm{model}}(\mu)\|_X \\
&\quad \approx \|\tilde{u}_{\mathrm{RB}}(\mu) - u^h(\mu)\|_X \; ; \qquad \text{OFFLINE-ONLINE}
\end{aligned}
$$

provide rigorous error bound

$$
\|\tilde{u}_{\mathrm{RB}}(\mu) - u^h(\mu)\| \le \Delta^h_{\mathrm{RB}}(\mu) \; ,
$$

where $\Delta^h_{\mathrm{RB}}(\mu) \equiv C^h_{\mathrm{stability}}(\mu) \, \|\mathcal{A}(\tilde{u}_{\mathrm{RB}}, \cdot \, ; \mu)\|_{(X^h)'}$.

OFFLINE-ONLINE Computational Strategy

OFFLINE Construct $\tilde{X}_{\mathcal{D}}$ (once): expensive.

ONLINE Evaluate $\mu \to \tilde{u}_{\mathrm{RB}}$, Δ^h_{RB}: inexpensive.

In the many-query (or real-time) context, *amortize* OFFLINE effort over many ONLINE evaluations.

Note: ONLINE cost independent of dim(X^h), hence choose X^h conservatively rich.

Parametric Manifold Models

Approximation Space

Reduced Basis (RB)

Empirical Interpolation (EI)

Collocation

OFFLINE: Given $\tilde{X}_{\mathcal{D}}$, identify

quasi optimal interpolation points $\tilde{x}_k$;

associated characteristic functions $V_k \in \tilde{X}_{\mathcal{D}}$;

for $1 \leq k \leq N$.

ONLINE: For $\mu \in \mathcal{D}$, form $\tilde{u}_{\mathrm{EI}}(\mu) \in \tilde{X}_{\mathcal{D}}$ as

$$\tilde{u}_{\mathrm{EI}}(x;\mu) = \sum_{k=1}^{N} u^h(\tilde{x}_k;\mu) V_k(x) \;.^{\dagger}$$

Advantage: $\Omega \subset \mathbb{R}^d$ replaced by $\{\tilde{x}_k\}_{k=1,\ldots,N}$.

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† In practice, EI applied to *functions* of *approximations* of $u^h(\mu)$.

Parameter Manifold Models

Approximation Space

Reduced Basis (RB)

Empirical Interpolation (EI)

Dirty Laundry

Issues

Difficulty	Palliative
Stability Constant, $C^h_{\text{stability}}$	Successive Constraint
$P \gg 1$: $\mu \in \mathcal{D} \subset \mathbb{R}^P$	Domain Decomposition in Ω
$\mathcal{D}$ Large: $\mu \in \mathcal{D} \subset \mathbb{R}^P$	Domain Decomposition in $\mathcal{D}$
Nonpolynomial Nonlinearity	Empirical Interpolation
Long-Time Integration	Space-Time Inf-Sup

Numerical Example

Cast of Characters

"Exact" Model:

$$(\mu_1, \mu_2) \in \mathcal{D} \to u^{\mathrm{model}}(t, x; \mu) \in X$$

FE Surrogate: $\dim(X^h) \approx 3{,}000$

$$(\mu_1, \mu_2) \in \mathcal{D} \to u^h(t, x; \mu) \in X^h$$

RB Approximate Model: $\dim(\tilde{X}_{\mathcal{D}}) \leq 40^{\dagger}$

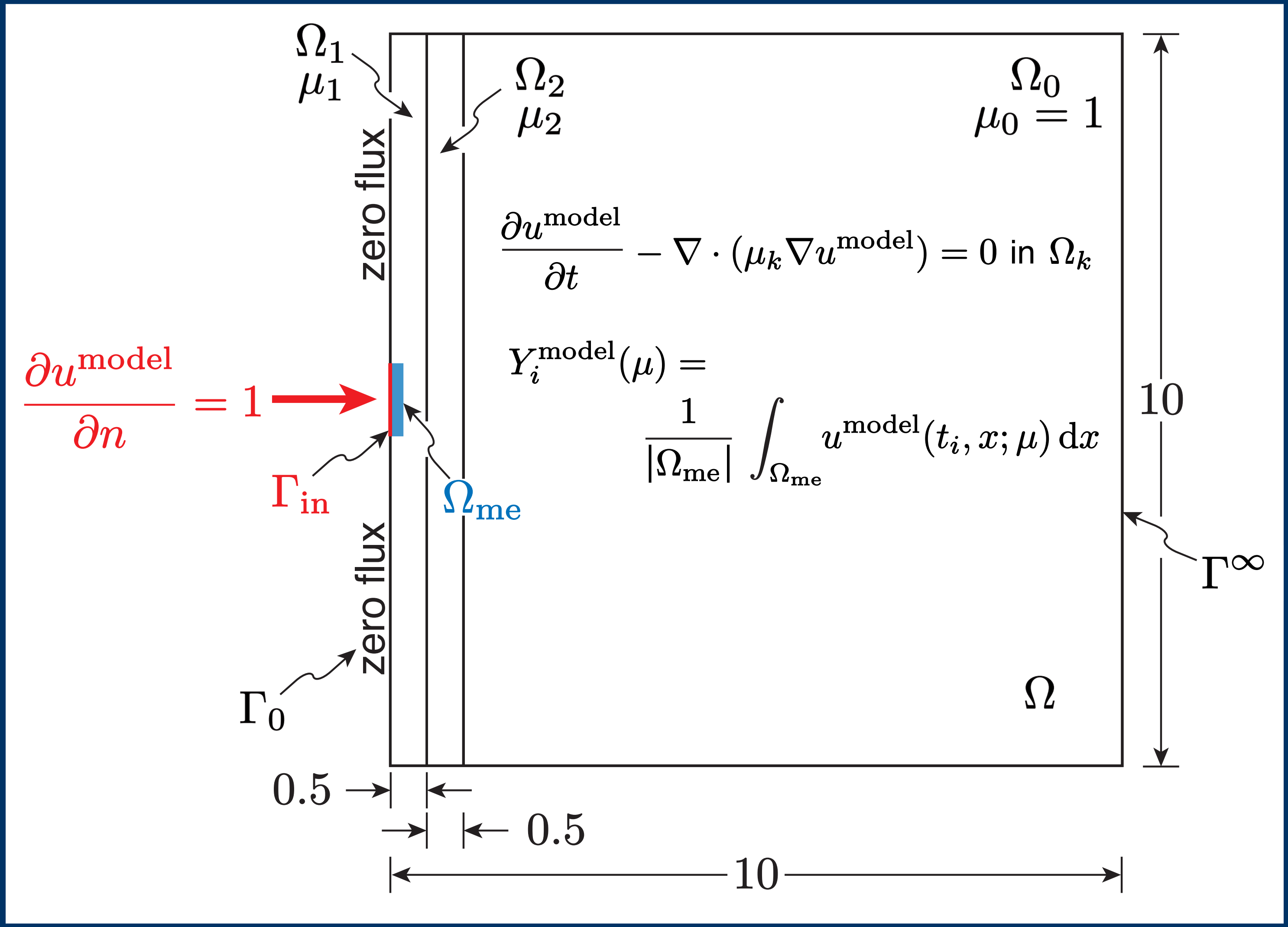
$$(\mu_1, \mu_2) \in \mathcal{D} \to \tilde{u}_{\mathrm{RB}}(t, x; \mu) \in \tilde{X}_{\mathcal{D}},\ \Delta^h_{\mathrm{RB}}(t, \mu)$$

Physical System: $u^{\mathrm{phy}}(t, x)$

---

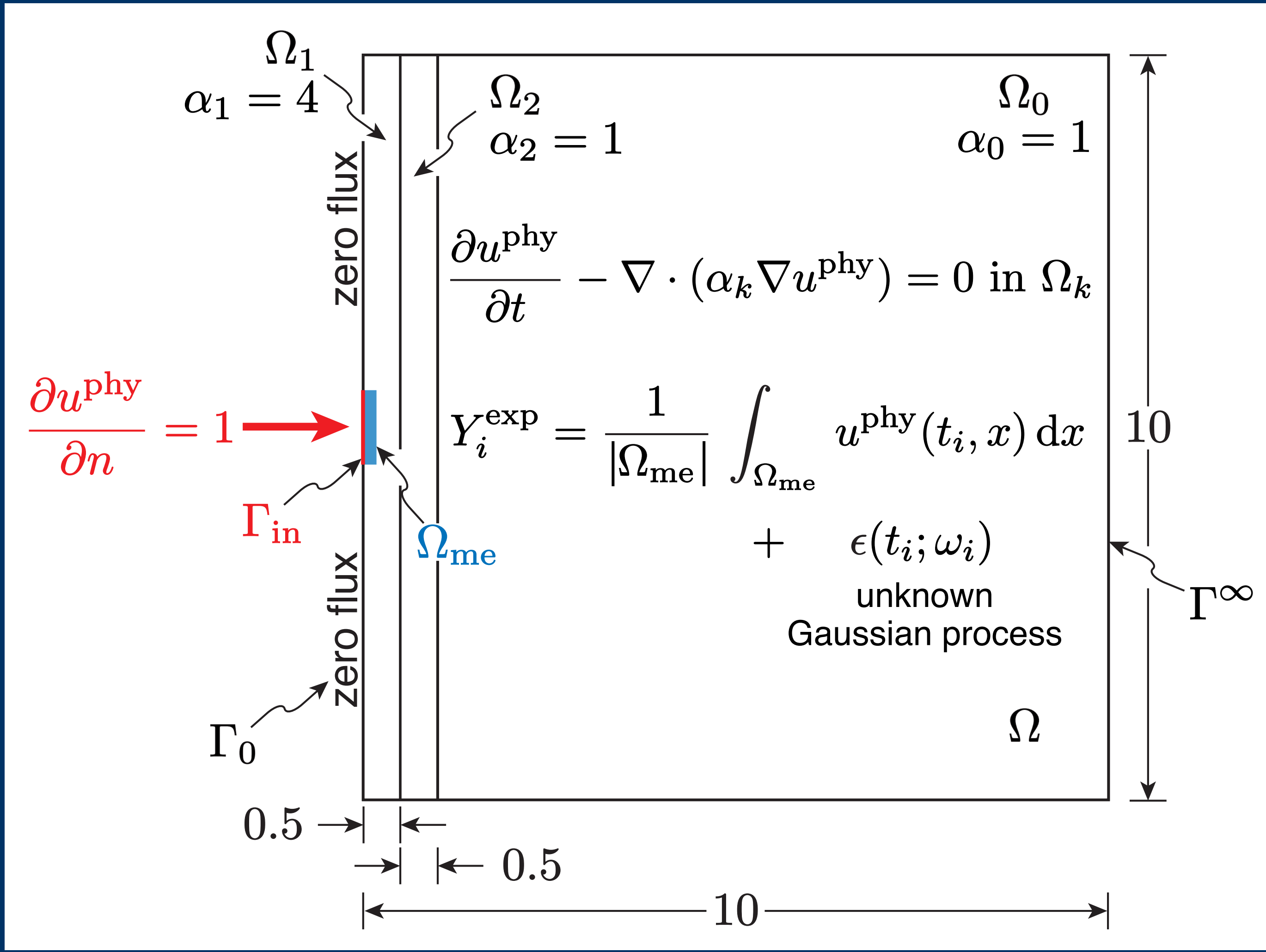
†RB $100\times$ faster (ONLINE) than FE.

Case I: Model



Parametrization: $\boldsymbol{\mu} \equiv (\boldsymbol{\mu_1}, \boldsymbol{\mu_2}) \in [\mathbf{0.2}, \mathbf{5}]^2 \equiv \boldsymbol{\mathcal{D}}$.

Case I: Physical System
(fully modeled physics)

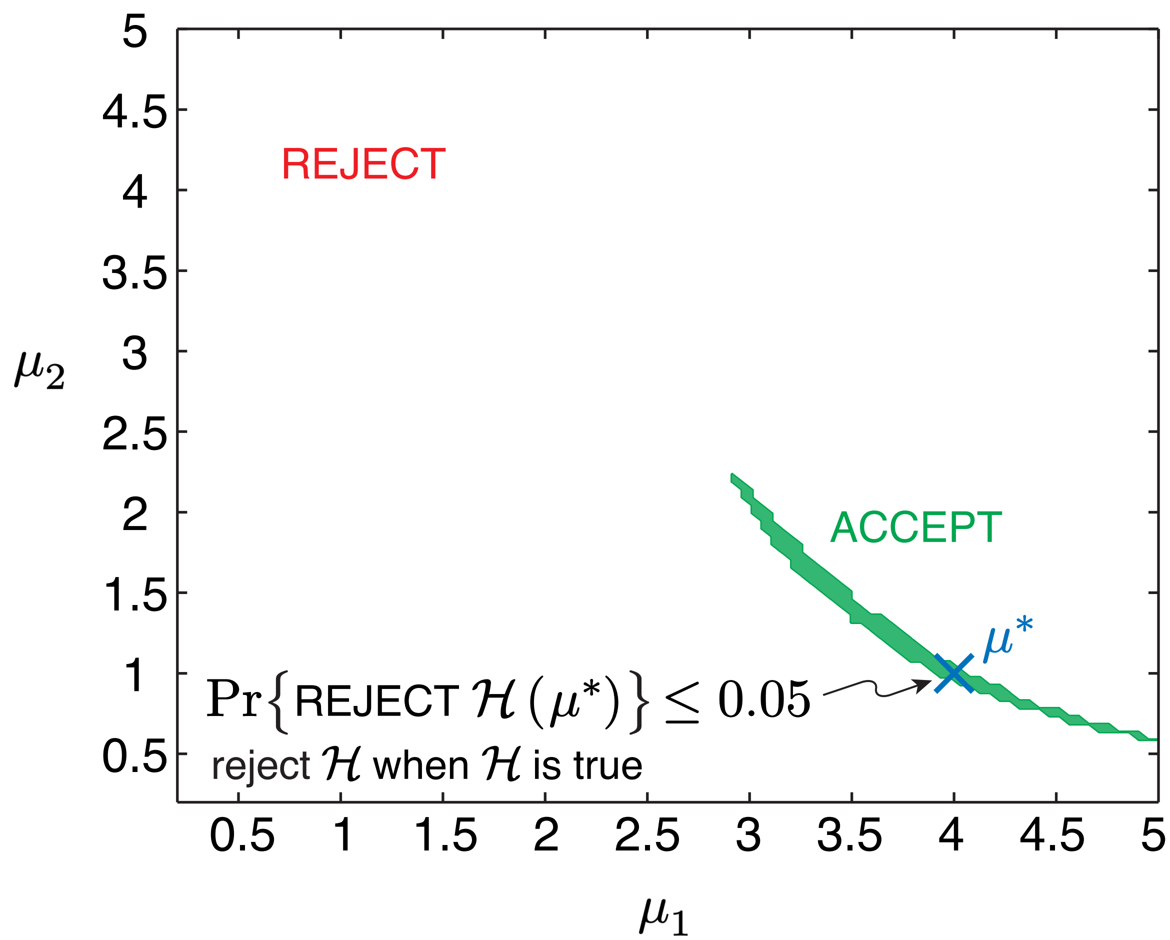


$$u^{\mathrm{phy}}(t,x) = u^{\mathrm{model}}(t,x;\mu^* \equiv \underbrace{(4,1)}_{(\alpha_1,\alpha_2)})^{\dagger}.$$

† In practice, $u^{\mathrm{model}}(t,x;\mu^*)$ replaced by $u^h(t,x;\mu^*)$.

Case I: Validation

(noise: $\approx 1\%$, uncorrelated)



Case I: Effort

Experiment (*synthetic*):

$$m = \mathbf{10} \text{ repeats} \times \mathbf{100} \text{ measurements in time}$$

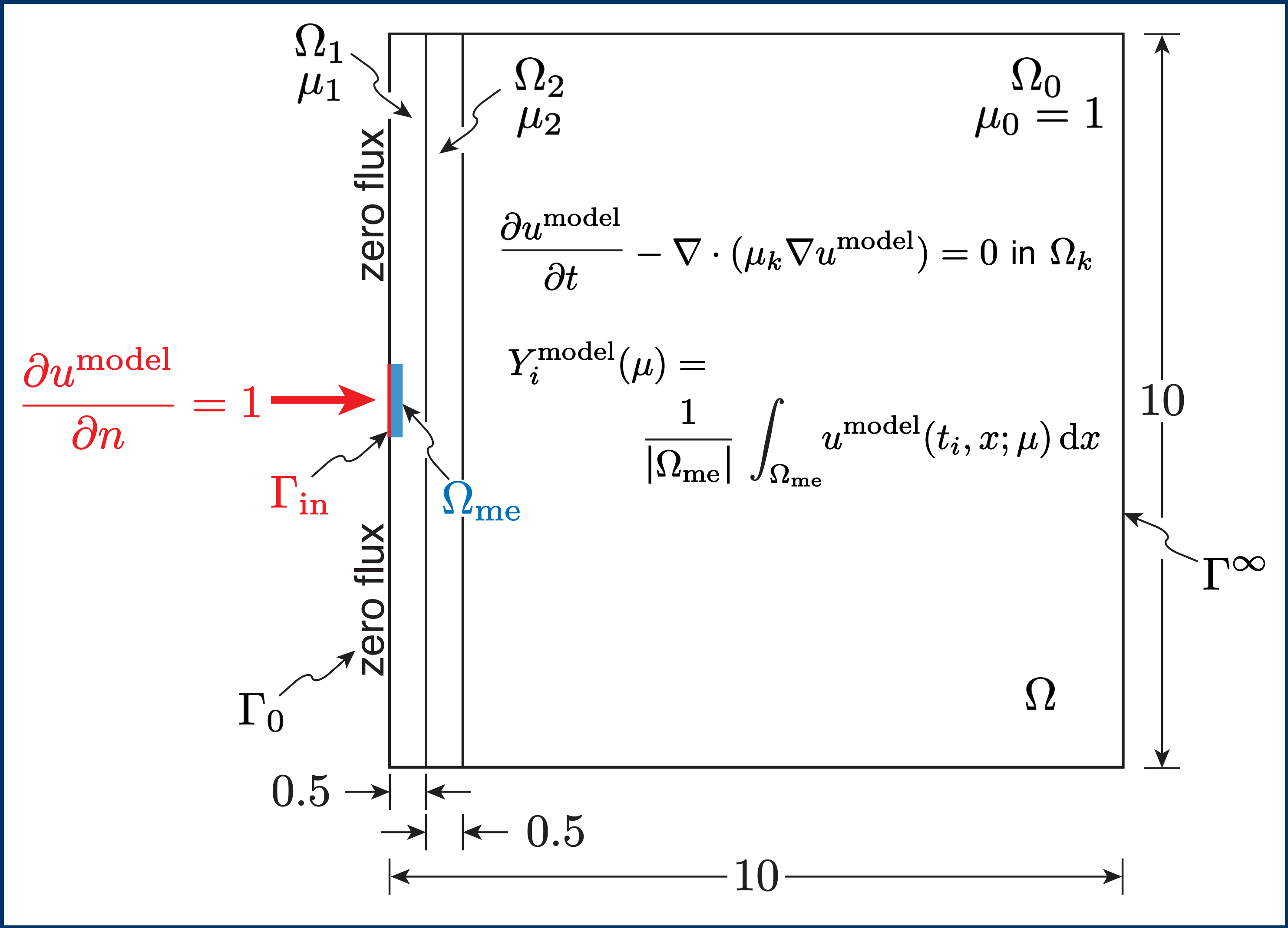
$$= \mathbf{1{,}000} \text{ data in total.}$$

Computation: $\mathbf{10{,}000}$ ONLINE evaluations

$$\boldsymbol{\mu \to \tilde{Y}^{\mathrm{model}}(\mu),\ \Delta^{h}_{\mathrm{RB}}(\mu),\ \tilde{B}_{\delta}(\mu)}$$

$\Rightarrow$ ACCEPT or REJECT $\boldsymbol{\mathcal{H}(\mu)}$.

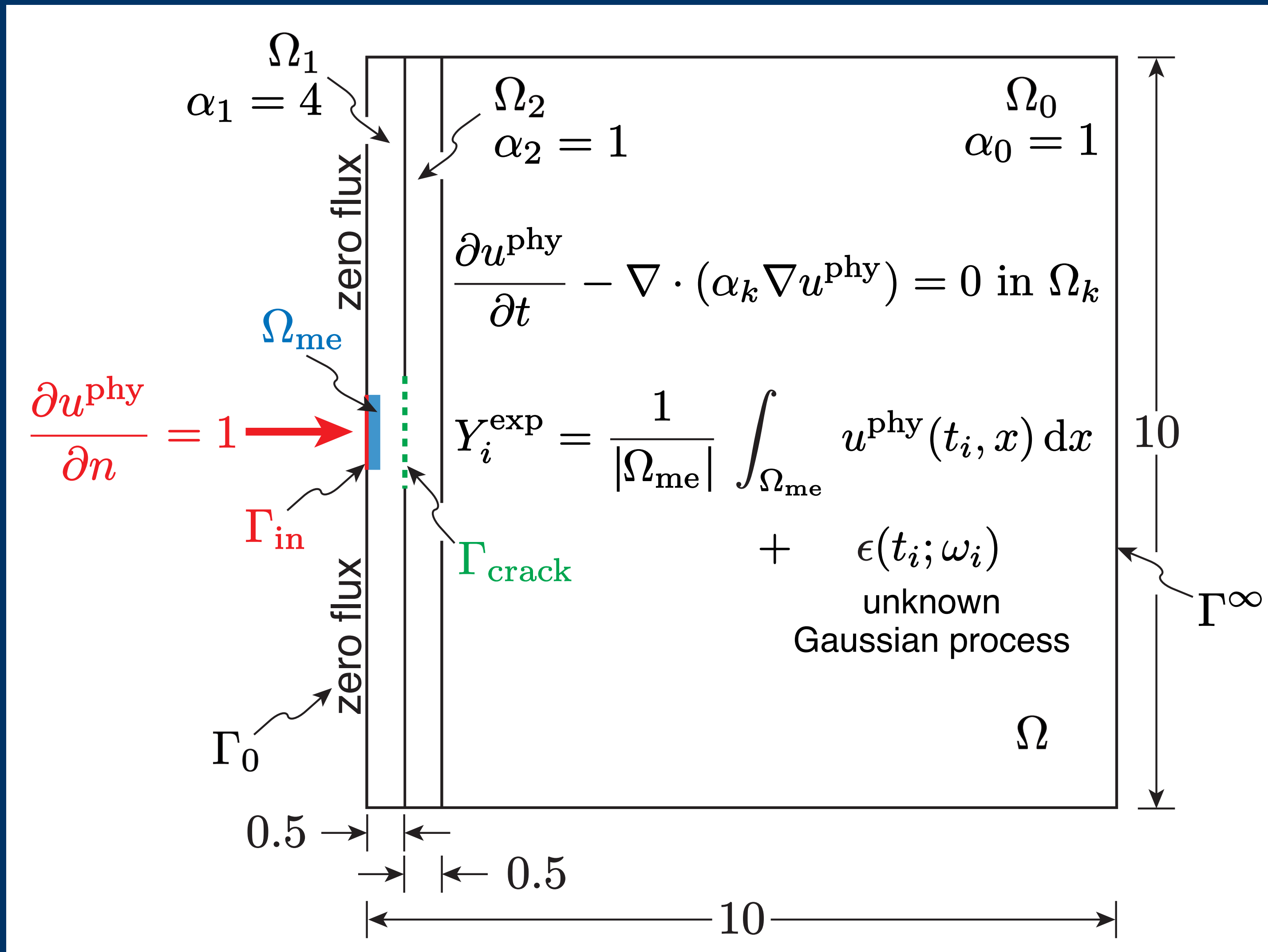
Case II: Model



Parametrization: $\mu \equiv (\mu_1, \mu_2) \in [0.2, 5]^2 \equiv \mathcal{D}$.

Case II: Physical System

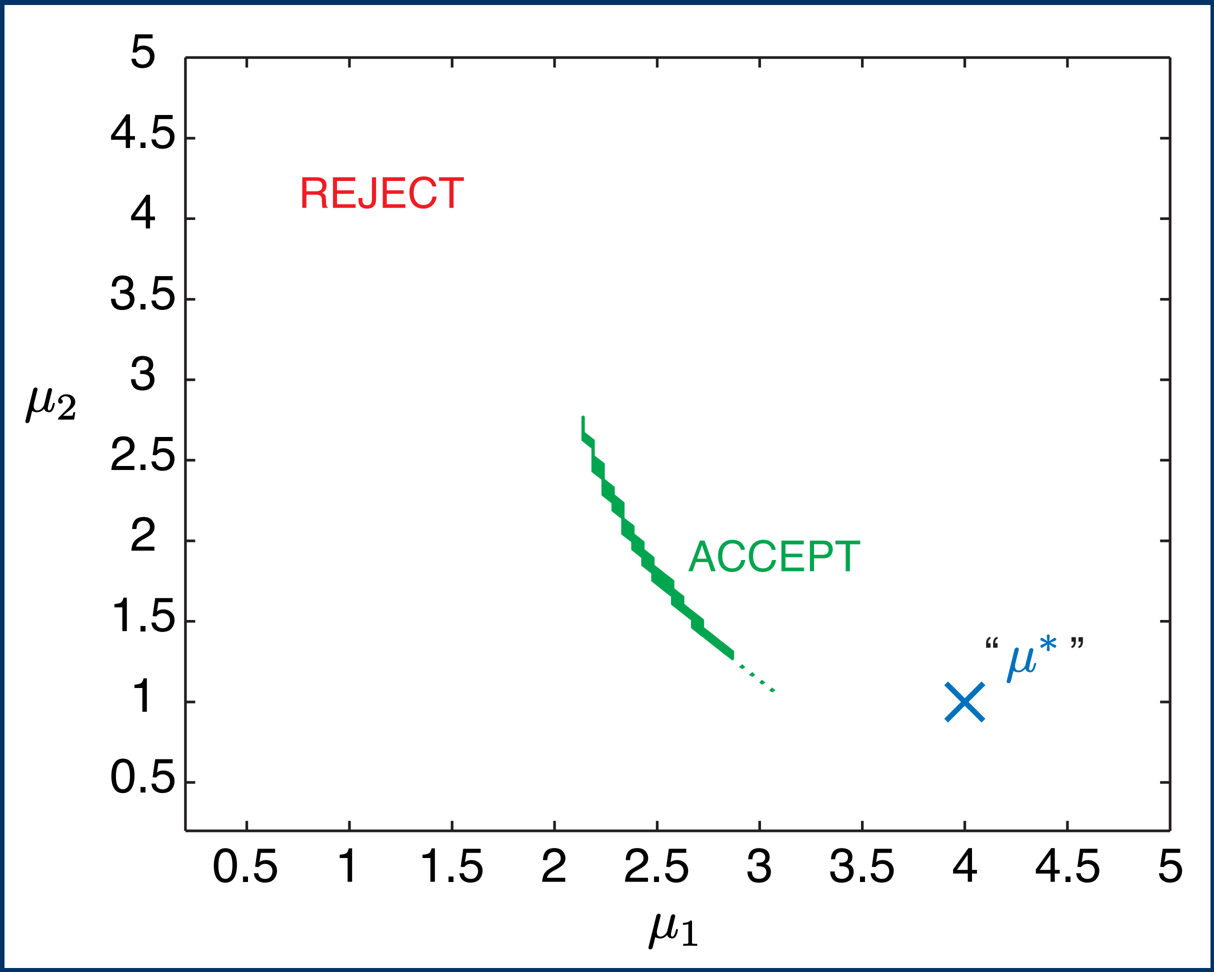
(unmodeled physics: crack)



$$u^{\rm phy}(t, x) \neq u^{\rm model}(t, x; \mu)$$ for any $\mu \in \mathcal{D}$.

Case II: Validation

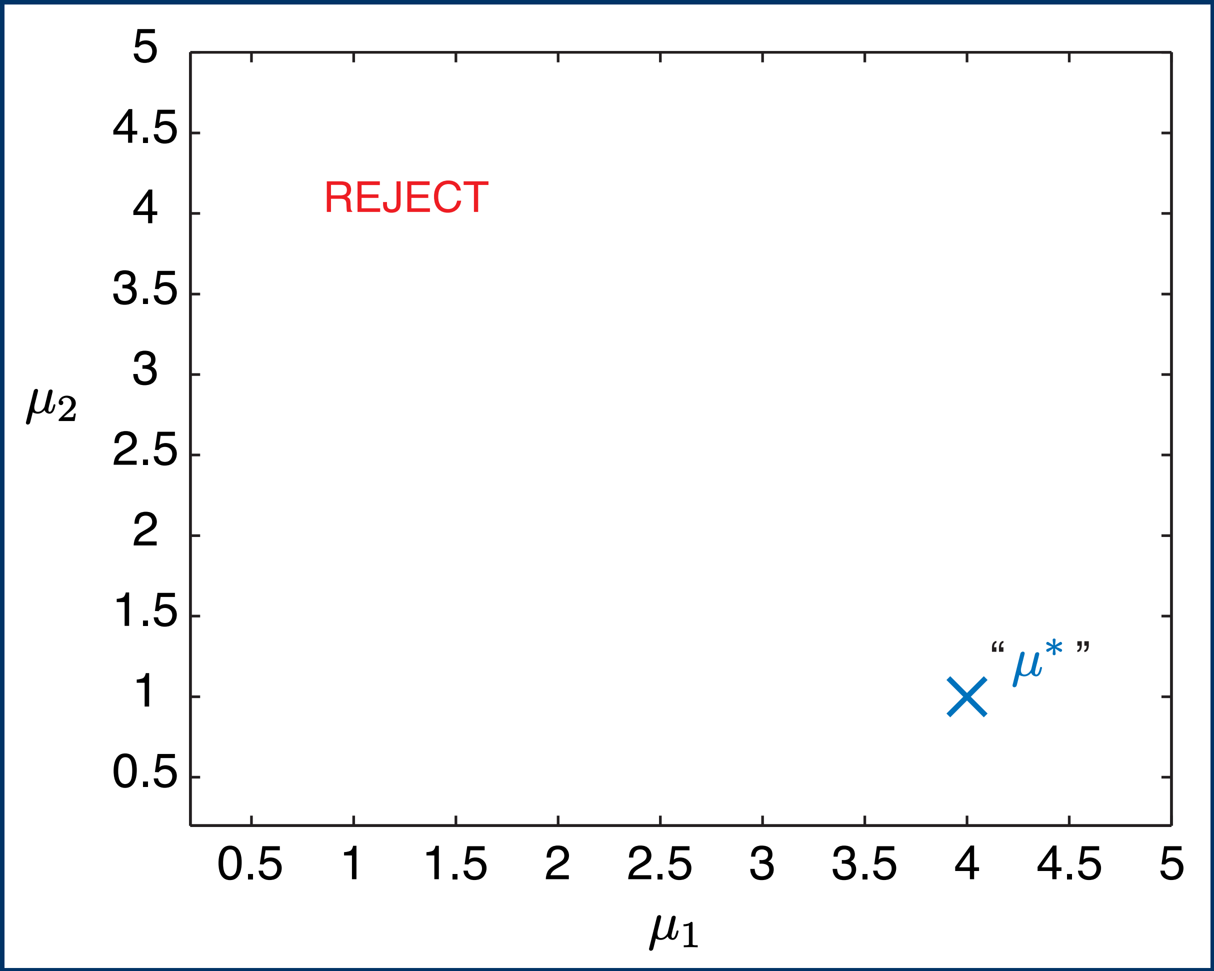
(noise: $\approx 1\%$, uncorrelated)



Crack Length $= 1$: crack conflated with lower conductivity medium.

Case II: Validation

(noise: ≈ 1%, uncorrelated)



Crack Length $= \mathbf{1.5}$: unmodeled physics detected.

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MURI Architecture

while (model insufficient)

propose/update model: μPDE, SPDE;

develop Reduced Order Model (ROM);

ISOMAP, ANOVA, RB/EI, MEPC, . . .

verify ROM;

validate model $\Leftarrow \mathcal{F}_\epsilon$ (data, ROM);

end

design under uncertainty $\Leftarrow$ ACCEPTED $\mathcal{H}(\mu)$;

MURI Domains & Applications

Thermofluids

Acoustics (for Noise Mitigation . . .)

Electromagnetics (for Stealth . . .)

(Multiscale) Materials

References

Frequentist Validation

V Chew, Confidence, prediction, and tolerance regions for the multivariate normal distribution. J Am Stat Ass 61(315): 605–617, 1966.

O Balci, R Sargent, Validation of simulation models via simultaneous confidence intervals. Am J Math Manage Sci 4: 375–406, 1984.

J McFarland, S Mahadevan, Multivariate significance testing and model calibration under uncertainty. Comput Methods Appl Mech Engrg 197(29– 32): 2467–2479, 2008.

DBP Huynh, DJ Knezevic, AT Patera, Certified reduced basis model validation: A frequentistic uncertainty framework. Comput Methods Appl Mech Engrg 201–204:13–24, 2012.

Parametric Manifold Models

AK Noor, Recent advances in reduction methods for nonlinear problems. Comput Struct 13:31–44, 1981.

BO Almroth, P Stern, FA Brogan, Automatic choice of global shape functions in structural analysis. AIAA J 16:525–528, 1978.

TA Porsching, Estimation of the error in the reduced basis method solution of nonlinear equations. Math Comput 45(172):487–496, 1985.

L Machiels, Y Maday, IB Oliveira, AT Patera, DV Rovas, Output Bounds for Reduced-Basis Approximations of Symmetric Positive Definite Eigenvalue Problems. CR Acad Sci Paris Series I 331:153–158, 2000.

G Rozza, DBP Huynh, AT Patera, Reduced Basis Approximation and A Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations — Application to Transport and Continuum Mechanics. Arch Comput Methods Eng 15(3):229–275, 2008.

M Barrault, Y Maday, NC Nguyen, AT Patera, An ‘Empirical Interpolation’ Method: Application to Efficient Reduced-Basis Discretization of Partial Differential Equations. CR Acad Sci Paris Series I 339:667–672, 2004.

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