Real-Time Reliable Solution of Partial Differential Equations on Smartphones; Application to Parameter Estimation, Design, and Optimization "in the Field"

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Acknowledgements

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Outline

The Big Picture

An Acoustics Example

A Heat Transfer Example

The Big Questions

Goal

We wish to perform

analyses . . .

in the field . . .

for design and operation of

distributed physical systems.

Analyses for Design & Operation

(Measurement and) Characterization

Prediction

Visualization

Optimization

Control and Decision

“In the Field”

In Situ:

calibrate model to instance/environment;

explore model implications in context;

initiate appropriate actions on site.

A Tempo: “real-time”

respond/intervene on relevant timescales.

Distributed Physical Systems

Continua described by PDE$_{\mu}$

Temperature$(\boldsymbol{x}, t)$: Heat Transfer,

Displacement$(\boldsymbol{x}, t \text{ or } \omega)$: Solid Mechanics,

Pressure$(\boldsymbol{x}, t \text{ or } \omega)$: Acoustics,[†]

Velocity$(\boldsymbol{x}, t)$: Fluid Dynamics.

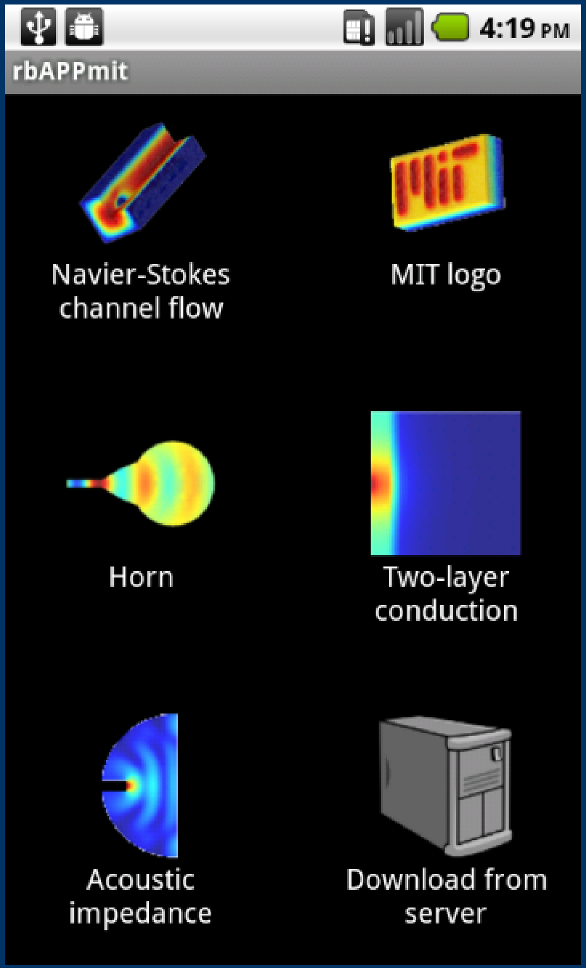
[†] Also, vicariously [He *et al.*], electromagnetics: $(\boldsymbol{E}, \boldsymbol{B})(\boldsymbol{x}, t \text{ or } \omega)$.

Distributed Physical Systems

Examples

Distributed Physical Systems

Examples



Outline

The Big Picture

An Acoustics Example

A Heat Transfer Example

The Big Questions

An Acoustics Example: In Situ Impedance

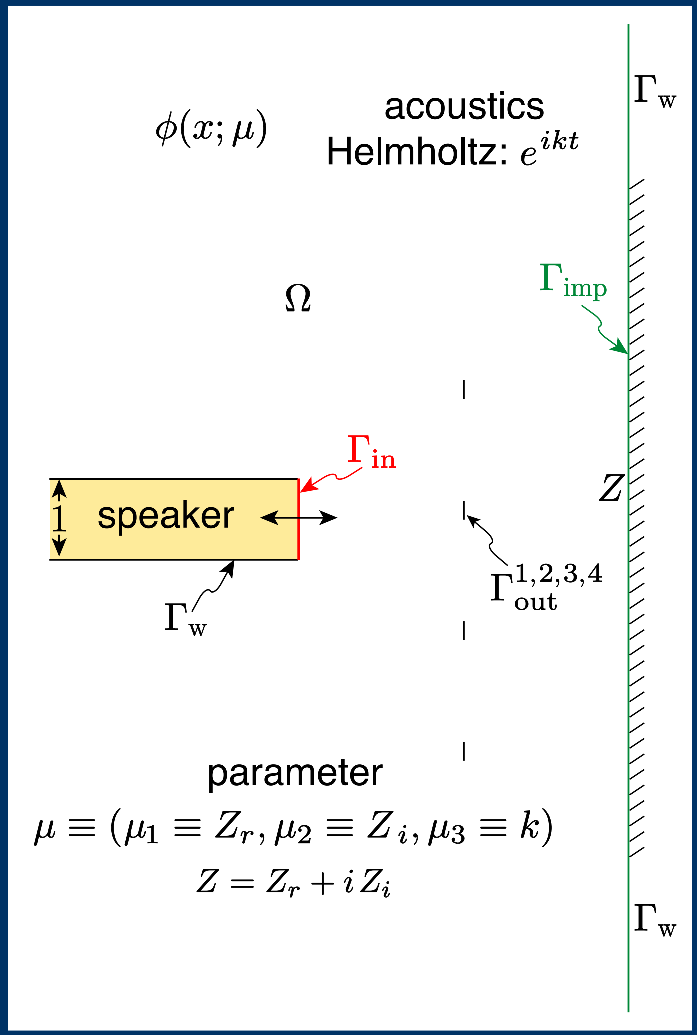
(Inverse) Problem Formulation

Computational Approach

Parametrized Model $\mathcal{M}$

Domain

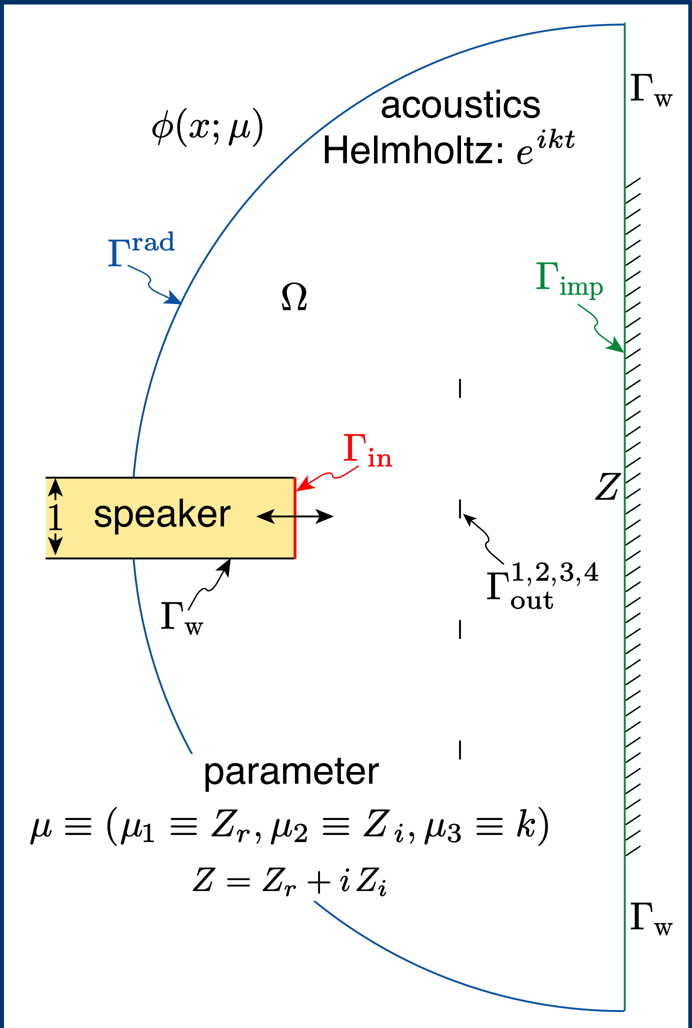
Semi-Infinite



Parametrized Model $\mathcal{M}$

Domain

Truncated



Parametrized Model $\mathcal{M}$

Governing Equations

Strong Form

Given $\mu \equiv (Z_r, Z_i, k) \in \mathcal{D}$, $\phi(x; \mu)$ satisfies

$$-\nabla^2 \phi - k^2 \phi = 0 \quad \text{in} \quad \Omega ,$$

with boundary conditions

$$\frac{\partial \phi}{\partial n} = -ik \ \text{ on } \ \Gamma_{\text{in}} , \qquad \frac{\partial \phi}{\partial n} + \frac{ik}{Z} \phi = 0 \ \text{ on } \ \Gamma_{\text{imp}} .^{\dagger}$$

Outputs: $\Phi^\ell(\mu) = \frac{1}{|\Gamma^\ell_{\text{out}}|} \int_{\Gamma^\ell_{\text{out}}} \phi(x; \mu), \, 1 \leq \ell \leq 4 .$

† We also impose $\partial \phi / \partial n = 0$ on Γ_{w} and radiation conditions on Γ^{rad}.

Parametrized Model $\mathcal{M}$

Governing Equations

Weak Form...

Given $\mu \equiv (Z_r, Z_i, k) \in \mathcal{D}$, $\phi(\mu) \in X$ satisfies

$$\int_\Omega \underset{-\nabla^2\phi\,\overline{v}\,+\,\cdots}{\nabla\phi \cdot \nabla\overline{v}} - \int_\Omega k^2\,\phi\,\overline{v} + \int_{\Gamma_{\text{imp}}} \frac{ik}{Z}\,\phi\,\overline{v}$$

$$+ \int_{\Gamma^{\text{rad}}} \cdots = \int_{\Gamma_{\text{in}}} -\,ik\,\overline{v},\ \forall\, v \in X\,.$$

Outputs: $\Phi^\ell(\mu) = \dfrac{1}{|\Gamma^\ell_{\text{out}}|} \displaystyle\int_{\Gamma^\ell_{\text{out}}} \phi(\mu),\ 1 \le \ell \le 4\,.$

Parametrized Model $\mathcal{M}$

Governing Equations

...Weak Form

Here derivatives square integrable

$$X(\Omega) = H^1(\Omega) \qquad \text{(complex fields)}$$

with inner product and norm

$$(w, v)_X = \int_\Omega \nabla w \cdot \nabla \bar{v}, \quad \|v\|_X^2 \equiv \int_\Omega |\nabla v|^2.$$

Define also $L^2(\Omega)$ inner product and norm

$$(w, v) = \int_\Omega w \, \bar{v}, \quad \|v\|^2 \equiv \int_\Omega |v|^2.$$

Parametrized Model $\mathcal{M}$

Governing Equations

Parameter (Domain)

Here $P = 3$

$\mu \ (\mu_1 \equiv Z_r, \mu_2 \equiv Z_i, \mu_3 \equiv k)$ is the *parameter*;

$\mathcal{D} \equiv [1, 4]^2 \times [1, 2]$ is the *parameter domain*.

More generally,

$\mu \ = (\mu_1, \ldots, \mu_P)$ is the *parameter*;

$\mathcal{D} \subset \mathbb{R}^P$ is the *parameter domain*.

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Introduce a Finite Element (FE) space

$$X_h(\Omega; \mathcal{T}_h) \subset X(\Omega) ,$$

where h is the diameter of a "triangulation" $\mathcal{T}_h$.

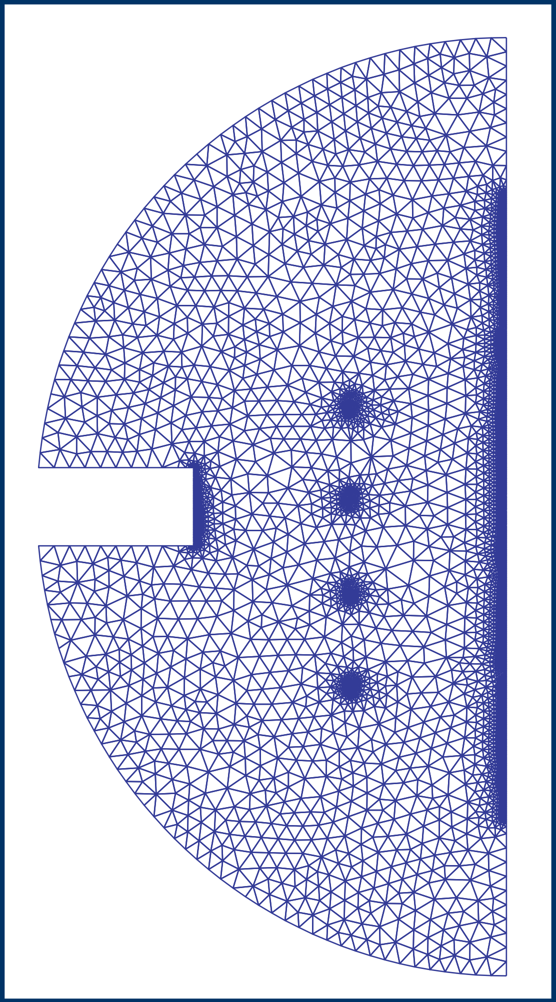
Find given $\mu \in \mathcal{D}$

$$\phi_h(\mu) \in X_h \approx \phi(\mu) \in X .$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Space



X_h: $\mathbb{P}_2$ elements

over

Triangulation $\mathcal{T}_h$

$\Downarrow$

$$\mathbf{dim}(X_h) = \mathbf{16{,}919}$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Galerkin Projection

Given $\mu \in \mathcal{D}$, $\phi_h(\mu) \in X_h$ satisfies

$$\int_\Omega \nabla \phi_h \cdot \nabla \overline{v} - \int_\Omega k^2 \, \phi_h \, \overline{v} + \int_{\Gamma_{\rm imp}} \frac{ik}{Z} \, \phi_h \, \overline{v}$$

$$+ \int_{\Gamma^{\rm rad}} \cdots = \int_{\Gamma_{\rm in}} -\, ik \, \overline{v}, \ \forall \, v \in X_h \, .$$

Outputs: $\Phi_h^\ell(\mu) = \dfrac{1}{|\Gamma_{\rm out}^\ell|} \displaystyle\int_{\Gamma_{\rm out}^\ell} \phi_h(\mu), \, 1 \le \ell \le 4 \, .$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Algebraic System...

Express $\phi_h(\mu) \in X_h$ as $\mathcal{N}_h = \dim(X_h)$

$$\phi_h(\boldsymbol{x};\mu) = \sum_{n=1}^{\mathcal{N}_h} [c_h(\mu)]_n \varphi_n(\boldsymbol{x}),$$

where

$\varphi_n(\boldsymbol{x})$: (nodal) basis functions $\Leftarrow X_h$;

$[c_h(\mu)]_n$: ($\mathbb{C}$) coefficients $\Leftarrow$ Galerkin projection ...

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

...Algebraic System

Given $\mu \in \mathcal{D}$, $c_h(\mu) \in \mathbb{C}^{\mathcal{N}_h}$ satisfies

$$A_h(\mu)\, c_h(\mu) = F_h\ .$$

Outputs: $1 \le \ell \le 4$,

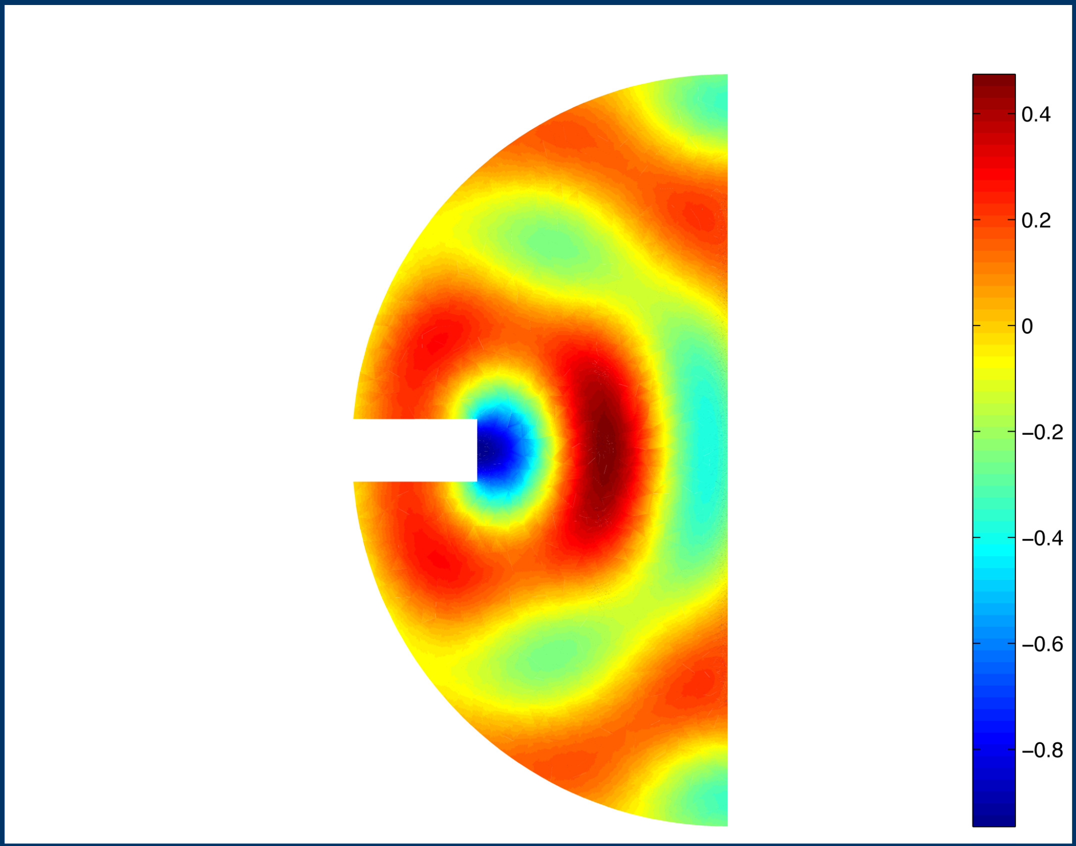
$$\Phi_h^\ell(\mu) = \sum_{n=1}^{\mathcal{N}_h} [c_h(\mu)]_n \left(\frac{1}{|\Gamma_{\text{out}}^\ell|} \int_{\Gamma_{\text{out}}^\ell} \varphi_n \right)\ .$$

Here $c_h(\mu) \in \mathbb{C}^{\mathcal{N}_h}$, $F_h \in \mathbb{C}^{\mathcal{N}_h}$, and $A_h(\mu) \in \mathbb{C}^{\mathcal{N}_h \times \mathcal{N}_h}$ but *sparse*.

Parametrized Model $\mathcal{M}_h$ (FE)

Illustrative Solutions

Pressure Field

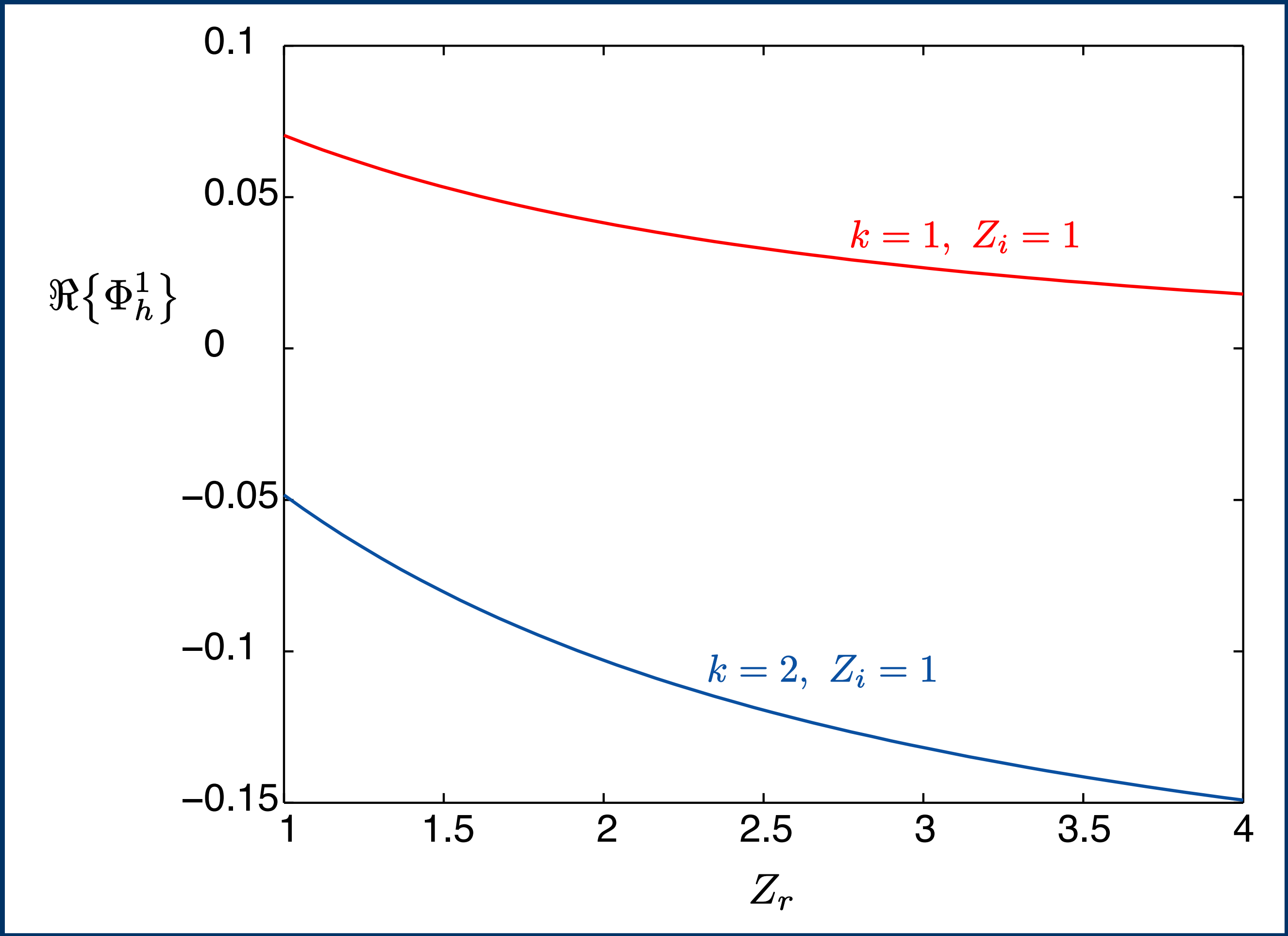


$$\mu = (1, 1, 2)$$

Parametrized Model $\mathcal{M}_h$ (FE)

Illustrative Solutions

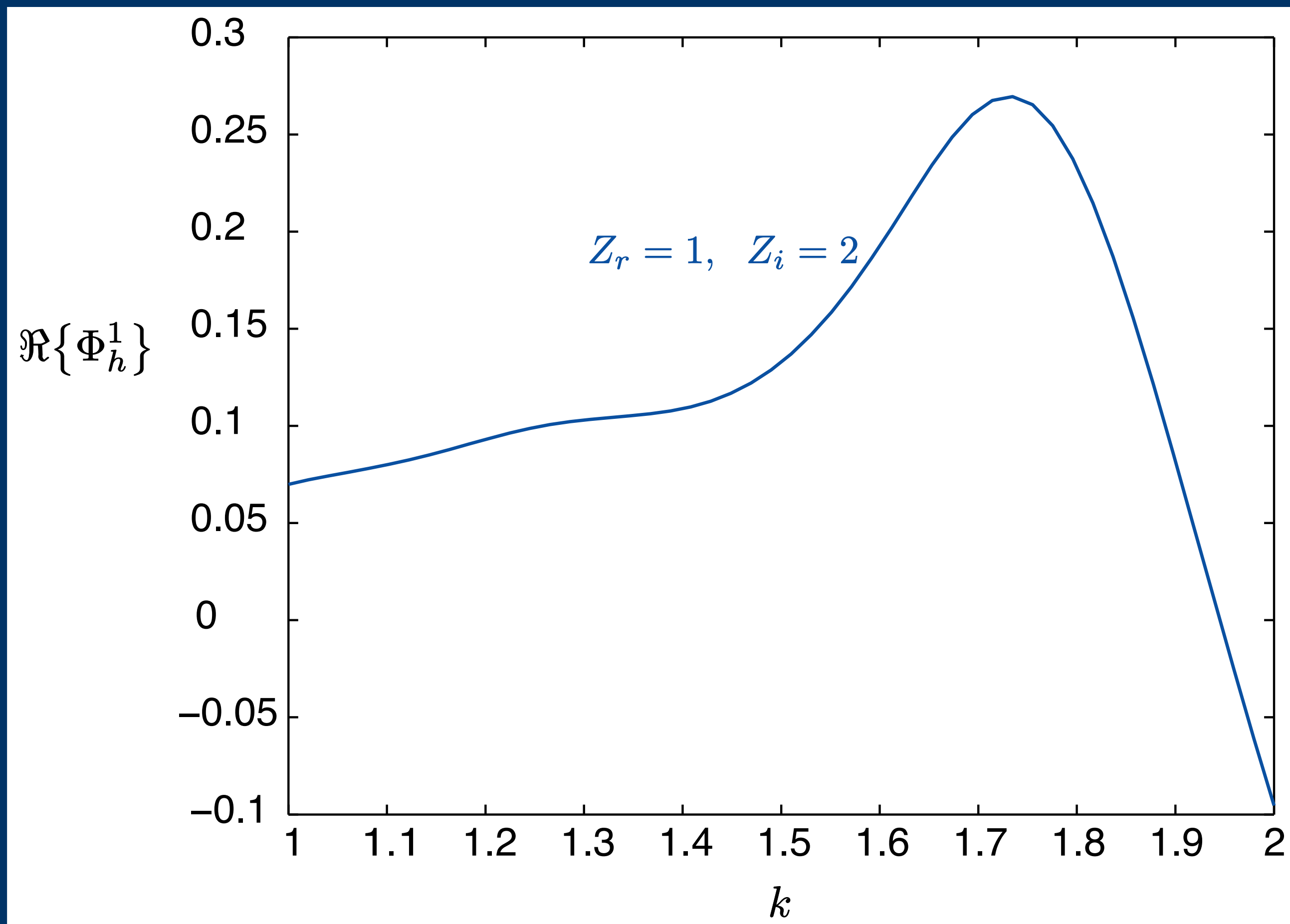
Output Variation...



Parametrized Model $\mathcal{M}_h$ (FE)

Illustrative Solutions

...Output Variation



Inverse Problem$_h$ [KT]

Impedance Estimate$_h$

Least Squares

Given $k = [1, 2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\exp}(k) \in \mathbb{C}, \;\; 1 \le \ell \le 4 \,,$$

find $(Z^*_r, Z^*_i)_h$: no regularization

$$(Z^*_r, Z^*_i)_h = \arg \min_{(Z_r, Z_i) \in [1,4]^2} \mathcal{E}_h(Z_r, Z_i, k) \;,$$

$$\mathcal{E}_h(Z_r, Z_i, k) \equiv \sum_{\ell=1}^{4} \left| \Phi^{\ell}_{\exp}(k) - \Phi^{\ell}_h(Z_r, Z_i, k) \right|^2 .$$

Inverse Problem$_h$

Uncertainty Analysis$_h$

Likelihood Ratio: $\Lambda_h(\mu)$

Given $k \in [1, 2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\exp}(k) = \Phi^{\ell}_h(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\exp}\,\mathcal{N}(0, 1)\ ,$$

hypothesis

define (pre-Bayesian) $\forall\ (Z_r, Z_i) \in [1, 4]^2$

$$\mathcal{L}_h(Z_r, Z_i, k) \equiv e^{\left\{-\mathcal{E}_h(Z_r, Z_i, k)/2\epsilon^2_{\exp}\right\}}\ ,$$

$$\Lambda_h(Z_r, Z_i, k) \equiv \frac{\mathcal{L}_h(Z_r, Z_i, k)}{\mathcal{L}_h(Z^*_{r\,h}, Z^*_{i\,h}, k)}\ .$$

An Acoustics Example: In Situ Impedance

(Inverse) Problem Formulation

Computational Approach

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\mu_h^* \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \mu_{h,N}^* \left(\mathcal{M}_{h,N} \text{ (RB)}\right),$$

$$\Lambda_h \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \left(\mathcal{M}_{h,N} \text{ (RB)}\right).$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Introduce a Finite Element (FE) space

$$X_h(\Omega; \mathcal{T}_h) \subset X(\Omega) ,$$

where h is the diameter of a "triangulation" $\mathcal{T}_h$.

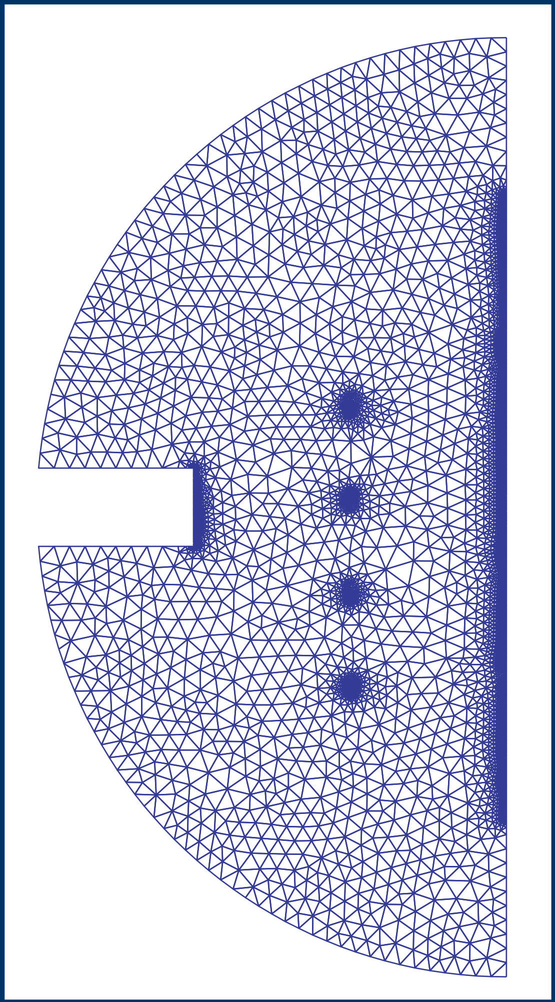
Find given $\mu \in \mathcal{D}$

$$\phi_h(\mu) \in X_h \approx \phi(\mu) \in X .$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Space



X_h: $\mathbb{P}_2$ elements

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Triangulation $\mathcal{T}_h$

$\Downarrow$

$$\dim(X_h) = 16{,}919$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Galerkin Projection

Given $\mu \in \mathcal{D}$, $\phi_h(\mu)$ satisfies

$$\int_\Omega \nabla\phi_h \cdot \nabla\overline{v} - \int_\Omega k^2\,\phi_h\,\overline{v} + \int_{\Gamma_{\rm imp}} \frac{ik}{Z}\,\phi_h\,\overline{v}$$

$$+ \int_{\Gamma^{\rm rad}} \cdots = \int_{\Gamma_{\rm in}} -\,ik\,\overline{v},\ \ \forall\, v \in X_h\,.$$

Outputs: $\Phi_h^\ell(\mu) = \dfrac{1}{|\Gamma_{\rm out}^\ell|}\displaystyle\int_{\Gamma_{\rm out}^\ell} \phi_h(\mu),\ 1 \le \ell \le 4\,.^\dagger$

$^\dagger\Re\ \Im\ \Phi_h^\ell$: consider *separately* real and imaginary parts.

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Algebraic System...

Express $\phi_h(\mu) \in \boldsymbol{X}_h$ as $\qquad \mathcal{N}_h = \mathbf{dim}(\boldsymbol{X}_h)$

$$\phi_h(\boldsymbol{x};\mu) = \sum_{n=1}^{\mathcal{N}_h} [\boldsymbol{c}_h(\mu)]_n \, \varphi_n(\boldsymbol{x}),$$

where

$\varphi_n(\boldsymbol{x})$: (nodal) basis functions $\Leftarrow \boldsymbol{X}_h$;

$[\boldsymbol{c}_h(\mu)]_n$: ($\mathbb{C}$) coefficients $\Leftarrow$ Galerkin projection ...

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

...Algebraic System

Given $\mu \in \mathcal{D}$, $c_h(\mu) \in \mathbb{C}^{\mathcal{N}_h}$ satisfies

$$A_h(\mu)\, c_h(\mu) = F_h \;.$$

Outputs: $1 \le \ell \le 4$,

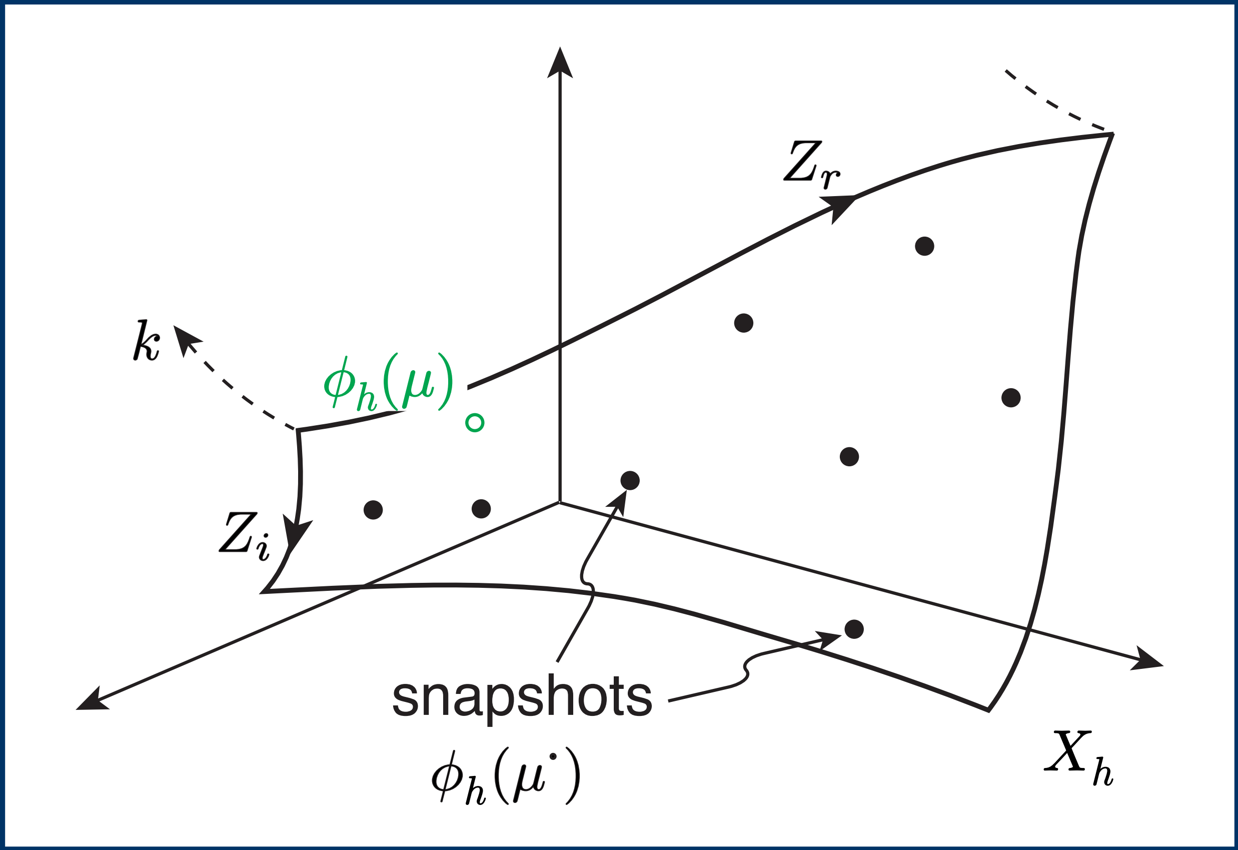
$$\Phi_h^\ell(\mu) = \sum_{n=1}^{\mathcal{N}_h} [c_h(\mu)]_n \left(\frac{1}{|\Gamma_{\text{out}}^\ell|} \int_{\Gamma_{\text{out}}^\ell} \varphi_n \right) .$$

Here $c_h(\mu) \in \mathbb{C}^{\mathcal{N}_h}$, $F_h \in \mathbb{C}^{\mathcal{N}_h}$, and $A_h(\mu) \in \mathbb{C}^{\mathcal{N}_h \times \mathcal{N}_h}$ but *sparse*.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Parametric Manifold $\mathcal{P}_h$...



$$\mathcal{P}_h = \{\phi_h(\mu) \mid \forall\, \mu \in \mathcal{D}\}$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Parametric Manifold $\mathcal{P}_h$

Introduce a Reduced Basis† (RB) space

$$\boldsymbol{X_{h,N} \subset \mathrm{span}\{\mathcal{P}_h\} \subset X_h}$$

of dimension $\boldsymbol{\dim(X_{h,N}) = N}$.

Find given $\boldsymbol{\mu}$

$$\boldsymbol{\phi_{h,N}(\mu) \in X_{h,N} \approx \phi_h(\mu) \in X_h}\ .$$

†Early work: [ASB], [NPe], [FR], [Po], [G], . . .

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Spaces...

Greedy heuristic: $N_{\max}$

$$\zeta_n = \phi_h(\mu^n \in \mathcal{D}), \ \ 1 \leq n \leq N_{\max} \, , \qquad \perp_X$$

and associated hierarchical spaces

$$X_{h,N} = \text{span}\{\zeta_n, 1 \leq n \leq N\}, 1 \leq N \leq N_{\max} \, .$$

Optimality: $\{\mu^n\}_{1 \leq n \leq N_{\max}}$ $\qquad \dim(Y_N) = N$

$$X_{h,N} \approx \arg \min_{Y_N} \mathbb{D}_{L^\infty(\mathcal{D};X)} \left(\mathcal{P}_h, Y_N\right).$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Spaces...

Algorithm Greedy $(\mu^1, N_{\max})$:

for $N = 1\colon\ N_{\max} - 1$ % tol

$$\mu^{n+1} = \arg\max_{\mu \in \mathcal{D}} \|\phi_h(\mu) - \phi_{h,N}(\mu)\|_X;^\dagger$$

$$\zeta^{n+1} = \phi_h(\mu^{n+1});$$ % $\perp_X$

$$X_{h,N} = \text{span}\{\zeta_n,\ 1 \le n \le N\};$$

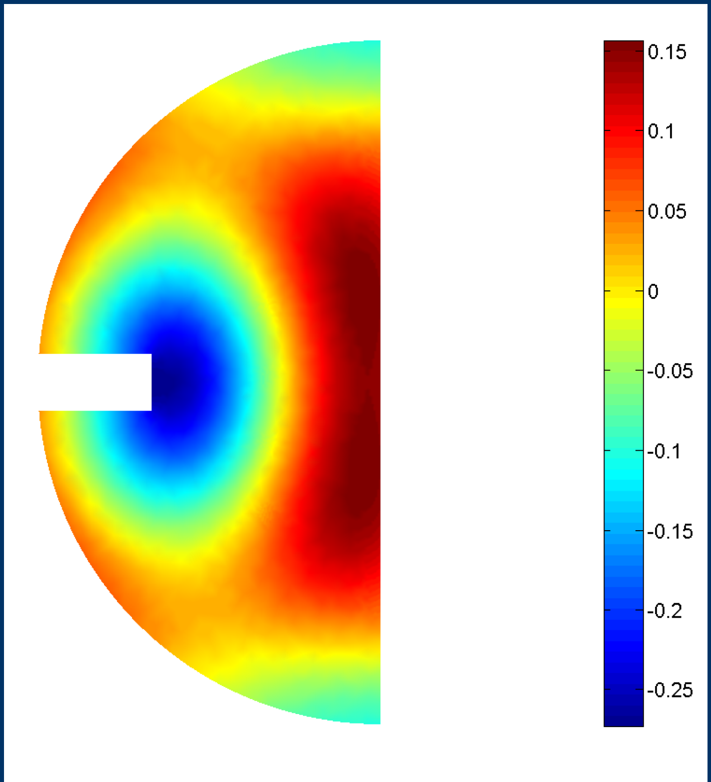
end

[†] In practice: $\mathcal{D} \leftarrow \Xi_{\text{train}}$; $\|\phi_h(\mu) - \phi_{h,N}(\mu)\|_X \leftarrow$ *error bound*.

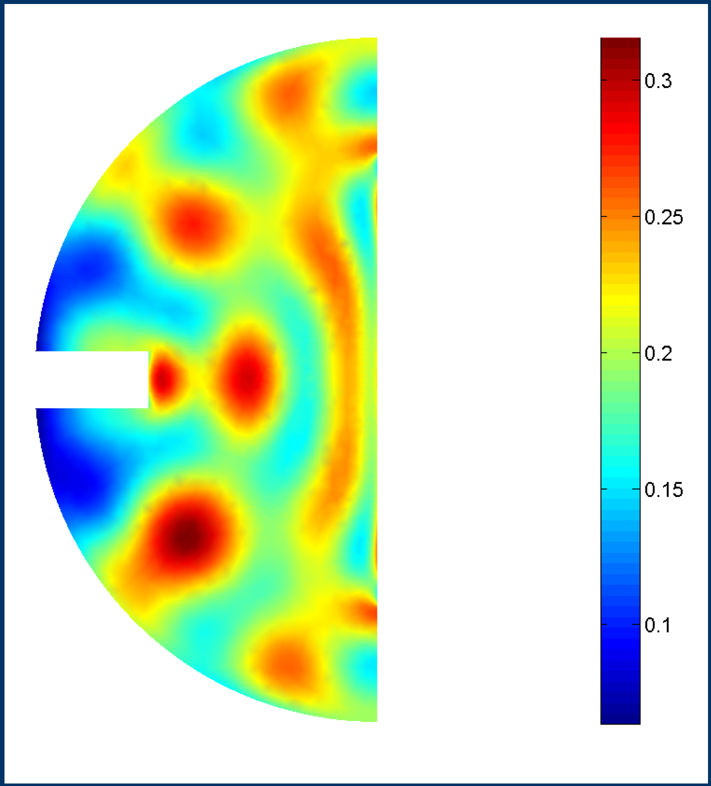
Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Spaces



$\Re(\zeta_1)$



$\Im(\zeta_{N_{\max}=25})$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

(Petrov) Galerkin Projection...

Given $\mu \in \mathcal{D}$, $\phi_{h,N}(\mu) \in X_{h,N}$ satisfies

$$\int_\Omega \nabla \phi_{h,N} \cdot \nabla \overline{v} - \int_\Omega k^2\, \phi_{h,N}\, \overline{v} + \int_{\Gamma_{\text{imp}}} \frac{ik}{Z}\, \phi_{h,N}\, \overline{v}$$

$$+ \int_{\Gamma^{\text{rad}}} \cdots = \int_{\Gamma_{\text{in}}} -\, ik\, \overline{v}, \;\; \forall\, v \in X_{h,N}\ .$$

Outputs: $\Phi^{\ell}_{h,N}(\mu) = \dfrac{1}{|\Gamma^{\ell}_{\text{out}}|} \displaystyle\int_{\Gamma^{\ell}_{\text{out}}} \phi_{h,N}(\mu),\ 1 \le \ell \le 4\ .$

Optimality: $\phi_{h,N} \approx$ Best_Fit$_{X_{h,N}}(\phi_h)$ in $\|\cdot\|_X$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...(Petrov) Galerkin Projection...

Output

and

'State' (Field)†

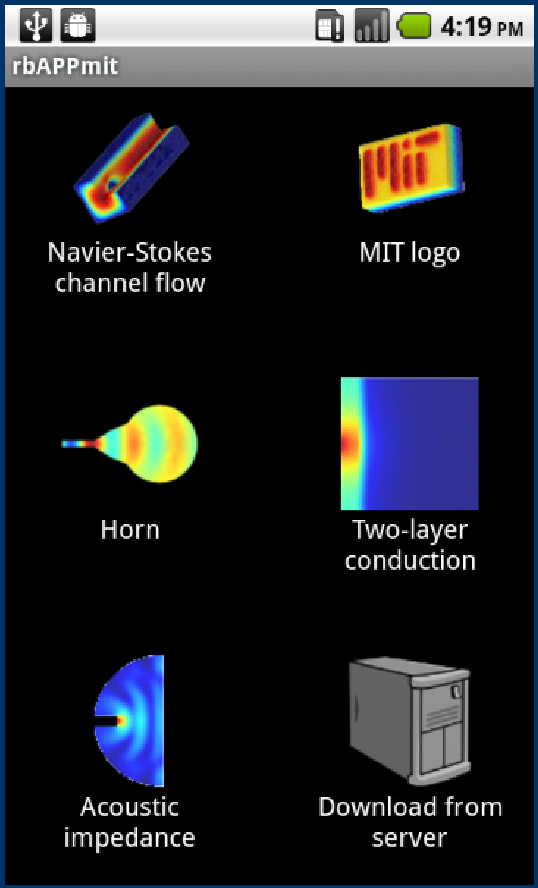
↑

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

…(Petrov) Galerkin Projection…



Output

and

'State' (Field)†

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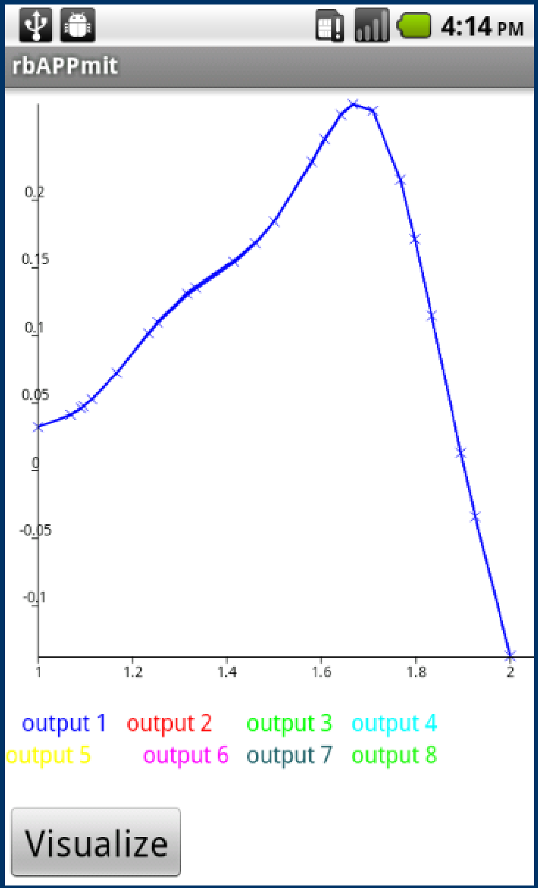
Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...(Petrov) Galerkin Projection...



Output

and

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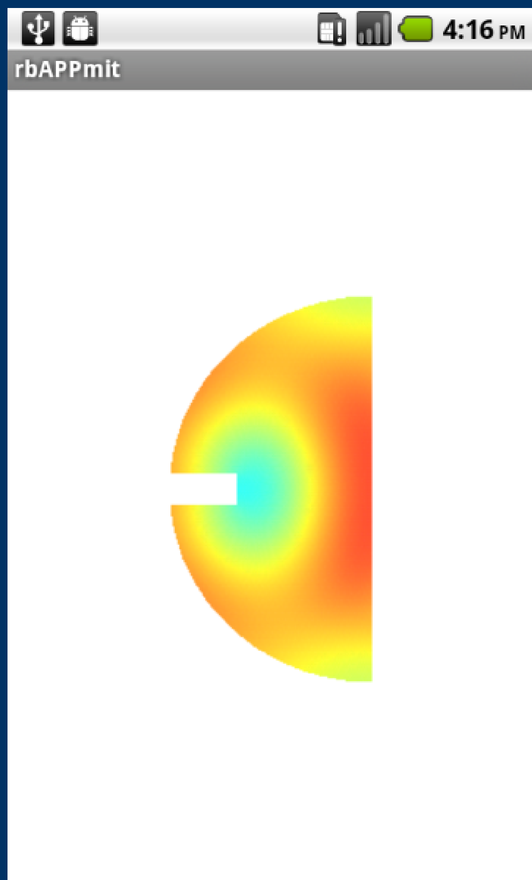
Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...(Petrov) Galerkin Projection...



Output

and

'State' (Field)†

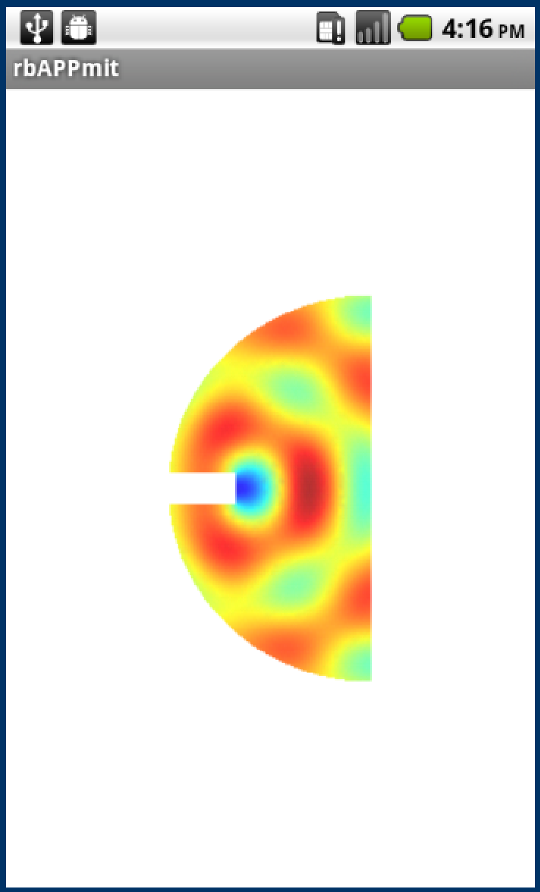
$\uparrow$

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...(Petrov) Galerkin Projection



Output

and

'State' (Field)†

↑

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Algebraic System...

Express $\phi_{h,N}(\boldsymbol{\mu}) \in X_{h,N}$ as

$$\phi_{h,N}(\boldsymbol{x};\boldsymbol{\mu}) = \sum_{n=1}^{N} [c_{h,N}(\boldsymbol{\mu})]_n \; \zeta_n(\boldsymbol{x}),$$

where

$\zeta_n(\boldsymbol{x})$: basis functions $\Leftarrow$ Greedy$(\boldsymbol{\mu})$;

$[c_{h,N}(\boldsymbol{\mu})]_n$: $(\mathbb{C})$ coefficients $\Leftarrow$ Galerkin Projection . . .

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Algebraic System

Given $\mu \in \mathcal{D}$, $c_{h,N}(\mu) \in \mathbb{C}^N$ satisfies

$$A_{h,N}(\mu)\, c_{h,N}(\mu) = F_{h,N}\ .$$

Outputs: $1 \le \ell \le 4$,

$$\Phi^{\ell}_{h,N}(\mu) = \sum_{n=1}^{N} [c_{h,N}(\mu)]_n \left(\frac{1}{|\Gamma^{\ell}_{\text{out}}|} \int_{\Gamma^{\ell}_{\text{out}}} \zeta_n \right) .$$

Here $c_{h,N}(\mu) \in \mathbb{C}^N$, $F_{h,N} \in \mathbb{C}^N$, and $A_{h,N}(\mu) \in \mathbb{C}^{N \times N}$ but *full*.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

We present

rigorous, sharp(ish), inexpensive†

a posteriori bounds crucial for

efficient Greedy search $\Rightarrow$ $\boldsymbol{X}_{h,N}$;

effective error control $\Rightarrow$ $\boldsymbol{N}$;

uncertainty assessment $\Rightarrow$ design & operation.

†We discuss efficient calculation of the bounds subsequently.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

Residual

Introduce residual: $\forall\, v \in X_h$,

$$R_{h,N}(v;\mu) \equiv \int_{\Gamma_{\text{in}}} - ik\,\overline{v} - \int_{\Omega} \nabla\phi_{h,N} \cdot \nabla\overline{v}$$

$$+ \int_{\Omega} k^2\,\phi_{h,N}\,\overline{v} - \int_{\Gamma_{\text{imp}}} \frac{ik}{Z}\,\phi_{h,N}\,\overline{v} - \int_{\Gamma^{\text{rad}}} \cdots \quad .$$

Define dual norm

$$\|v\|_X = \int_{\Omega} |\nabla v|^2$$

$$\delta_{h,N}(\mu) \equiv \sup_{v \in X_h} \frac{|R_{h,N}(v;\mu)|}{\|v\|_X}\,.$$

Output Error Bound...

Introduce error bounds: $1 \le \ell \le 4$,

$$\Delta^{\ell}_{h,N}(\mu) \equiv \underbrace{\left(\beta^{\mathrm{LB}}_h(\mu)\right)^{-1}}_{\text{stability}} \underbrace{C^{\ell}_{\mathrm{out}}}_{\text{output}} \delta_{h,N}(\mu) \; ;$$

$\beta^{\mathrm{LB}}_h(\mu) \leftarrow$ Successive Constraint Method (SCM),†

$$C^{\ell}_{\mathrm{out}} = \sup_{v \in X_h} \frac{\left| \frac{1}{|\Gamma^{\ell}_{\mathrm{out}}|} \int_{\Gamma^{\ell}_{\mathrm{out}}} \overline{v} \right|}{\|v\|_X}, \; 1 \le \ell \le 4 \, .$$

† Smartphone shortcut: $\beta^{\mathrm{LB}}_h(\mu)$ replaced by minimum of $\beta^{\mathrm{LB}}_h(\mu)$ over dense sample in $\mathcal{D}$.

Stability: $\beta_h^{\mathrm{LB}}(\mu)$ satisfies

$$0 < \beta_h^{\mathrm{LB}}(\mu) \leq \beta_h(\mu), \ \forall\, \mu \in \mathcal{D}\ ,$$

where

$$\beta_h(\mu) = \inf_{w \in X_h} \sup_{v \in X_h} \frac{\left| \int_\Omega \nabla w \cdot \nabla \bar{v} - \int_\Omega k^2\, w\, \bar{v} + \cdots \right|}{\|w\|_X\, \|v\|_X}$$

is a (generalized) minimum singular value.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Error Bound

Proposition 1.0A. Given $\mu \in \mathcal{D}$,

$$| \underbrace{\Phi^{\ell}_{h}(\mu)}_{\text{FE (Truth)}} - \underbrace{\Phi^{\ell}_{h,N}(\mu)}_{\text{RB}} | \leq \Delta^{\ell}_{h,N}(\mu), \; 1 \leq \ell \leq 4 \,,$$

for any $N \in \{1, \ldots, N_{\max}\}$.†

Rigorous error bounds for the output;

in practice, bounds also quite *sharp*.

†We can also obtain error bounds for the field variable in the X norm.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

Output Bounds...

Introduce output bounds $1 \leq \ell \leq 4$

$$\Phi^{-\,\ell}_{h,N}(\mu) \equiv \Phi^{\ell}_{h,N}(\mu) - (1+i)\Delta^{\ell}_{h,N}(\mu)\ ,$$

and

$$\Phi^{+\,\ell}_{h,N}(\mu) \equiv \Phi^{\ell}_{h,N}(\mu) + (1+i)\Delta^{\ell}_{h,N}(\mu)\ .$$

Bound gap (uncertainty): $1 \leq \ell \leq 4$

$$\Phi^{+\,\ell}_{h,N}(\mu) - \Phi^{-\,\ell}_{h,N}(\mu) = 2(1+i)\Delta^{\ell}_{h,N}(\mu)\ .$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Bounds...

Corollary 1.1A. Given $\mu \in \mathcal{D}$, $\Re$ $\Im$

$$\Phi^{-\ell}_{h,N}(\mu) \le \Phi^{\ell}_{h}(\mu) \le \Phi^{+\ell}_{h,N}(\mu)\;, \quad 1 \le \ell \le 4\;,$$

RB — FE (Truth) — RB

for any $N \in \{1, \ldots, N_{\max}\}$.

Rigorous lower and upper bounds
for the *FE (Truth)* outputs.†

† Note: output bounds calculated *without reference to* $\phi_h(\mu)$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

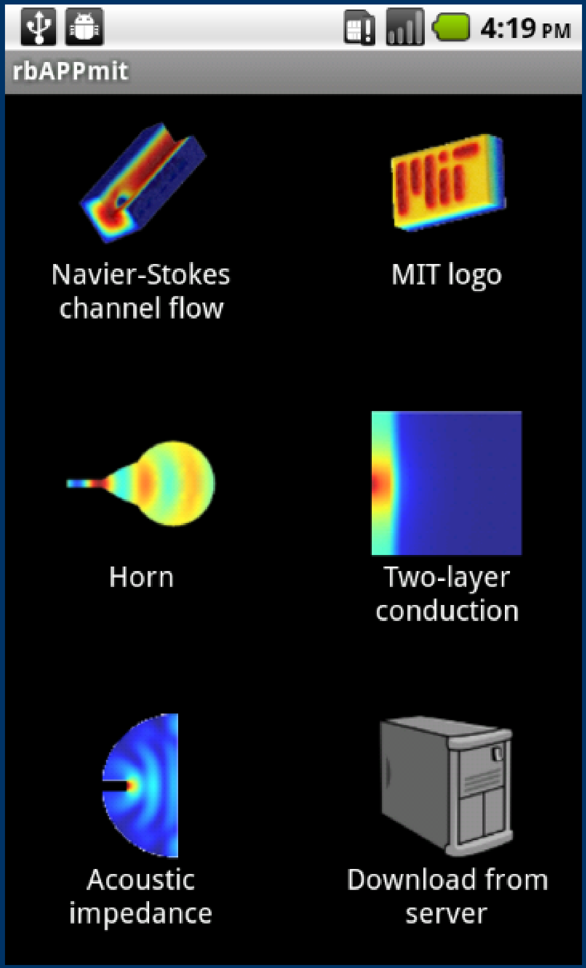
a posteriori Bounds

...Output Bounds...

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

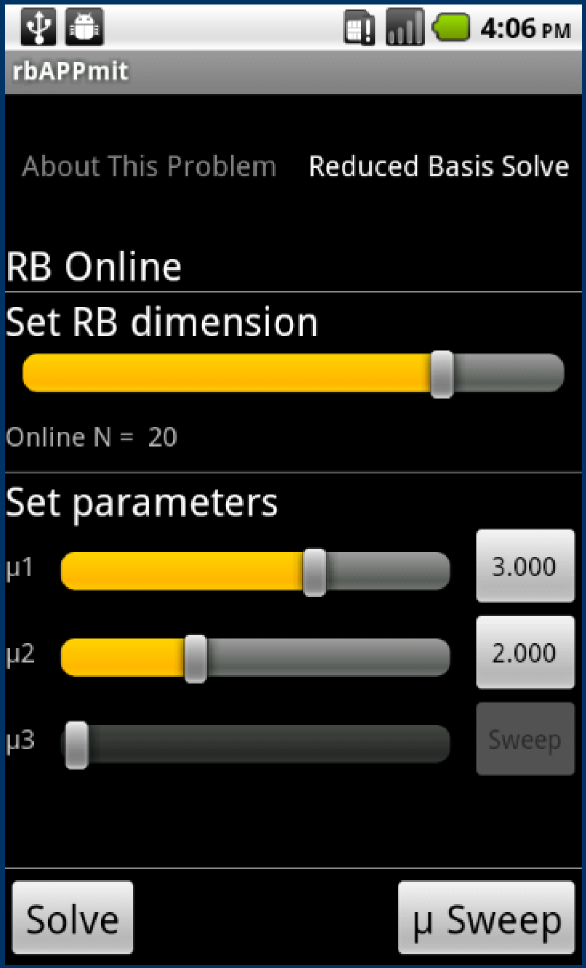
...Output Bounds...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

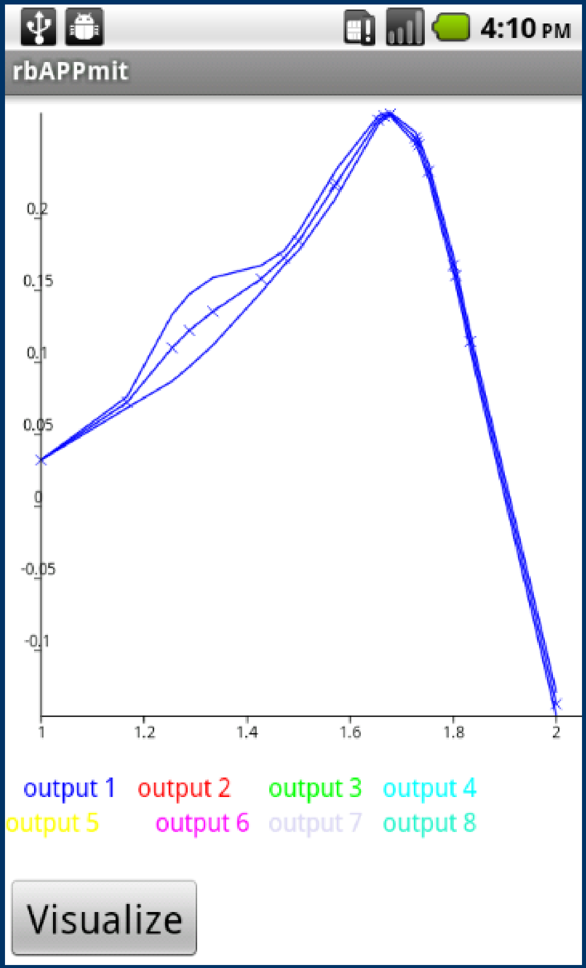
...Output Bounds...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Bounds



Given $\varepsilon > 0$, define

$$N_\varepsilon \equiv \max_{\mu \in \mathcal{D}} \left(\min_{2\Delta^{\ell}_{h,N}(\mu) \le \varepsilon,\, 1 \le \ell \le 4} N \right) .$$

Observation 2.0A. As $h \to 0$ ($\mathcal{N}_h \to \infty$)

(i) N_ε is independent of $\mathcal{N}_h$;

(ii) $N_\varepsilon \sim -\mathrm{Const} \ln(\varepsilon)$ as $\varepsilon \to 0$.

(Proof is possible in some simpler cases.)

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

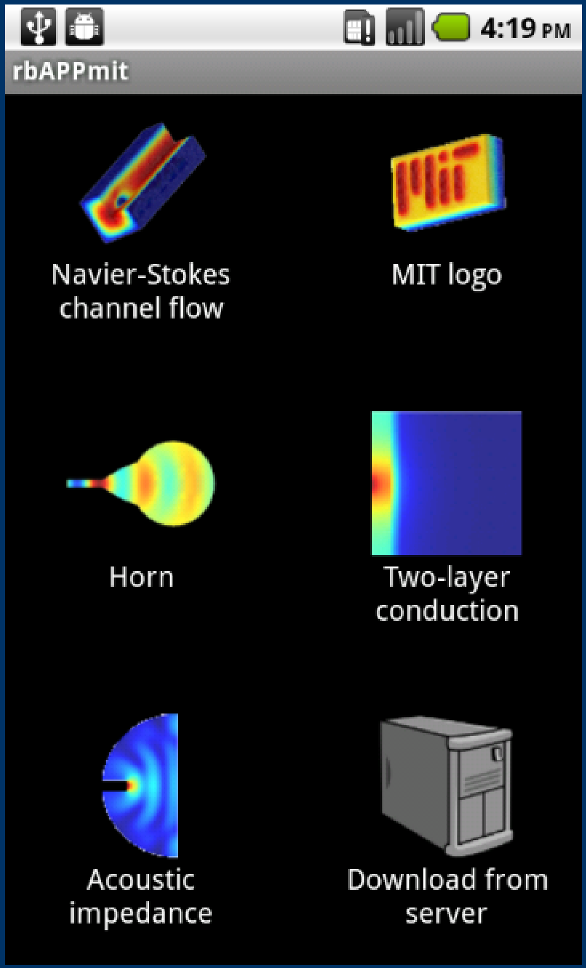
a posteriori Bounds

...Convergence...

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

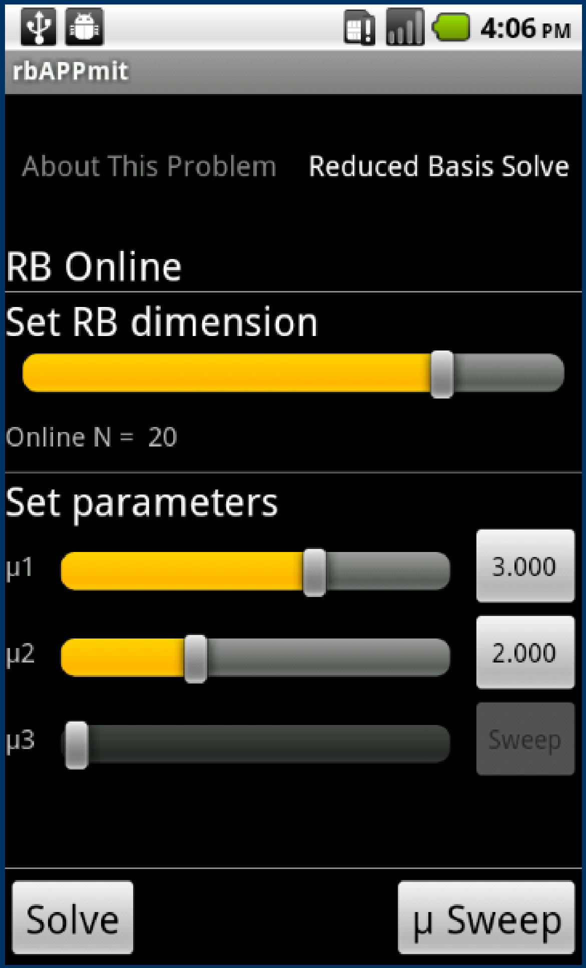
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

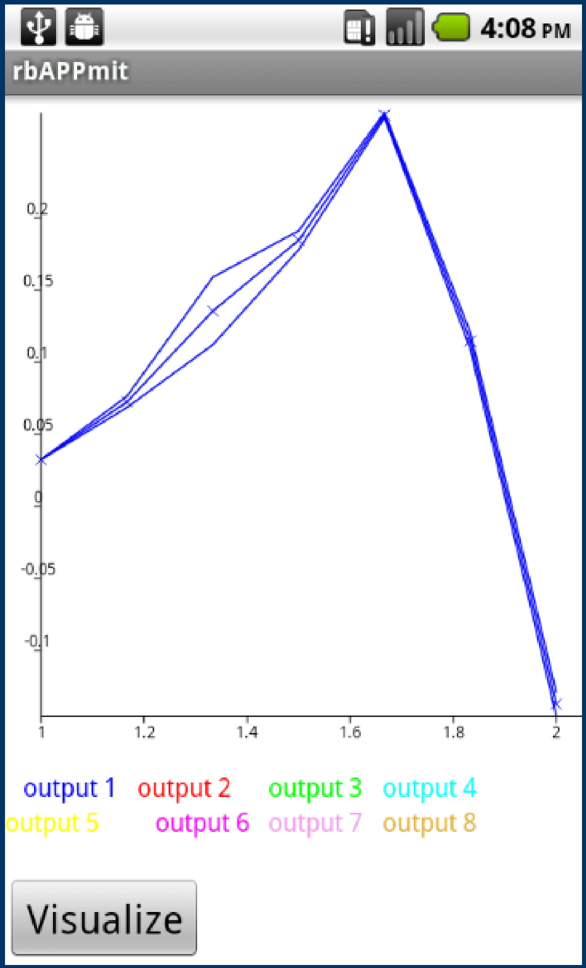
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

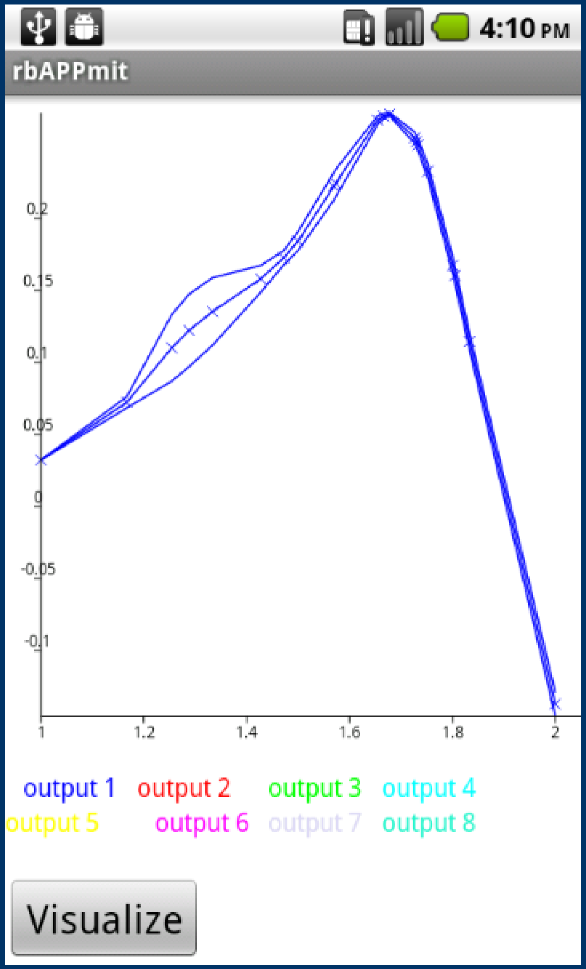
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

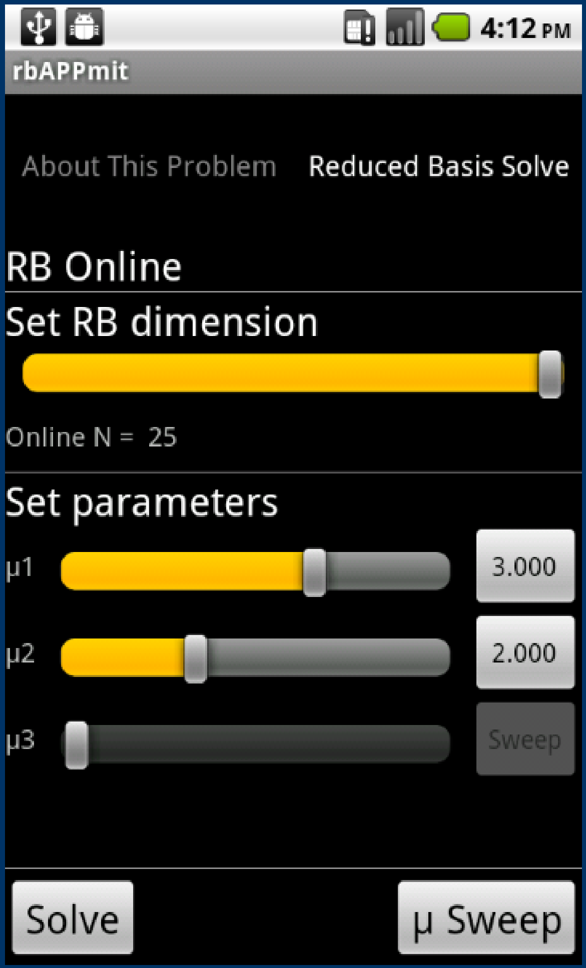
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

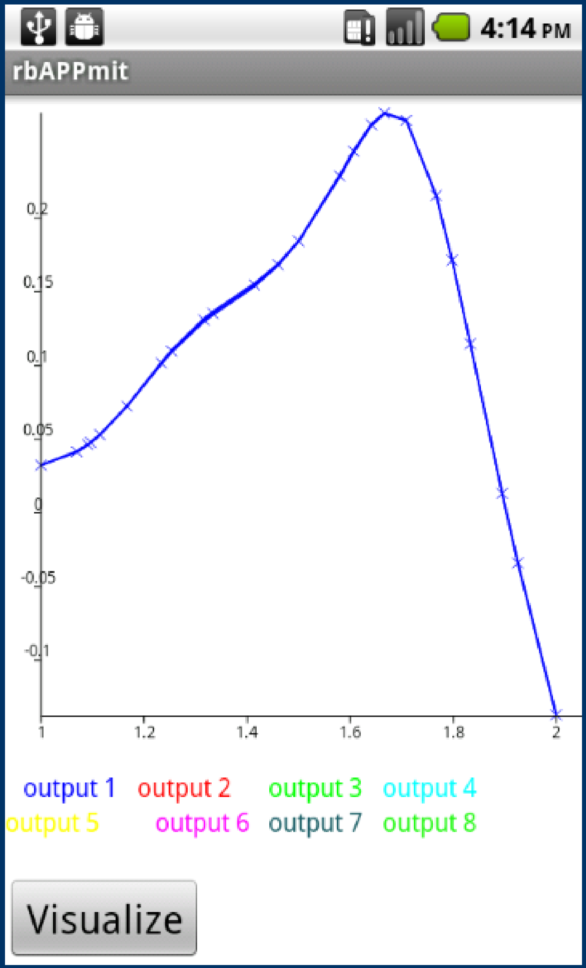
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Convergence



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

Offline-Online...

Key requirement:

weak form *affine* in *(functions of) the parameter*.

Key ingredients:

linear approximation space $\boldsymbol{X}_{h,N}$ ($\Rightarrow \boldsymbol{\phi}_{h,N}$);

Riesz representation of $\boldsymbol{R}_{h,N}$ ($\Rightarrow \boldsymbol{\delta}_{h,N}$);

Successive Constraint Method ($\boldsymbol{\Delta}^{\ell}_{h,N}$, $\boldsymbol{\Phi}^{\pm\,\ell}_{h,N}$).

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online...

Given $\mu \in \mathcal{D}$, $\phi(\mu) \in X$ satisfies

$$1 \int_\Omega \nabla\phi \cdot \nabla\overline{v} - k^2 \int_\Omega \phi\,\overline{v} + \frac{ik}{Z} \int_{\Gamma_{\mathrm{imp}}} \phi\,\overline{v}$$

$$+ \int_{\Gamma_{\mathrm{rad}}} \cdots = -ik \int_{\Gamma_{\mathrm{in}}} \overline{v}, \ \forall\, v \in X\ .$$

Outputs: $\Phi^\ell(\mu) = \frac{1}{|\Gamma^\ell_{\mathrm{out}}|} \int_{\Gamma^\ell_{\mathrm{out}}} \phi(\mu), 1 \le \ell \le 4\ .$

Affine: $\sum_{q=1}^{Q}$ function$_q$ (μ) $\times$ (bi)linear form$_q$ (*no* μ).

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online...

Offline Stage:

$$\mathcal{N}_h \equiv \dim(X_h)$$

$$\mathcal{M}_h \xrightarrow[O(\mathcal{N}_h) \text{ FLOPS}]{} \mathcal{S}_{\text{Online}}[\mathcal{M}_h]\ ;$$

$$\mathcal{S}_{\text{Online}}[\mathcal{M}_h]\text{: } O(N^2_{\max}) \text{ FPNS}\ .$$

Online Stage ($\mathcal{S}_{\text{Online}}[\mathcal{M}_h]$):

$$\mu, N \xrightarrow[O(N^3+Q^2N^2) \text{ FLOPs}]{} \Phi^{\pm\,\ell}_{h,N}(\mu),\ 1 \le \ell \le 4\ .$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online

Proposition 3.0A. Given

$$\mathcal{S}_{\text{Online}}[\mathcal{M}_h] \text{ of size } O(N_{\max}^2)\ ,$$

then

$$\mu, N \longrightarrow \Phi_{h,N}^{\pm\,\ell}(\mu),\ 1 \le \ell \le 4\,,$$

may be calculated in $O(N^3 + Q^2N^2)$ FLOPs.

Online operation count *independent* of $\mathcal{N}_h$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Hierarchical Architecture

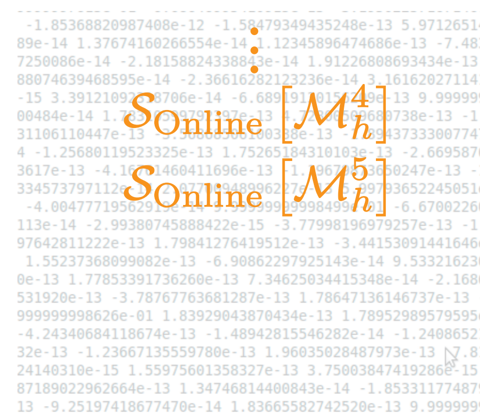
“In-the-Lab”

$\vdots$

$\mathcal{M}_h^5$ →

Offline:
Supercomputer[†]

- - - - →



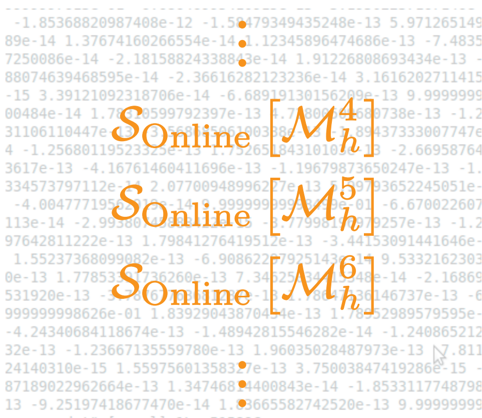
Library:
www

[†]Exploit parallelism over Ω and over $\mathcal{D}$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Hierarchical Architecture

"In-the-Field"...



$\leftarrow \mu, N$

$\rightarrow \Phi^{\pm\ell}_{h,N},\ 1 \le \ell \le 4$

Library:
www

Online:
Smartphone†

†More generally: any small, lightweight, inexpensive portable or embedded platform.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Hierarchical Architecture

...“In-the-Field”

Corollary 1.1A

Smartphone prediction suffices without appeal to expensive Truth.

In Situ *A Tempo*

Observation 2.0A

Smartphone memory suffices to accommodate $\mathcal{S}_{\text{Online}}[\mathcal{M}_h]$.

Proposition 3.0A

Smartphone processor suffices to calculate $\Phi^{\pm\,\ell}_{h,N}(\mu), 1 \leq \ell \leq 4$.

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\mu_h^* \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \mu_{h,N}^* \left(\mathcal{M}_{h,N} \text{ (RB)}\right),$$

$$\Lambda_h \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \left(\mathcal{M}_{h,N} \text{ (RB)}\right).$$

Inverse Problem$_h$ [KT]

Impedance Estimate$_h$

Least Squares

Given $k = [1, 2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\text{exp}}(k) \in \mathbb{C}, \;\; 1 \le \ell \le 4\,,$$

find $(Z_r^*, Z_i^*)_h$: no regularization

$$(Z_r^*, Z_i^*)_h = \arg \min_{(Z_r, Z_i) \in [1,4]^2} \mathcal{E}_h(Z_r, Z_i, k)\,,$$

$$\mathcal{E}_h(Z_r, Z_i, k) \equiv \sum_{\ell=1}^{4} \left| \Phi^{\ell}_{\text{exp}}(k) - \Phi^{\ell}_h(Z_r, Z_i, k) \right|^2 .$$

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

Least Squares

Given $k = [1, 2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\exp}(k) \in \mathbb{C}, \;\; 1 \le \ell \le 4\,,$$

find $(Z_r^*, Z_i^*)_{h,N}$: no regularization

$$(Z_r^*, Z_i^*)_{h,N} = \arg \min_{(Z_r, Z_i) \in [1,4]^2} \mathcal{E}_{h,N}(Z_r, Z_i, k)\;,$$

$$\mathcal{E}_{h,N}(Z_r, Z_i, k) \equiv \sum_{\ell=1}^{4} \left| \Phi^{\ell}_{\exp}(k) - \Phi^{\ell}_{h,N}(Z_r, Z_i, k) \right|^2 .$$

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

Parametric Derivatives...

Field Sensitivity: $1 \le p \le P - 1\ (= 2)$

$$\partial_p\, \phi_{h,N}(\boldsymbol{x};\boldsymbol{\mu}) \equiv \frac{\partial \phi_{h,N}}{\partial \mu_p}(\boldsymbol{x};\boldsymbol{\mu})\ .^\dagger$$

Output Sensitivity: $1 \le \ell \le 4$,

$$\partial_p\, \Phi^\ell_{h,N}(\boldsymbol{\mu}) = \frac{1}{|\Gamma^\ell_{\rm out}|} \int_{\Gamma_{\rm out}} \partial_p\, \phi_{h,N}(\boldsymbol{x};\boldsymbol{\mu})\ .$$

Jacobian $\mathcal{J} \in \mathbb{R}^{8\times 2}$: $1 \le \ell \le 4, 1 \le p \le 2,$

$$\left[\mathcal{J}_{h,N}(\boldsymbol{\mu})\right] = \left[\Re\, \partial_p\, \Phi^\ell_{h,N}; \Im\, \partial_p\, \Phi^\ell_{h,N}\right]\ .$$

†Recall $\boldsymbol{\mu} = (\mu_1 = Z_r,\ \mu_2 = Z_i,\ \mu_3 = k)$.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Parametric Derivatives...

Given $\mu \in \mathcal{D}$, $\partial_p\, \phi_{h,N}(\mu) \in X_{h,N}$ satisfies $\quad p = 1, 2$

$$\int_\Omega \nabla \partial_p\, \phi_{h,N} \cdot \nabla \overline{v} - \int_\Omega k^2\, \partial_p\, \phi_{h,N}\, \overline{v} + \int_{\Gamma_{\mathrm{imp}}} \frac{i\,k}{Z}\, \partial_p\, \phi_{h,N}\, \overline{v}$$

$$+ \int_{\Gamma^{\mathrm{rad}}} \cdots = \frac{-k\, i^p}{Z^2} \int_{\Gamma_{\mathrm{imp}}} \phi_{h,N}\, \overline{v}, \;\; \forall\, v \in X_{h,N}\,;$$

recall $Z = Z_r + i\, Z_i = \mu_1 + i\, \mu_2$.

Note $\partial_p\, \phi_{h,N} \equiv \dfrac{\partial \phi_{h,N}}{\partial \mu_p} \in X_{h,N} \approx \dfrac{\partial \phi_h}{\partial \mu_p} \in X_h$.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Parametric Derivatives

Corollary 3.1A. Given $(P = 3)$

$$\mathcal{S}_{\text{Online}}\,[\mathcal{M}_h] \text{ of size } O(N_{\max}^2)\ ,$$

then DIRECT APPROACH

$$\mu, N \to \mathcal{J}_{h,N}(\mu) \in \mathbb{R}^{8\times 2}$$

may be calculated in $O(N^3 + PN^2)$ FLOPs.

Note for very large P ADJOINT APPROACH is preferred.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

Levenberg-Marquardt...

Given $\mathcal{J}_{h,N}(\mu) \in \mathbb{R}^{8\times 2}$: $\mu = (Z_r, Z_i, k)$

$$\underset{2\times 2}{G(\mu)} \equiv \mathcal{J}^{\mathrm{T}}_{h,N}(\mu)\, \mathcal{J}_{h,N}(\mu) + \lambda_{\mathrm{L}M}\, \mathbf{diag}\left(\mathcal{J}^{\mathrm{T}}_{h,N}(\mu)\, \mathcal{J}_{h,N}(\mu)\right),$$

and

$$\underset{2\times 1}{b\,(\mu)} \equiv \mathcal{J}^{\mathrm{T}}_{h,N}(\mu) \begin{pmatrix} \Re\, \Phi^1_{\exp}(k) - \Re\, \Phi^1_{h,N}(\mu) \\ \vdots \\ \Im\, \Phi^4_{\exp}(k) - \Im\, \Phi^4_{h,N}(\mu) \end{pmatrix}.$$

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...

Algorithm Levenberg-Marquardt†: given k

set $(Z_r^*, Z_i^*)_{h,N} = (Z_r, Z_i)_{\text{guess}} \in [1,4]^2$

while $|\nabla\, \mathcal{E}_{h,N}\, ((Z_r^*, Z_i^*)_{h,N}, k)| > \text{tol}$

$G((Z_r^*, Z_i^*)_{h,N}, k)\; (\delta Z_r; \delta Z_i) = b((Z_r^*, Z_i^*)_{h,N}, k)$;

$(Z_r^*, Z_i^*)_{h,N} \leftarrow (Z_r^*, Z_i^*)_{h,N} + (\delta Z_r, \delta Z_i)$;

end while % $N^3 + PN^2$

†Apache Math Commons (Java) implementation; unconstrained.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...

$$\epsilon_{\text{exp}} = 0.015$$

$$Z_r^{**} = 3, \quad Z_i^{**} = 2^{\dagger}$$
$$k = 2$$

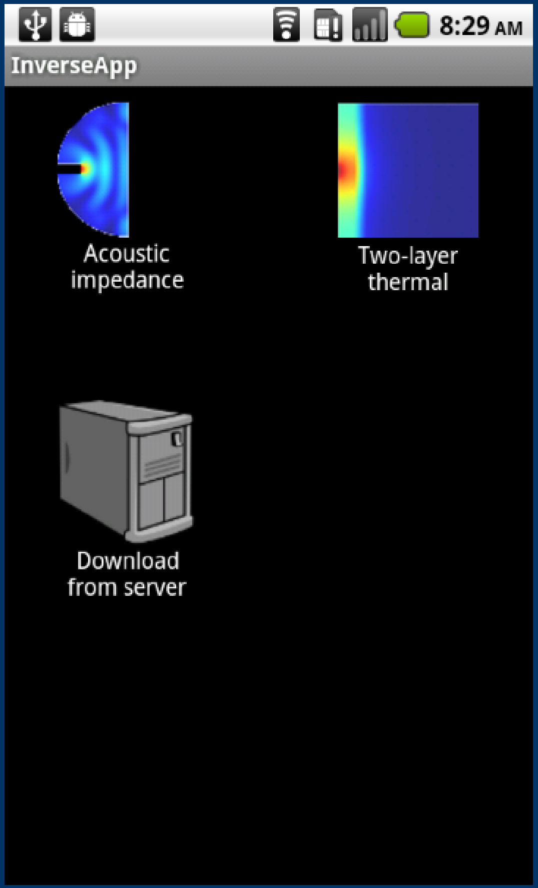
$$N = 25$$
$$(Z_r, Z_i)_{\text{guess}} = (2.5, 2.5)$$

† Here $\Phi^{\ell}_{\text{exp}}(k) = \Phi^{\ell}_{h,N_{\max}}(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\text{exp}} \mathcal{N}(0,1)$.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...



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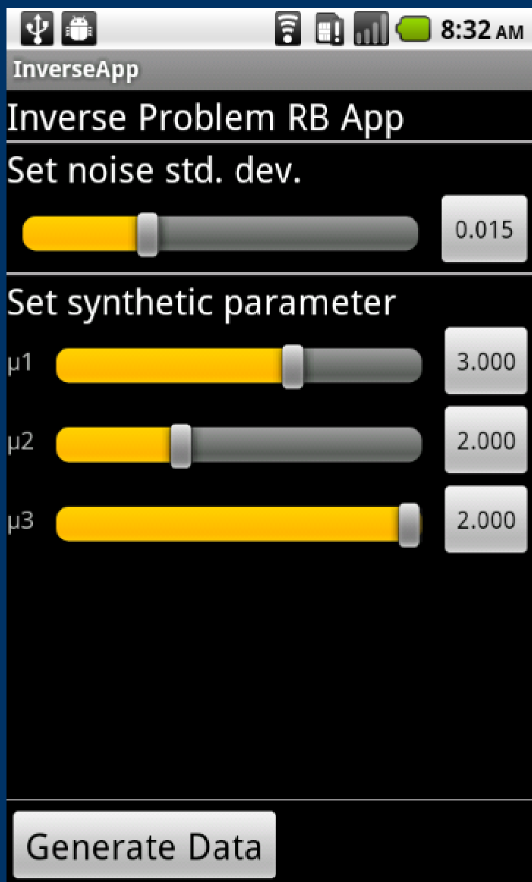
Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...



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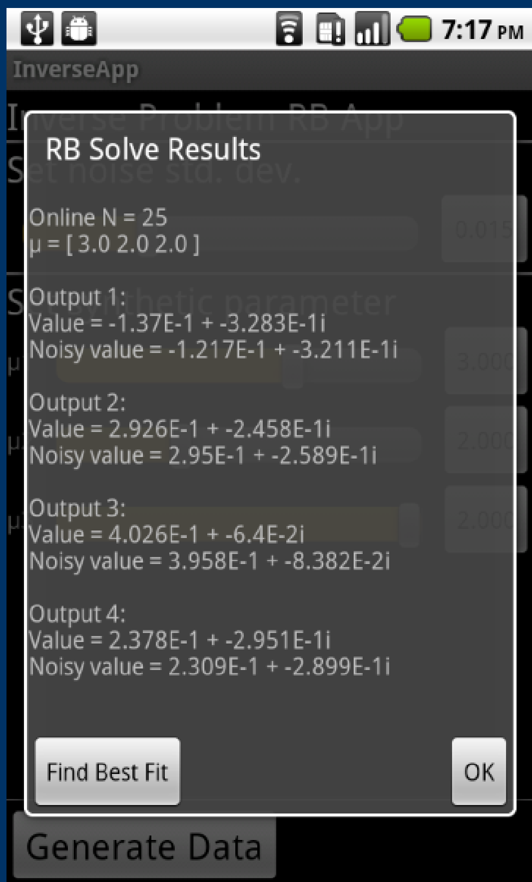
Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...



$$\epsilon_{\text{exp}} = 0.015$$

$$Z_r^{**} = 3, \quad Z_i^{**} = 2^{\dagger}$$

$$k = 2$$

$$N = 25$$

$$(Z_r, Z_i)_{\text{guess}} = (2.5, 2.5)$$

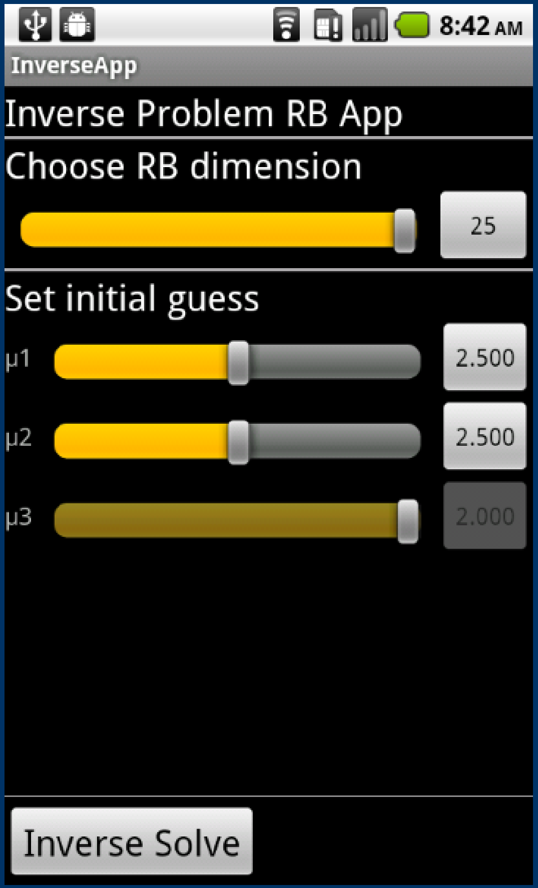
---

†Here $\Phi^{\ell}_{\text{exp}}(k) = \Phi^{\ell}_{h,N_{\max}}(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\text{exp}} \mathcal{N}(0,1)$.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt...



$$\epsilon_{\rm exp} = 0.015$$

$$Z_r^{**} = 3, \quad Z_i^{**} = 2^\dagger$$

$$k = 2$$

$$N = 25$$

$$(Z_r, Z_i)_{\rm guess} = (2.5, 2.5)$$

†Here $\Phi^\ell_{\rm exp}(k) = \Phi^\ell_{h,N_{\max}}(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\rm exp}\mathcal{N}(0,1)$.

Inverse Problem$_{h,N}$

Impedance Estimate$_{h,N}$

...Levenberg-Marquardt

$$\epsilon_{\text{exp}} = 0.015$$

$$Z_r^{**} = 3, \quad Z_i^{**} = 2^\dagger$$
$$k = 2$$

$$N = 25$$
$$(Z_r, Z_i)_{\text{guess}} = (2.5, 2.5)$$

---

†Here $\Phi^\ell_{\text{exp}}(k) = \Phi^\ell_{h,N_{\max}}(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\text{exp}}\mathcal{N}(0,1)$.

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\mu_h^* \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \mu_{h,N}^* \left(\mathcal{M}_{h,N} \text{ (RB)}\right),$$

$$\Lambda_h \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \left(\mathcal{M}_{h,N} \text{ (RB)}\right).$$

Inverse Problem$_h$

Uncertainty Analysis$_h$

Likelihood Ratio: $\Lambda_h(\mu)$

Given $k \in [1, 2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\exp}(k) = \Phi^{\ell}_h(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\exp}\,\mathcal{N}(0, 1)\ ,$$

hypothesis

define (pre-Bayesian) $\forall\ (Z_r, Z_i) \in [1, 4]^2$

$$\mathcal{L}_h(Z_r, Z_i, k) \equiv e^{\left\{-\mathcal{E}_h(Z_r, Z_i, k)/2\epsilon^2_{\exp}\right\}}\ ,$$

$$\Lambda_h(Z_r, Z_i, k) \equiv \frac{\mathcal{L}_h(Z_r, Z_i, k)}{\mathcal{L}_h(Z^*_{r\,h}, Z^*_{i\,h}, k)}\ .$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Strategy

Given $k \in [1,2]$ and $\mu = (Z_r, Z_i, k)$

$$\Phi^{\ell}_{\exp}(k) = \Phi^{\ell}_{h}(Z_r^{**}, Z_i^{**}, k) + \epsilon_{\exp}\, \mathcal{N}(0,1) \; ,$$

hypothesis

form

$$\Lambda^{\mathrm{U}}_{h,N}(Z_r, Z_i, k)\left[\Phi^{\pm\,\ell}_{h,N}(Z_r, Z_i, k)\right]_{1 \le \ell \le 4}$$

such that $\forall\ (Z_r, Z_i) \in [1,4]^2$

$$\Lambda_h(Z_r, Z_i, k) \le \Lambda^{\mathrm{U}}_{h,N}(Z_r, Z_i, k) \; .$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Likelihood Bounds...

Define $\mathcal{L}^{\mathrm{L}}_{h,N}(\mu) \equiv e^{\{-\mathcal{E}^{\mathrm{U}}_{h,N}(\mu)/2\epsilon^2_{\exp}\}}$,

where $\mu = (Z_r, Z_i, k)$

$$\mathcal{E}^{\mathrm{U}}_{h,N}(\mu) \equiv \sum_{\ell=1}^{4} \left|\Phi^{\ell}_{\exp}(k) - \Phi^{\mathrm{U}\,\ell}_{h,N}(\mu)\right|^2;$$

$$\Re\,\Im\,\Phi^{\mathrm{U}\,\ell}_{h,N}(\mu) =$$

$$\arg \max_{z\in[\Re\,\Im\,\Phi^{-\,\ell}_{h,N}(\mu),\Re\,\Im\,\Phi^{+\,\ell}_{h,N}(\mu)]^{\dagger}} \left|\Re\,\Im\,\Phi^{\ell}_{\exp}(k) - z\right|.$$

---

†Minimum obtained for $z = \Re\,\Im\,\Phi^{-\,\ell}_{h,N}(\mu)$ or $z = \Re\,\Im\,\Phi^{+\,\ell}_{h,N}(\mu)$.

...Likelihood Bounds...

Define $\mathcal{L}^{\mathrm{U}}_{h,N}(\mu) \equiv e^{\{-\mathcal{E}^{\mathrm{L}}_{h,N}(\mu)/2\epsilon^2_{\exp}\}}$,

where $\mu = (Z_r, Z_i, k)$

$$\mathcal{E}^{\mathrm{L}}_{h,N}(\mu) \equiv \sum_{\ell=1}^{4} \left|\Phi^{\ell}_{\exp}(k) - \Phi^{\mathrm{L}\,\ell}_{h,N}(\mu)\right|^2;$$

$$\Re\,\Im\,\Phi^{\mathrm{L}\,\ell}_{h,N}(\mu) =$$

$$\arg \min_{z \in [\Re\,\Im\,\Phi^{-\,\ell}_{h,N}(\mu),\, \Re\,\Im\,\Phi^{+\,\ell}_{h,N}(\mu)]^{\dagger}} \left|\Re\,\Im\,\Phi^{\ell}_{\exp}(k) - z\right|.$$

---

†Minimum obtained for $z = \Re\,\Im\,\Phi^{-\,\ell}_{h,N}(\mu)$, $\Re\,\Im\,\Phi^{+\,\ell}_{h,N}(\mu)$, *or* $\Re\,\Im\,\Phi^{\ell}_{\exp}(k)$.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Bounds

Proposition 4.0A: Given $k, \{\Phi^\ell_{\exp}(k)\}_{1\le\ell\le4} \in \mathbb{C}$,

$$\mathcal{L}^{\mathrm{L}}_{h,N}(Z_r, Z_i, k) \le \mathcal{L}_h(Z_r, Z_i, k) \le \mathcal{L}^{\mathrm{U}}_{h,N}(Z_r, Z_i, k), \quad \forall\, (Z_r, Z_i) \in [1,4]^2,$$

for any $N \in \{1, \ldots, N_{\max}\}$.

Likelihood bounds include effects of

approximation error ($\Delta^\ell_{h,N}(Z_r, Z_i, k)$), and

experimental error ($\epsilon_{\exp}\mathcal{N}(0,1)$).

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)$...

Given $k \in [1,2]$ $\qquad \mu = (Z_r, Z_i, k)$

$$\Lambda^{\mathrm{U}}_{h,N}(Z_r, Z_i, k) \equiv \frac{\mathcal{L}^{\mathrm{U}}_{h,N}(Z_r, Z_i, k)}{\mathcal{L}^{\mathrm{L}}_{h,N}((Z_r^*, Z_i^*)_{h,N}, k)},$$

for all $(Z_r, Z_i) \in [1,4]^2$.

Similar construction possible for $\Lambda^{\mathrm{L}}_{h,N}(Z_r, Z_i, k)$.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)$...

Corollary 4.1A: Given $k, \{\Phi^{\ell}_{\mathrm{exp}}(k)\}_{1 \le \ell \le 4} \in \mathbb{C}$,

$$\Lambda_h(Z_r, Z_i, k) \le \Lambda^{\mathrm{U}}_{h,N}(Z_r, Z_i, k) \; ,$$

$$\forall \, (Z_r, Z_i) \in [1, 4]^2 \; ,$$

for any $N \in \{1, \ldots, N_{\max}\}$.

Rigorous constructions for parametric uncertainty.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)$

Corollary 3.2A: Given

$$\mathcal{S}_{\mathrm{Online}}\,[\mathcal{M}_h] \text{ of size } O(N^2_{\max}) \ ,$$

then given k

$$(Z_r, Z_i) \in [1,4]^2,\ N \rightarrow \Lambda^{\mathrm{U}}_{h,N}(Z_r, Z_i, k)$$

may be calculated in

$$O(N^3 + Q^2 N^2) \text{ FLOPs } + 8 \text{ exp's.}$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)^{\dagger}$...

$$\epsilon_{\mathrm{exp}} = 0.015$$

$$Z_r^{**} = 3, \;\; Z_i^{**} = 2^{\dagger}$$
$$k = 2$$

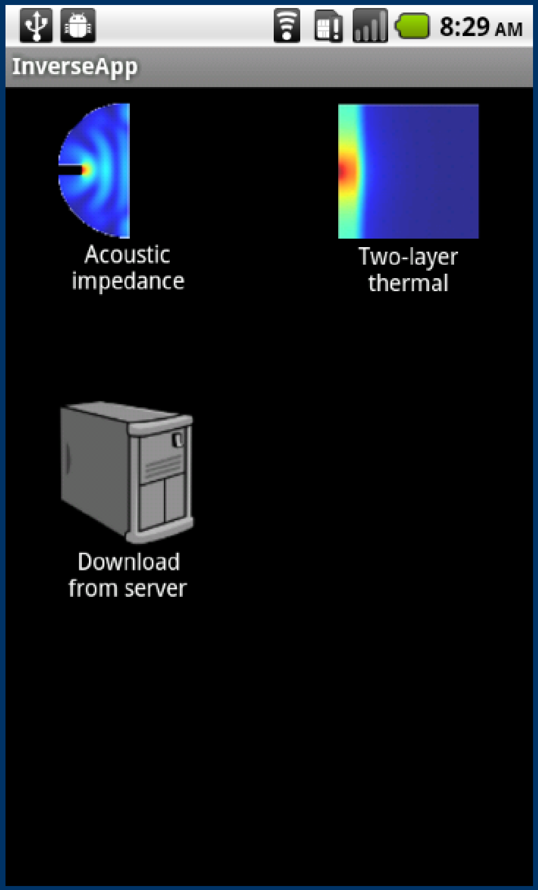
$$N = 25, \;\; 8$$
$$(Z_r, Z_i)_{\mathrm{guess}} = (2.5, 2.5)$$

† Here $\min(\Lambda^{\mathrm{U}}_{h,N}, 1)$ is plotted near $(Z_r^*, Z_i^*)_{h,N}$ based on 64^2 evaluations.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)^{\dagger}$...



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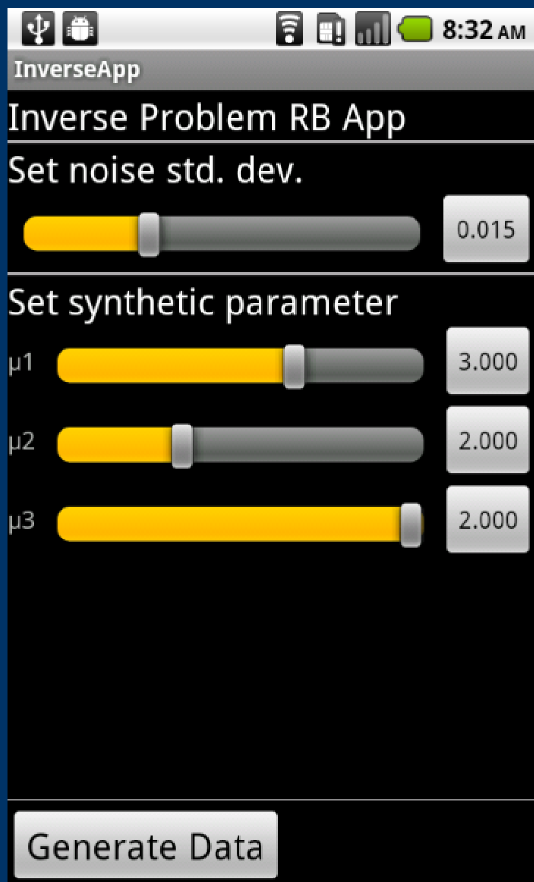
Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)^{\dagger}$...



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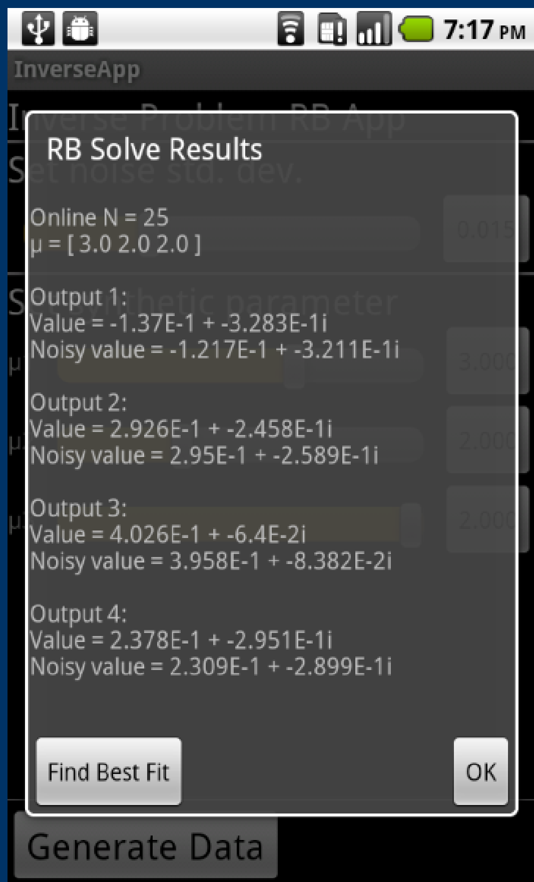
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\mu)^{\dagger}$...



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Uncertainty Analysis$_{h,N}$

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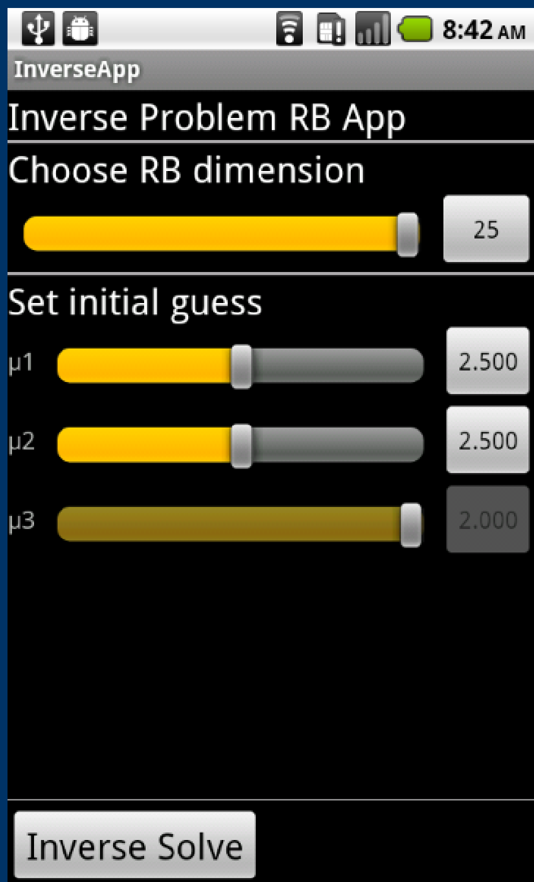

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Uncertainty Analysis$_{h,N}$

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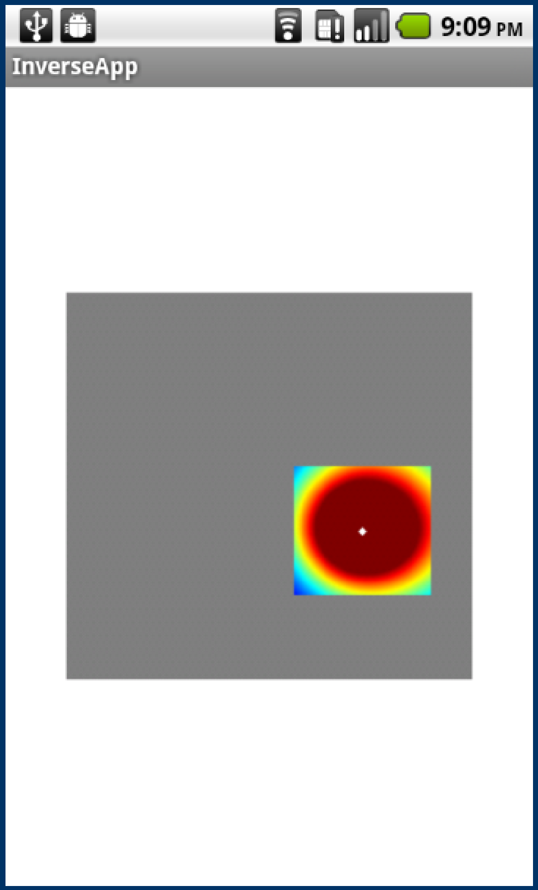

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Uncertainty Analysis$_{h,N}$

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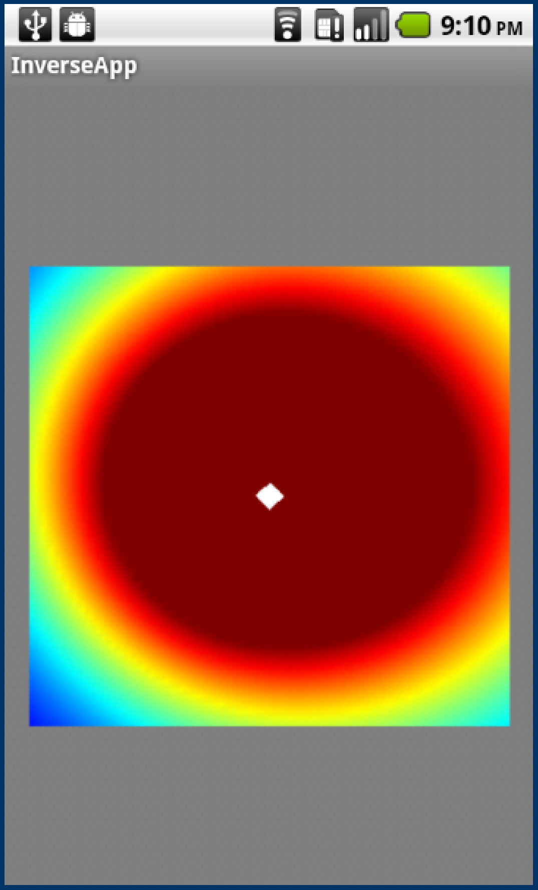

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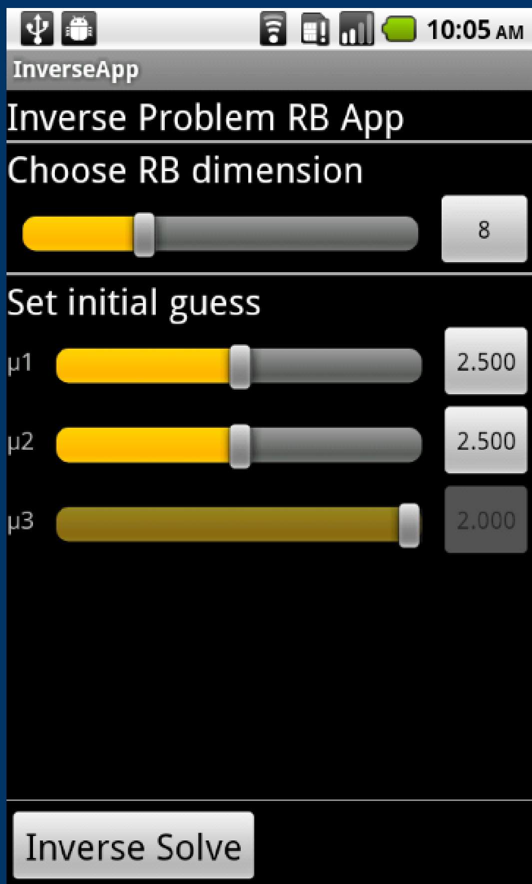

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Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

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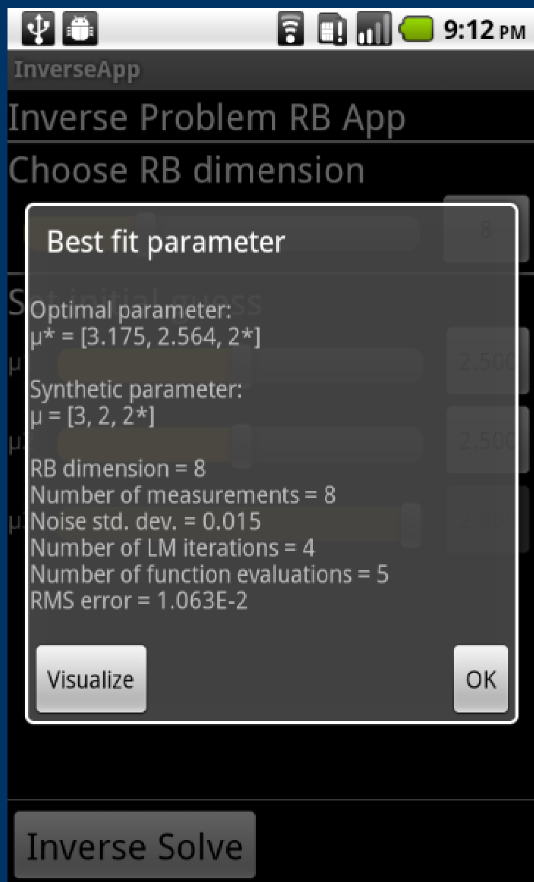

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Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

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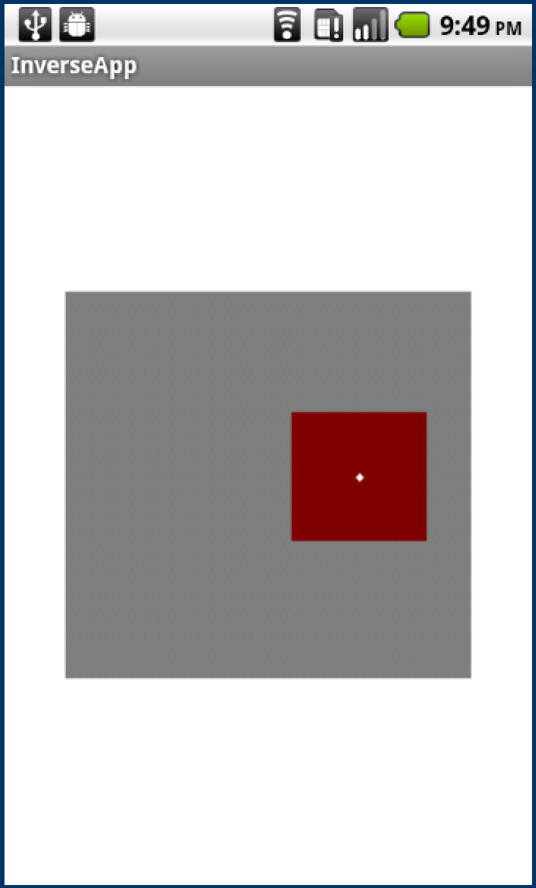

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Inverse Problem$_{h,N}$

Hierarchical Architecture

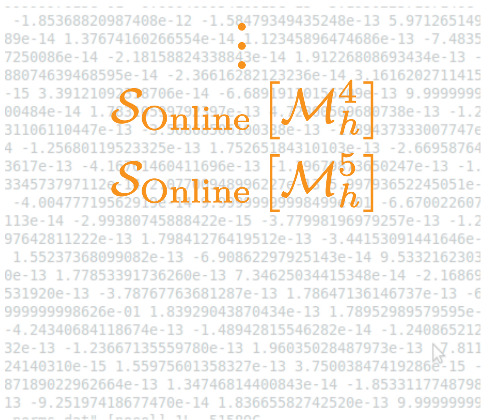
"In-the-Lab"

$\vdots$

$\mathcal{M}_h^5 \longrightarrow$

Offline:
Supercomputer†

$- - - \to$



$\vdots$

$\mathcal{S}_{\text{Online}}\left[\mathcal{M}_h^4\right]$

$\mathcal{S}_{\text{Online}}\left[\mathcal{M}_h^5\right]$

Library:
www

†Exploit parallelism over Ω and over $\mathcal{D}$.

Inverse Problem$_{h,N}$

Hierarchical Architecture

"In-the-Field"

$S_{\text{Online}}[\mathcal{M}_h^4]$

$\vdots$

$S_{\text{Online}}[\mathcal{M}_h^5]$

$\vdots$

$S_{\text{Online}}[\mathcal{M}_h^6]$

$\vdots$

$k, \{\Phi^\ell_{\text{exp}}(k)\}_{1\le\ell\le4};\ \epsilon_{\text{exp}} \qquad N$

$(Z_r^*, Z_i^*)_{h,N};\ \Lambda^{\text{U}}_{h,N}(Z_r, Z_i, k)$

Library:
www

Online:
Smartphone †

†More generally: any small, lightweight, inexpensive portable or embedded platform.

Outline

The Big Picture

An Acoustics Example

A Heat Transfer Example

The Big Questions

Heat Transfer Example: On-Site Energy Audit

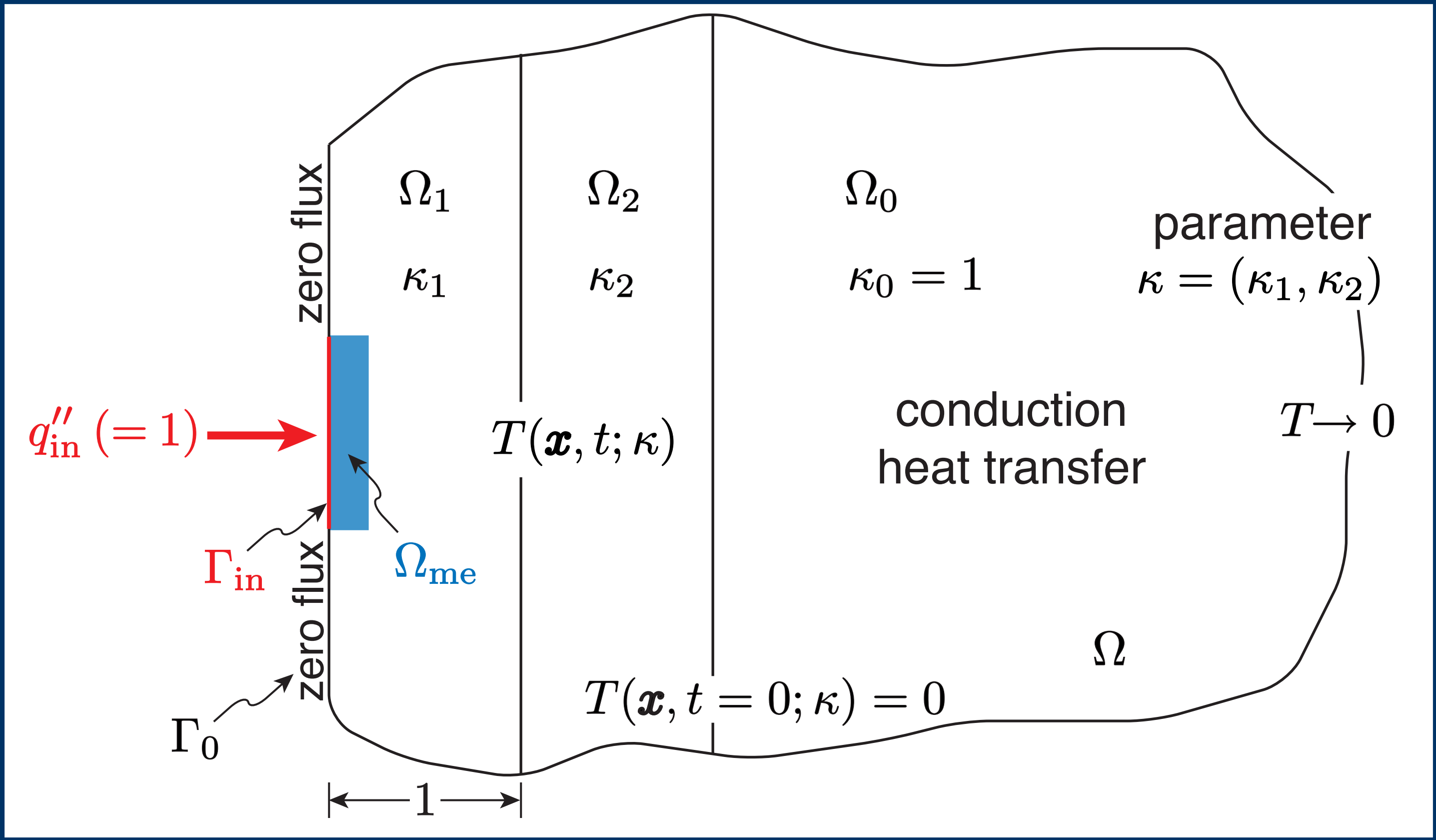
(Inverse) Problem Formulation

Computational Approach

Parametrized Model $\mathcal{M}$

Domain

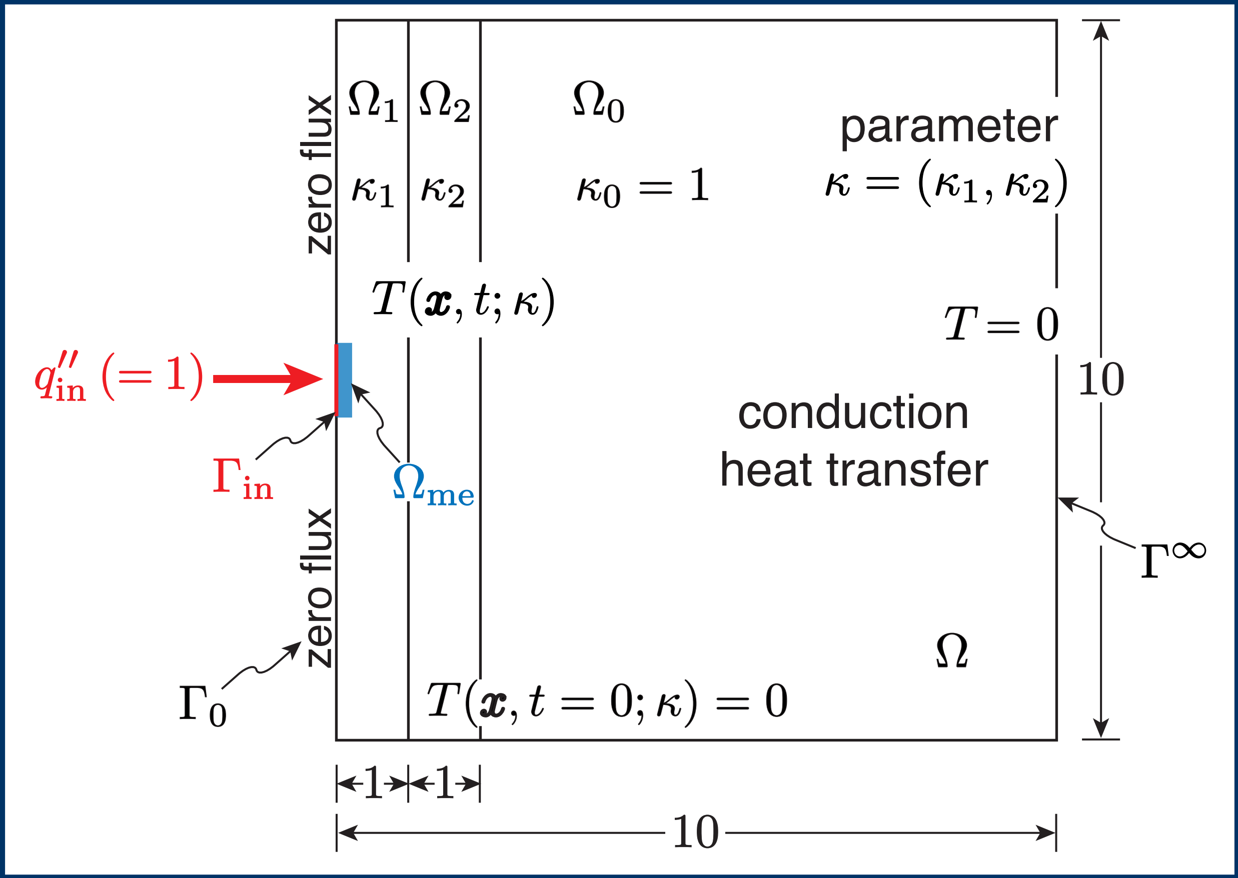
Semi-Infinite



Parametrized Model $\mathcal{M}$

Domain

Truncated



Parametrized Model $\mathcal{M}$

Governing Equations

Strong Form

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $T(\boldsymbol{x}, t; \boldsymbol{\kappa})$ satisfies $\quad T(\boldsymbol{x}, 0; \boldsymbol{\kappa}) = 0$

$$\frac{\partial T}{\partial t} - \kappa_\ell \, \nabla^2 T = 0 \text{ in } \Omega_{\ell=0,1,2} \,,$$

with boundary conditions

$$\kappa_1 \frac{\partial T}{\partial n} = q''_{\text{in}} \text{ on } \Gamma_{\text{in}} \qquad (= 0 \text{ on } \Gamma_0) \,.^{\dagger}$$

Output: $\overline{T}(t; \boldsymbol{\kappa}) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} T(\boldsymbol{x}, t; \boldsymbol{\kappa}) \, d\boldsymbol{x}$.

---

†We also impose continuity of T and flux at interfaces and $T|_{\Gamma^\infty} = 0$.

Parametrized Model $\mathcal{M}$

Governing Equations

Weak Form...

Given $\kappa \in \mathcal{D}$, $T(t;\kappa)$ satisfies $\qquad T(0;\kappa) = 0$

$$\int_\Omega \underbrace{\frac{\partial T}{\partial t}}_{\partial T/\partial t} v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \underbrace{\kappa_\ell \nabla T \cdot \nabla}_{-\kappa_\ell \nabla^2 T} v$$

$$= \int_{\Gamma_{\text{in}}} \underbrace{q''_{\text{in}}}_{q''_{\text{in}} - \kappa_1 \partial T/\partial n} v, \ \forall\, v \in X.$$

Output: $\overline{T}(t;\kappa) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} T(t;\kappa).$

Here derivatives square integrable

$$X(\Omega) = \{v \in H^1(\Omega) \mid v|_{\Gamma^\infty} = 0\}$$

with inner product and norm

$$(w, v)_X = \int_\Omega \nabla w \cdot \nabla v, \quad \|v\|_X^2 \equiv \int_\Omega |\nabla v|^2.$$

Define also $L^2(\Omega)$ inner product and norm

$$(w, v) = \int_\Omega w \; v, \quad \|v\|^2 \equiv \int_\Omega v^2.$$

Parametrized Model $\mathcal{M}$

Governing Equations

Discrete Time...

Replace continuous time

$$t \in \,]0, t_f]$$

by discrete levels $\qquad \Delta t = t_f / J = 5.0/100$

$$t^j = j\Delta t, \;\; j \in \mathbb{J} \equiv \{(0), 1, 2, \ldots, J\}.$$

Implicit Finite Difference discretization†

$$\Rightarrow \widetilde{T}^j(\kappa) \approx T(t^j; \kappa), \quad j \in \mathbb{J}.$$

†We consider Euler Backward, $O(\Delta t)$, or Crank-Nicolson, $O(\Delta t^2)$.

Parametrized Model $\mathcal{M}$

Governing Equations

...Discrete Time...

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $\widetilde{T}^j(\boldsymbol{\kappa}) \in X$ satisfies $\qquad \widetilde{T}^0(\boldsymbol{\kappa}) = 0$

$$\int_\Omega \frac{\widetilde{T}^j - \widetilde{T}^{j-1}}{\Delta t} v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \, \nabla \widetilde{T} \cdot \nabla v$$

$$= \int_{\Gamma_{\text{in}}} q''_{\text{in}} v, \ \forall\, v \in X, \ \ j \in \mathbb{J}\,.$$

Output: $\overline{\widetilde{T}}^j(\boldsymbol{\kappa}) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} \widetilde{T}^j(\boldsymbol{\kappa}), \ \ j \in \mathbb{J}.$

Assumption: $\widetilde{T}^j(\boldsymbol{\kappa}) \equiv T(t^j; \boldsymbol{\kappa})$ — $O(\Delta t^{\cdot})$ errors negligible.

Parametrized Model $\mathcal{M}$

Governing Equations

...Discrete Time

Given $\kappa \in \mathcal{D}$, $T^j(\kappa) \in X$ satisfies $\qquad T^0(\kappa) = 0$

$$\int_\Omega \frac{T^j - T^{j-1}}{\Delta t} v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \nabla T \cdot \nabla v$$

$$= \int_{\Gamma_{\text{in}}} q''_{\text{in}} v, \ \forall\, v \in X, \ \ j \in \mathbb{J}\,.$$

Output: $\overline{T}^j(\kappa) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} T^j(\kappa), \ \ j \in \mathbb{J}\,.$

Norm: $|||v^j|||^2 = \|v^j\|^2 + \Delta t \ \sum_{j'=1}^{j} \|v\|_X^2.$

Parametrized Model $\mathcal{M}$

Governing Equations

Parameter (Domain)

Here $P = 2$

$\kappa \equiv (\kappa_1, \kappa_2)$ is the *parameter*;

$\mathcal{D} \equiv [0.25, 4]^2 \subset \mathbb{R}^2$ is the *parameter domain*.

More generally,

$\mu = (\mu_1, \ldots, \mu_P)$ is the *parameter*;[†]

$\mathcal{D} \subset \mathbb{R}^P$ is the *parameter domain*.

[†]Note μ may represent physical properties, sources and boundary conditions, or geometry.

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Introduce a Finite Element (FE) space

$$X_h(\Omega; \mathcal{T}_h) \subset X(\Omega) \ ,$$

where h is the diameter of a "triangulation" $\mathcal{T}_h$.

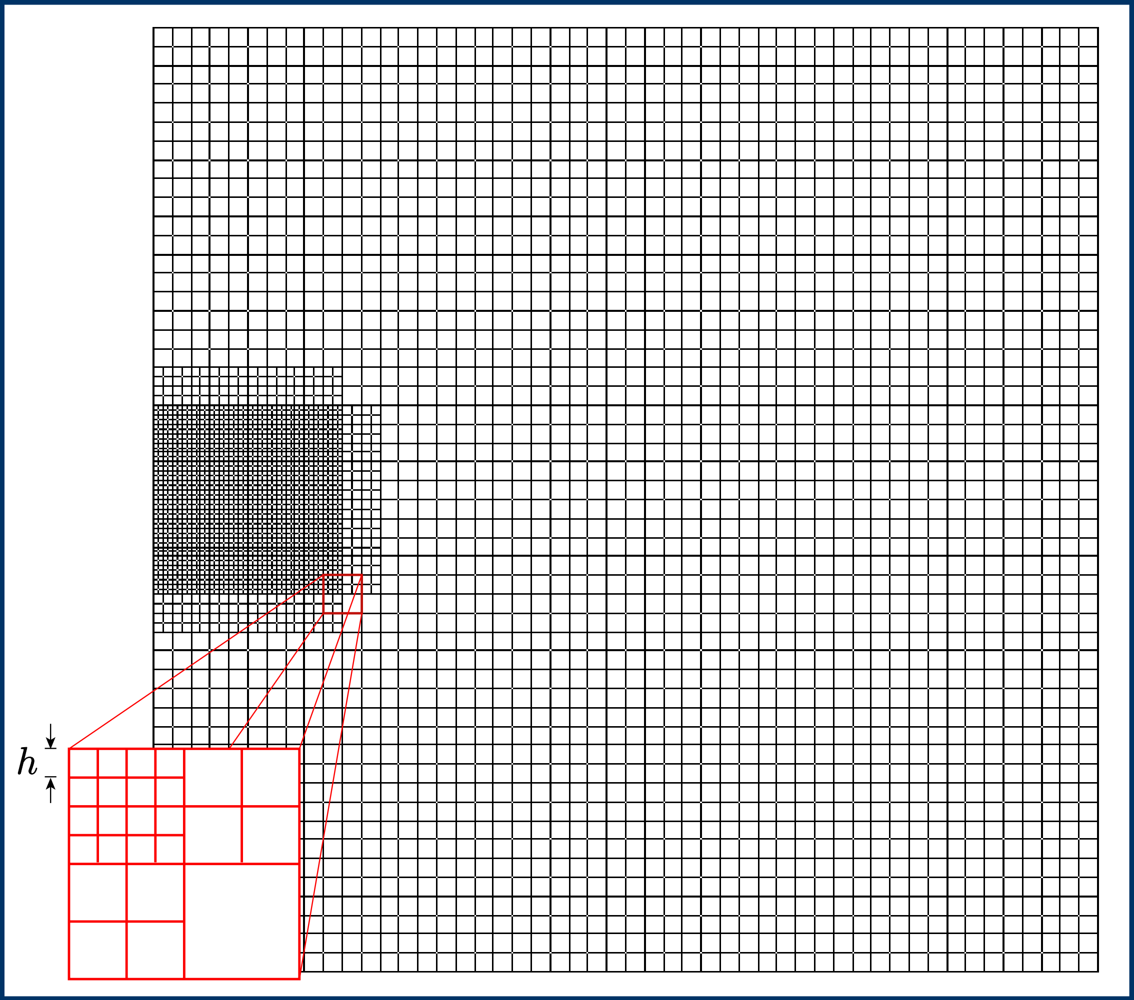
Find given $\kappa \in \mathcal{D}$

$$T_h^j(\kappa) \in X_h \approx T^j(\kappa) \in X, \quad j \in \mathbb{J} \ .$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Space



X_h: $\mathbb{Q}_2$ elements

over

Triangulation $\mathcal{T}_h$

$\Downarrow$

$$\dim(X_h) = 4{,}347$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Galerkin Projection

Given $\kappa \in \mathcal{D}$, $T_h^j(\kappa) \in X_h$ satisfies $\quad T_h^0 = 0$

$$\int_\Omega \frac{T_h^j - T_h^{j-1}}{\Delta t} v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \nabla T_h^j \cdot \nabla v$$

$$= \int_{\Gamma_{\text{in}}} q''_{\text{in}} v, \; \forall\, v \in X_h, \;\; j \in \mathbb{J} \, .$$

Output: $\overline{T}_h^j(\kappa) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} T_h^j(\kappa), \;\; j \in \mathbb{J}.$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Algebraic System...

Express $T_h^j(\kappa) \in X_h$ as $\quad\quad \mathcal{N}_h = \dim(X_h)$

$$T_h^j(x;\kappa) = \sum_{n=1}^{\mathcal{N}_h} \left[c_h^j(\kappa)\right]_n \varphi_n(x), \;\; j \in \mathbb{J},$$

where

$\varphi_n(x)$: (nodal) basis functions $\Leftarrow X_h$;

$[c_h^j(\kappa)]_n$: coefficients $\Leftarrow$ Galerkin projection . . .

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

...Algebraic System

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $\boldsymbol{c}_h^j(\boldsymbol{\kappa}) \in \mathbb{R}^{\mathcal{N}_h}$ satisfies $\boldsymbol{c}_h^0(\boldsymbol{\kappa}) = \mathbf{0}$

$$\left(\frac{\boldsymbol{M}_h}{\Delta t} + \boldsymbol{A}_h\right)\boldsymbol{c}_h^j = \frac{\boldsymbol{M}_h}{\Delta t}\,\boldsymbol{c}_h^{j-1} + \boldsymbol{F}_h\,, \quad j \in \mathbb{J}\,.$$

Output: $j \in \mathbb{J}$,

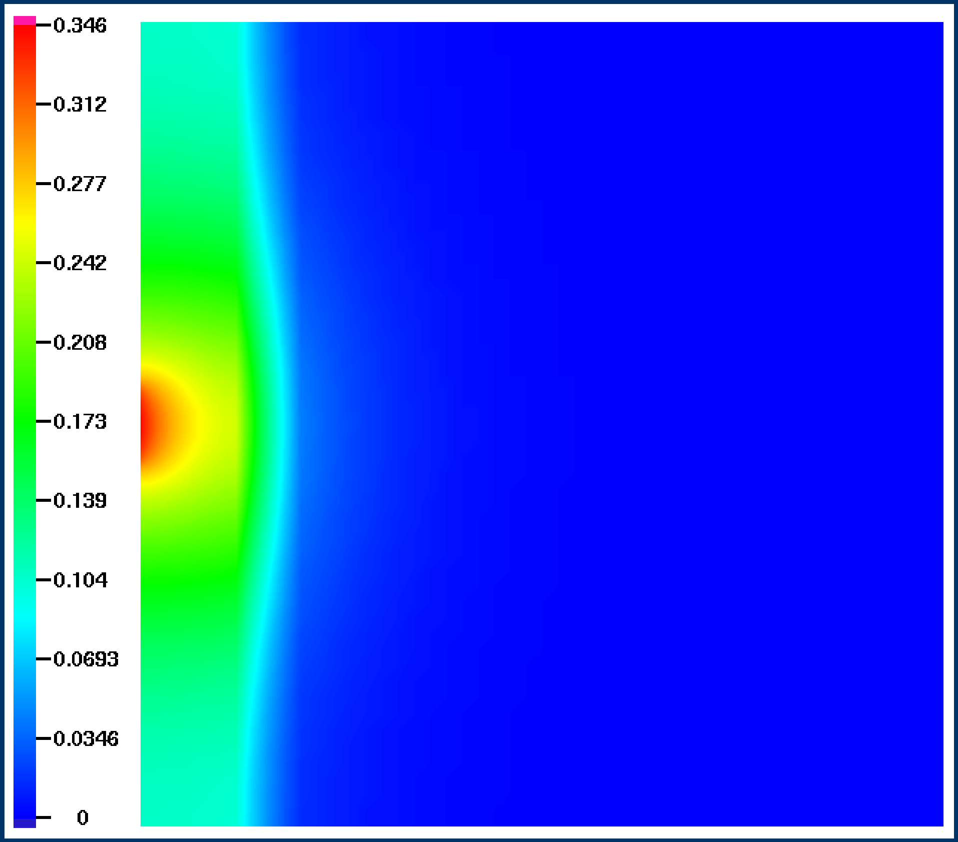
$$\overline{T}_h^j(\boldsymbol{\kappa}) = \sum_{n=1}^{\mathcal{N}_h} \left[\boldsymbol{c}_h^j(\boldsymbol{\kappa})\right]_n \left(\frac{1}{|\Omega_{\mathrm{me}}|}\int_{\Omega_{\mathrm{me}}} \varphi_n\right).$$

Here $\boldsymbol{c}_h^j(\boldsymbol{\kappa}) \in \mathbb{R}^{\mathcal{N}_h}$, $\boldsymbol{F}_h \in \mathbb{R}^{\mathcal{N}_h}$, and
$\boldsymbol{M}_h \in \mathbb{R}^{\mathcal{N}_h\times\mathcal{N}_h}$, $\boldsymbol{A}_h(\boldsymbol{\kappa}) \in \mathbb{R}^{\mathcal{N}_h\times\mathcal{N}_h}$ but *sparse*.

Parametrized Model $\mathcal{M}_h$ (FE)

Illustrative Solutions

Temperature Field

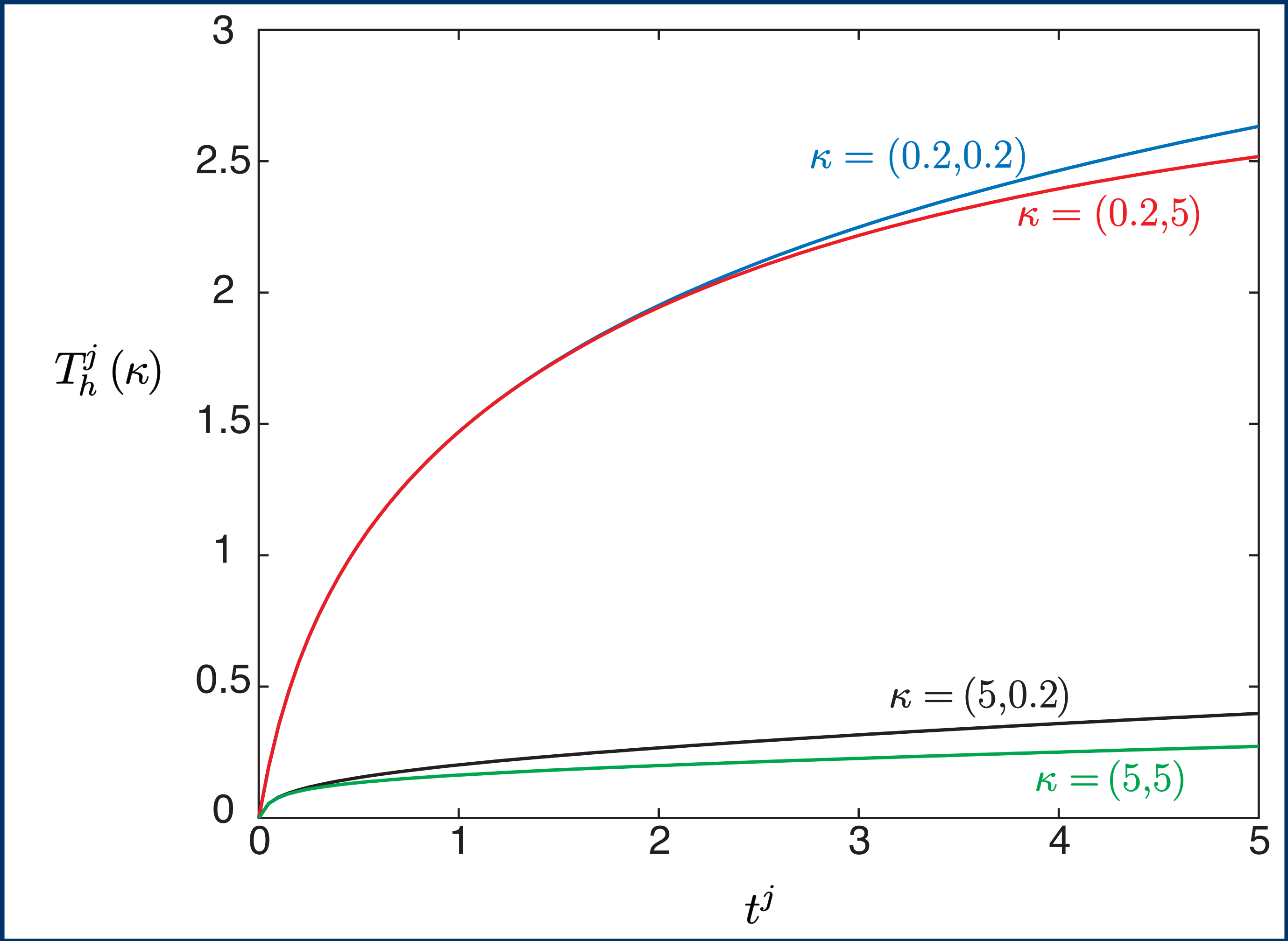


$$\kappa = (5.0, 0.2), \;\; t^j = 3$$

Parametrized Model $\mathcal{M}_h$ (FE)

Illustrative Solutions

Output Variation



Inverse Problem$_h$

Diffusivity Estimate$_h$

Least Squares

Given [St]

$$t_{\rm me}^m,\ \ \overline{T}_{\rm exp}(t_{\rm me}^m),\ \ 1 \le m \le M_{\rm me}\ ,$$

find (any) no regularization

$$\kappa_h^* = \arg\min_{\kappa\in\mathcal{D}} \mathcal{E}_h(\kappa)\ \ ,$$

$$\mathcal{E}_h(\kappa) \equiv \sum_{m=1}^{M_{\rm me}} \left(\overline{T}_{\rm exp}(t_{\rm me}^m) - \overline{T}_h(t_{\rm me}^m;\kappa)\right)^2 .^\dagger$$

---

†Note $\overline{T}_h(t_{\rm me}^m;\kappa) = \overline{T}_h^j(\kappa)$ for j: $t^j = t_{\rm me}^m$.

Inverse Problem$_h$

Uncertainty Analysis$_h$

Likelihood Ratio: $\Lambda_h(\kappa)$

Given *realization*

$$\overline{T}_{\exp}(t^m_{\mathrm{me}}) = \overline{T}_h(t^m_{\mathrm{me}}; \kappa^{**}) + \epsilon_{\exp}\, \mathcal{N}(0,1)$$

hypothesis

define (pre-Bayesian) $\forall\, \kappa \in \mathcal{D}$

$$\mathcal{L}_h(\kappa) \equiv e^{\left\{-\mathcal{E}_h(\kappa)/2\epsilon^2_{\exp}\right\}} ,$$

$$\Lambda_h(\kappa) \equiv \frac{\mathcal{L}_h(\kappa)}{\mathcal{L}_h(\kappa^*_h)} .$$

Heat Transfer Example: On-Site Energy Audit

(Inverse) Problem Formulation

Computational Approach

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\kappa_h^* \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \kappa_{h,N}^* \left(\mathcal{M}_{h,N} \text{ (RB)}\right),$$

$$\Lambda_h \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \left(\mathcal{M}_{h,N} \text{ (RB)}\right).$$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Introduce a Finite Element (FE) space

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where h is the diameter of a "triangulation" $\mathcal{T}_h$.

Find given $\kappa \in \mathcal{D}$

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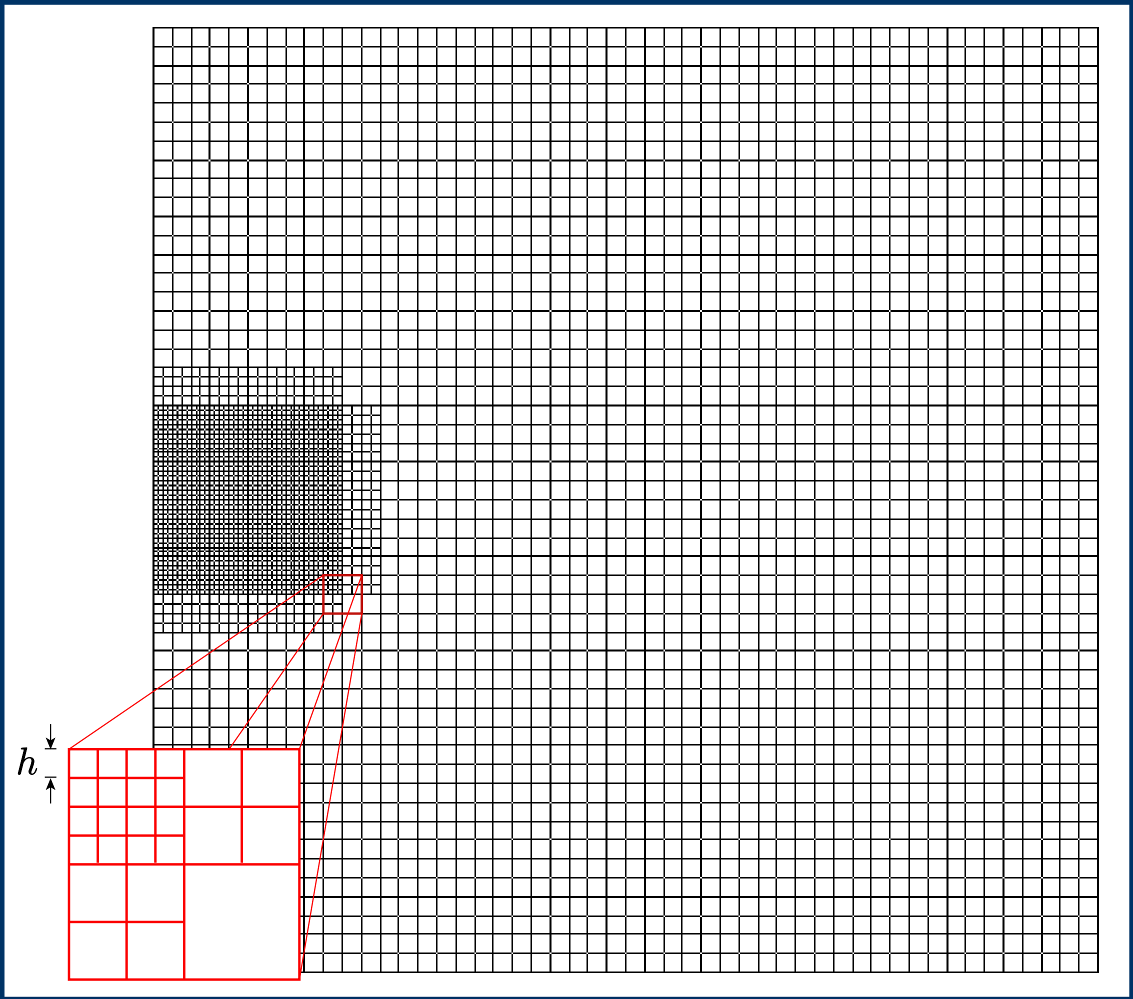
Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Space



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Triangulation $\mathcal{T}_h$

$\Downarrow$

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Parametrized Model $\mathcal{M}_h$ (FE)

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$$= \int_{\Gamma_{\text{in}}} q''_{\text{in}}\, v, \ \forall\, v \in X_h, \ \ j \in \mathbb{J} \ .$$

Output: $\overline{T}_h^j(\kappa) = \frac{1}{|\Omega_{\text{me}}|} \int_{\Omega_{\text{me}}} T_h^j(\kappa), \ \ j \in \mathbb{J}.$

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

Algebraic System...

Express $T_h^j(\kappa) \in X_h$ as $\mathcal{N}_h = \dim(X_h)$

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where

$\varphi_n(x)$: (nodal) basis functions $\Leftarrow X_h$;

$[c_h^j(\kappa)]_n$: coefficients $\Leftarrow$ Galerkin projection . . .

Parametrized Model $\mathcal{M}_h$ (FE)

(Truth) Approximation

...Algebraic System

Given $\kappa \in \mathcal{D}$, $c_h^j(\kappa) \in \mathbb{R}^{\mathcal{N}_h}$ satisfies $c_h^0(\kappa) = 0$

$$\left(\frac{M_h}{\Delta t} + A_h \right) c_h^j = \frac{M_h}{\Delta t} c_h^{j-1} + F_h \,, \quad j \in \mathbb{J} \,.$$

Output: $j \in \mathbb{J}$,

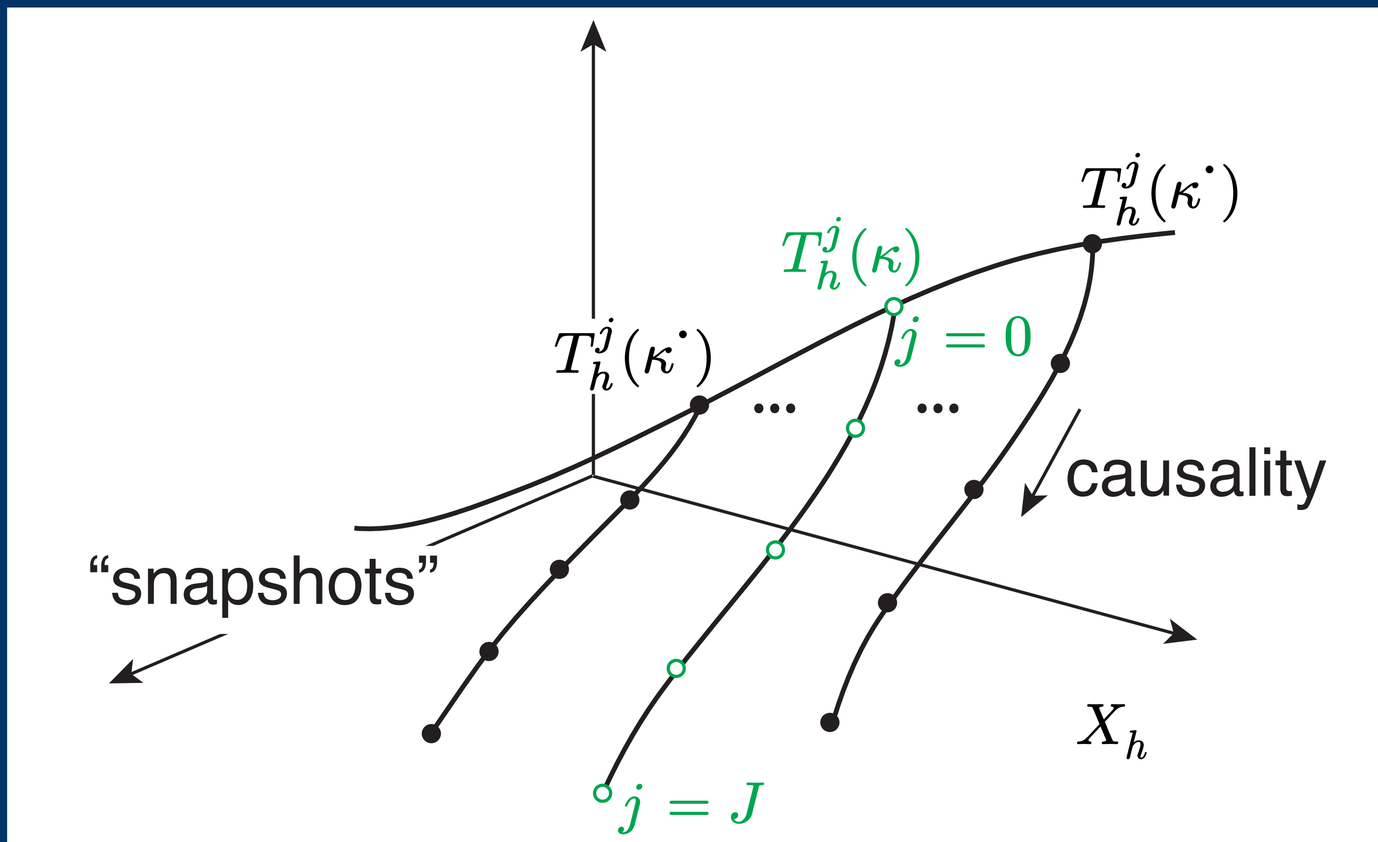
$$\overline{T}_h^j(\kappa) = \sum_{n=1}^{\mathcal{N}_h} \left[c_h^j(\kappa) \right]_n \left(\frac{1}{|\Omega_{\mathrm{me}}|} \int_{\Omega_{\mathrm{me}}} \varphi_n \right) .$$

Here $c_h^j(\kappa) \in \mathbb{R}^{\mathcal{N}_h}$, $F_h \in \mathbb{R}^{\mathcal{N}_h}$, and $M_h \in \mathbb{R}^{\mathcal{N}_h \times \mathcal{N}_h}$, $A_h(\kappa) \in \mathbb{R}^{\mathcal{N}_h \times \mathcal{N}_h}$ but *sparse*.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Parametric Manifold $\mathcal{P}_h$...



$$\mathcal{P}_h = \{T_h^j(\kappa) \mid \forall\, j \in \mathbb{J},\ \forall \kappa \in \mathcal{D}\}$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Parametric Manifold $\mathcal{P}_h$

Introduce a Reduced Basis† (RB) space

$$X_{h,N} \subset \mathrm{span}\{\mathcal{P}_h\} \subset X_h$$

of dimension $\dim(X_{h,N}) = N$.

Find given $\kappa \in \mathcal{D}$

$$T^j_{h,N}(\kappa) \in X_{h,N} \approx T^j_h(\kappa) \in X_h, \quad j \in \mathbb{J}\ .$$

---

†Early work: [ASB], [NPe], [FR], [Po], [G], . . .

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Spaces...

POD(t)-Greedy(κ) heuristic [HO] : $N_{\max}$

$$\{\zeta_n\}_{1 \le n \le N_{\max}} \in \text{span}\{\mathcal{P}_h\}\ , \qquad \text{(impulse control)}$$

and associated hierarchical spaces

$$X_{h,N} = \text{span}\{\zeta_n, 1 \le n \le N\}, 1 \le N \le N_{\max}\ .$$

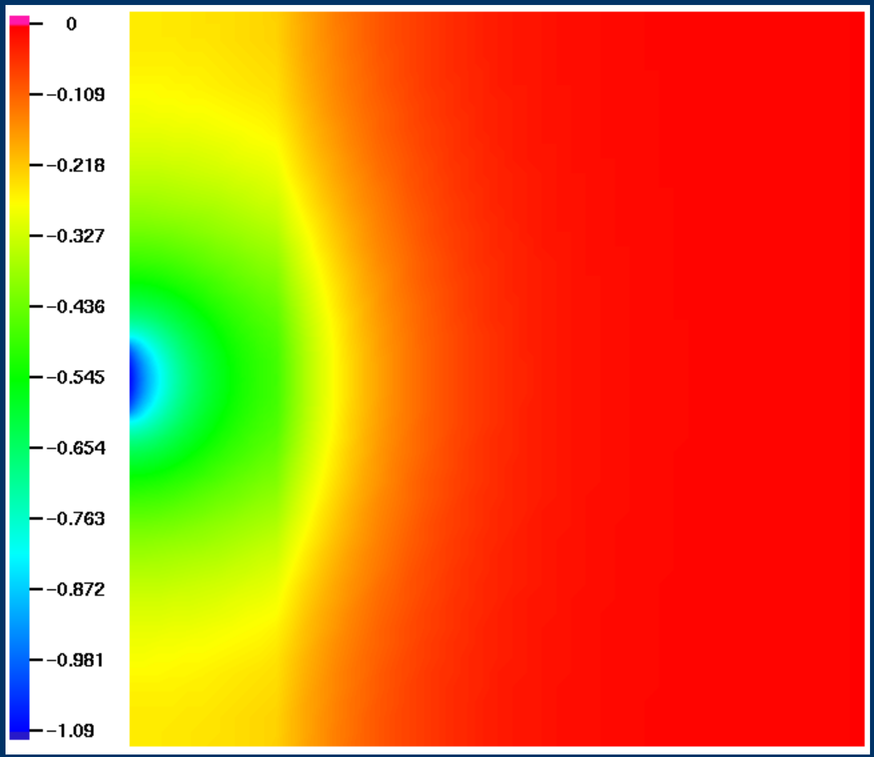
Optimality: $\dim(Y_N) = N$

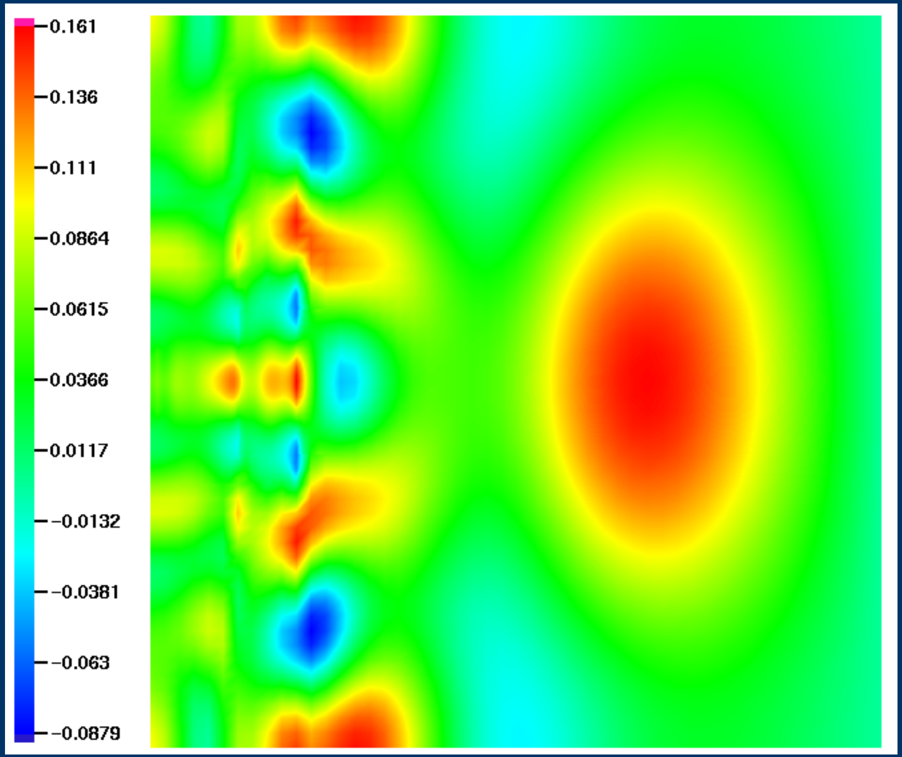
$$X_{h,N} \approx \arg\min_{Y_N} \mathbb{D}_{L^\infty(\mathcal{D};L^2(0,t^J;X))}(\mathcal{P}_h, Y_N).$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Spaces





ζ_1 $\qquad$ $\zeta_{N_{\max}=50}$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Galerkin Projection...

Given $\kappa \in \mathcal{D}$, $T^j_{h,N}(\kappa) \in X_{h,N}$ satisfies $\qquad T^0_{h,N} = 0$

$$\int_\Omega \frac{T^j_{h,N} - T^{j-1}_{h,N}}{\Delta t} v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \nabla T^j_{h,N} \cdot \nabla v$$

$$= \int_{\Gamma_{\text{in}}} q''_{\text{in}}\, v, \ \ \forall\, v \in X_{h,N}, \ \ j \in \mathbb{J}\ .$$

Output: $\overline{T}^j_{h,N}(\kappa) = \dfrac{1}{|\Omega_{\text{me}}|} \displaystyle\int_{\Omega_{\text{me}}} T^j_{h,N}(\kappa)$, $j \in \mathbb{J}$.

Optimality: $T^j_{h,N} \approx$ Best_Fit$_{X_{h,N}}(T^j_h)$ in $|||\cdot|||$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Galerkin Projection...

Output

and

'State' (Field)†

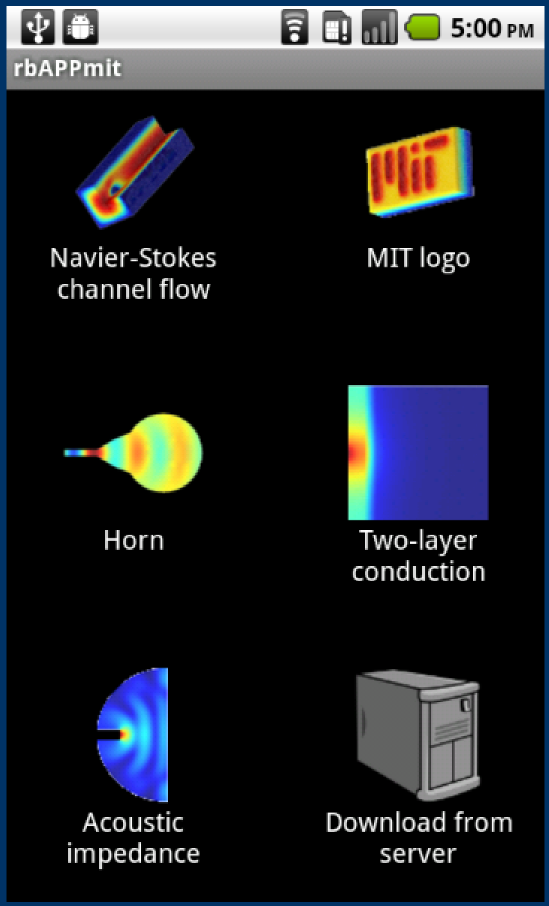
$\uparrow$

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Galerkin Projection...



Output

and

'State' (Field)†

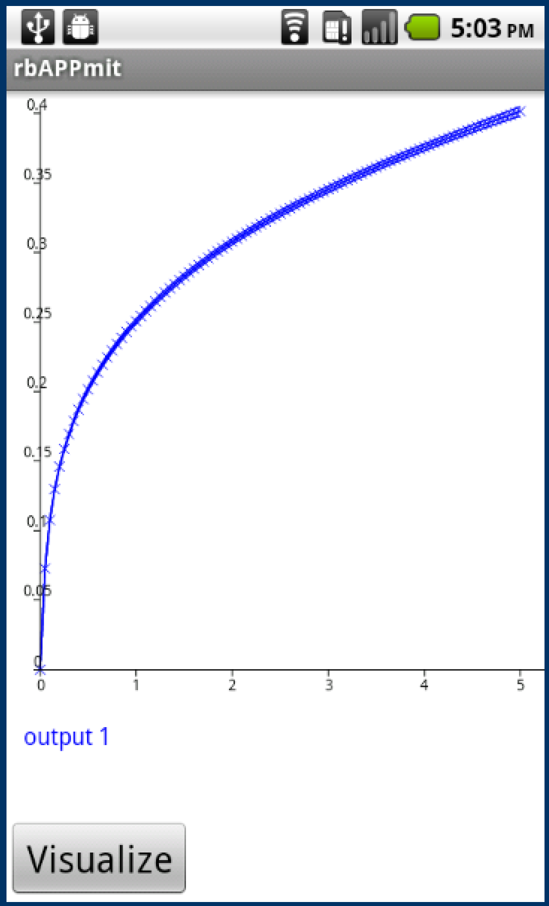
---

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Galerkin Projection...



Output

and

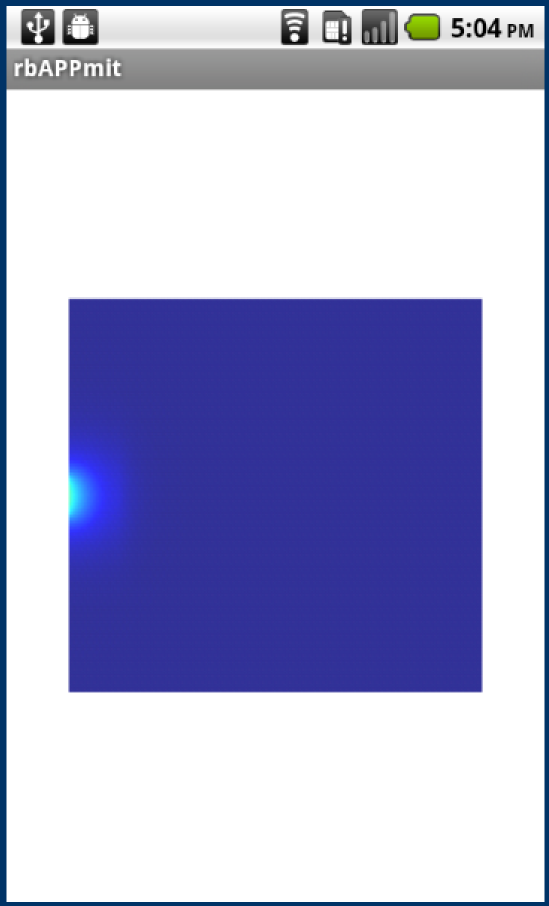
'State' (Field)[†]

[†]Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Galerkin Projection...



Output

and

'State' (Field)†

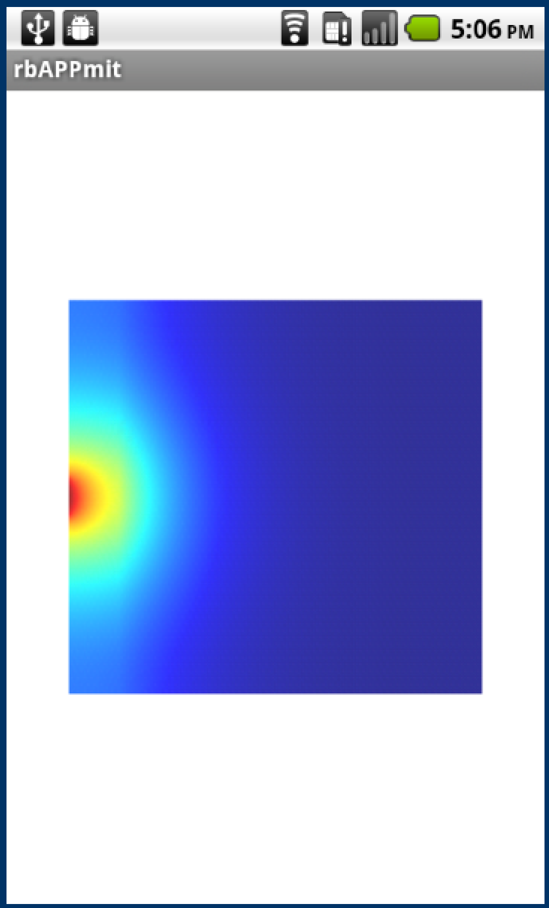
↑

† Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Galerkin Projection



Output

and

'State' (Field)†

†Primal-Dual techniques can also be considered.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

Algebraic System...

Express $T^j_{h,N}(\kappa) \in X_{h,N}$ as

$$T^j_{h,N}(x;\kappa) = \sum_{n=1}^{N} \left[c^j_{h,N}(\kappa)\right]_n \zeta_n(x), \; j \in \mathbb{J} \,,$$

where

$\zeta_n(x)$: basis functions $\Leftarrow$ POD(t)-Greedy(κ) ;

$[c^j_{h,N}(\kappa)]_n$: coefficients $\Leftarrow$ Galerkin Projection . . .

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Approximation

...Algebraic System

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $\boldsymbol{c}^j_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^N$ satisfies $\quad \boldsymbol{c}^0_{h,N}(\boldsymbol{\kappa}) = \mathbf{0}$

$$\left(\frac{\boldsymbol{M}_{h,N}}{\boldsymbol{\Delta t}} + \boldsymbol{A}_{h,N}\right)\boldsymbol{c}^j_{h,N} = \frac{\boldsymbol{M}_{h,N}}{\boldsymbol{\Delta t}}\,\boldsymbol{c}^{j-1}_{h,N} + \boldsymbol{F}_{h,N}\,, \quad j \in \mathbb{J}\,.$$

Output: $j \in \mathbb{J}$,

$$\overline{T}^j_{h,N}(\boldsymbol{\kappa}) = \sum_{n=1}^{N}\left[\boldsymbol{c}^j_{h,N}(\boldsymbol{\kappa})\right]_n \left(\frac{1}{|\boldsymbol{\Omega}_{\mathrm{me}}|}\int_{\boldsymbol{\Omega}_{\mathrm{me}}} \zeta_n\right).$$

Here $\boldsymbol{c}^j_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^N$, $\boldsymbol{F}_{h,N} \in \mathbb{R}^N$, and $\boldsymbol{M}_{h,N} \in \mathbb{R}^{N\times N}$, $\boldsymbol{A}_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^{N\times N}$ but *full*.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

We present

rigorous, sharp(ish), inexpensive†

a posteriori bounds crucial for

efficient Greedy$(\boldsymbol{\kappa})$ search $\Rightarrow \boldsymbol{X_{h,N}}$;

effective error control $\Rightarrow \boldsymbol{N}$;

uncertainty assessment $\Rightarrow$ design & operation.

---

†We discuss efficient calculation of the bounds subsequently.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

Residual

Introduce residual: $j \in \mathbb{J}$

$$R^j_{h,N}(v;\kappa) \equiv \int_{\Gamma_{\text{in}}} q''_{\text{in}}\, v - \int_{\Omega} \frac{T^j_{h,N} - T^{j-1}_{h,N}}{\Delta t}\, v$$

$$- \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \nabla T^j_{h,N} \cdot \nabla v, \ \forall\, v \in X_h\,,$$

and dual norm $\|v\|_X = \int_\Omega |\nabla v|^2$

$$\delta^j_{h,N}(\kappa) \equiv \sup_{v \in X_h} \frac{R^j_{h,N}(v;\kappa)}{\|v\|_X}\,.$$

Introduce error bound $j \in \mathbb{J}$

$$\Delta^j_{h,N}(\kappa) \equiv \left(C_\Delta(\kappa)\, \Delta t \sum_{j'=1}^{j} \left(\delta^j_{h,N}(\kappa)\right)^2 \right)^{1/2},$$

where

$$C_\Delta(\kappa) = \left(\min(\kappa_1, \kappa_2, 1)\, |\Omega_{\mathrm{me}}| \right)^{-1/2}$$

reflects (i) stability, and (ii) the particular output.†

†The Ω_{me} effect can be mitigated.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Error Bound

Proposition 1.0H. Given $\boldsymbol{\kappa} \in \mathcal{D}$,

$$| \overline{T}_h^j(\boldsymbol{\kappa}) - \overline{T}_{h,N}^j(\boldsymbol{\kappa}) | \leq \Delta_{h,N}^j(\boldsymbol{\kappa}), \;\; j \in \mathbb{J} \; ,$$

FE (Truth) — RB

for any $N \in \{1, \ldots, N_{\max}\}$.[†]

Rigorous error bounds for the output;

in practice, bounds also quite *sharp*.

[†]We can also obtain error bounds for the field variable in the $|||\cdot|||$ norm.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

Output Bounds...

Introduce output bounds $j \in \mathbb{J}$

$$\overline{T}^{-\,j}_{h,N}(\boldsymbol{\kappa}) \equiv \overline{T}^{\,j}_{h,N}(\boldsymbol{\kappa}) - \boldsymbol{\Delta}^{j}_{h,N}(\boldsymbol{\kappa}) ,$$

and

$$\overline{T}^{+\,j}_{h,N}(\boldsymbol{\kappa}) \equiv \overline{T}^{\,j}_{h,N}(\boldsymbol{\kappa}) + \boldsymbol{\Delta}^{j}_{h,N}(\boldsymbol{\kappa}) .$$

Bound gap (uncertainty):

$$\overline{T}^{+\,j}_{h,N}(\boldsymbol{\kappa}) - \overline{T}^{-\,j}_{h,N}(\boldsymbol{\kappa}) = 2\boldsymbol{\Delta}^{j}_{h,N}(\boldsymbol{\kappa}),\ \ j \in \mathbb{J}.$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Bounds...

Corollary 1.1H. Given $\kappa \in \mathcal{D}$,

$$\underbrace{\overline{T}^{-\,j}_{h,N}(\kappa)}_{\text{RB}} \;\le\; \underbrace{\overline{T}^{j}_{h}(\kappa)}_{\text{FE (Truth)}} \;\le\; \underbrace{\overline{T}^{+\,j}_{h,N}(\kappa)}_{\text{RB}}\ ,\quad j \in \mathbb{J}\ ,$$

for any $N \in \{1, \ldots, N_{\max}\}$.

Rigorous lower and upper bounds
for the *FE (Truth)* output.†

† Note: output bounds calculated *without reference to* $T_h^j(\kappa)$, $1 \le j \le J$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

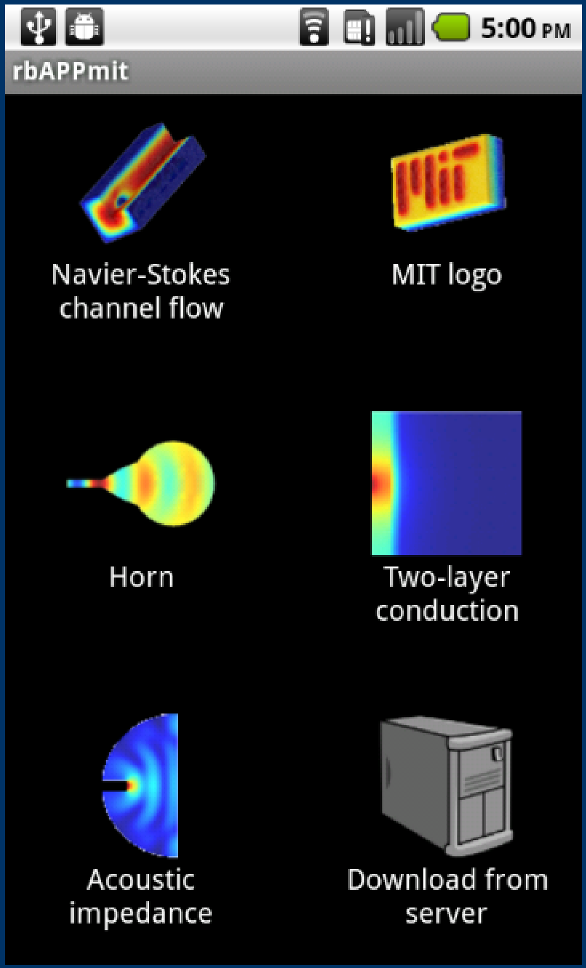
a posteriori Bounds

...Output Bounds...

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

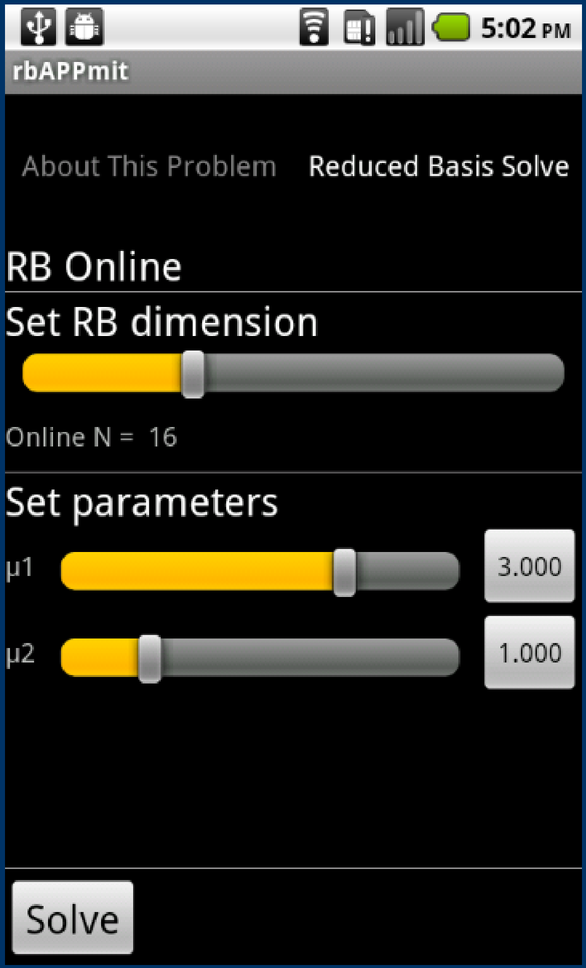
...Output Bounds...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

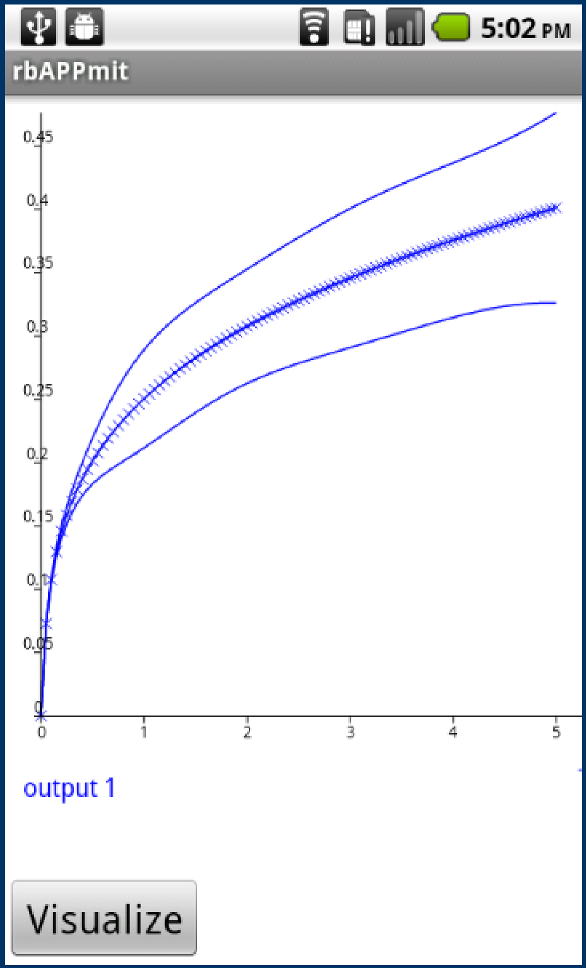
...Output Bounds...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Output Bounds



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

Convergence...

Given $\varepsilon > 0$, define

$$N_\varepsilon \equiv \max_{\kappa \in \mathcal{D}} \left(\min_{2\Delta^J_{h,N}(\kappa) \le \varepsilon} N \right).$$

Observation 2.0H. As $h \to 0$ ($\mathcal{N}_h \to \infty$)

(i) N_ε is independent of $\mathcal{N}_h$;

(ii) $N_\varepsilon \sim -\mathrm{Const}\,\ln(\varepsilon)$ as $\varepsilon \to 0$.

(Proof is possible in some simpler cases.)

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

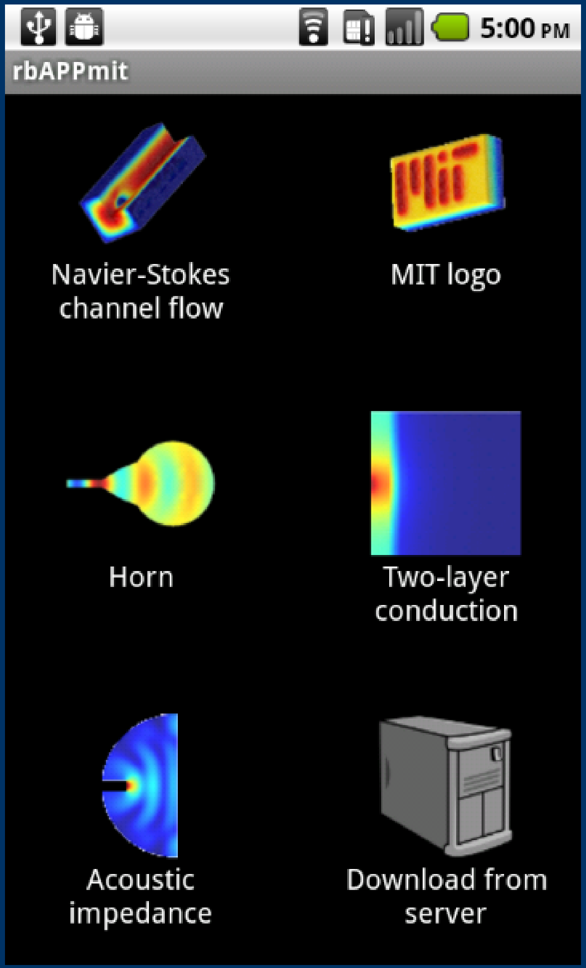
a posteriori Bounds

...Convergence...

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

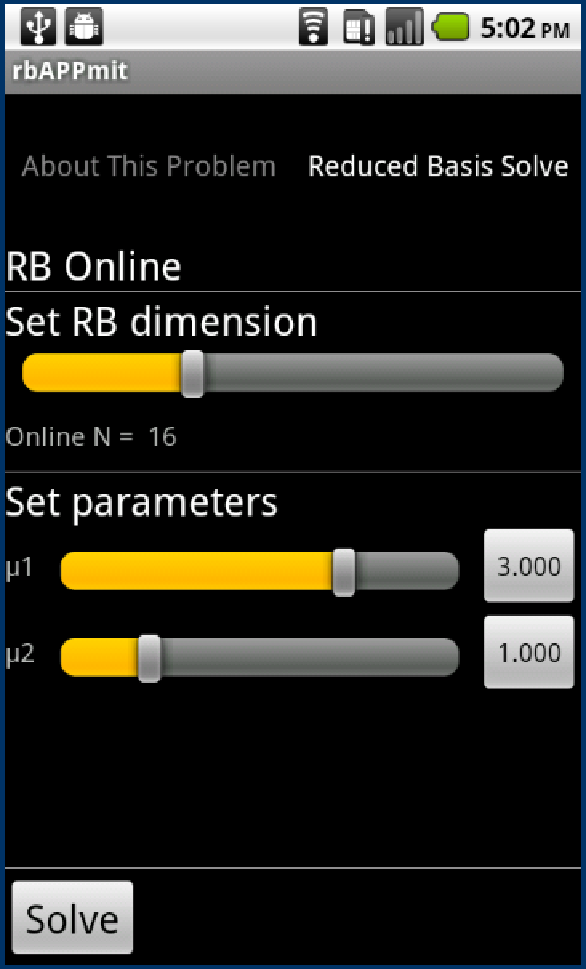
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

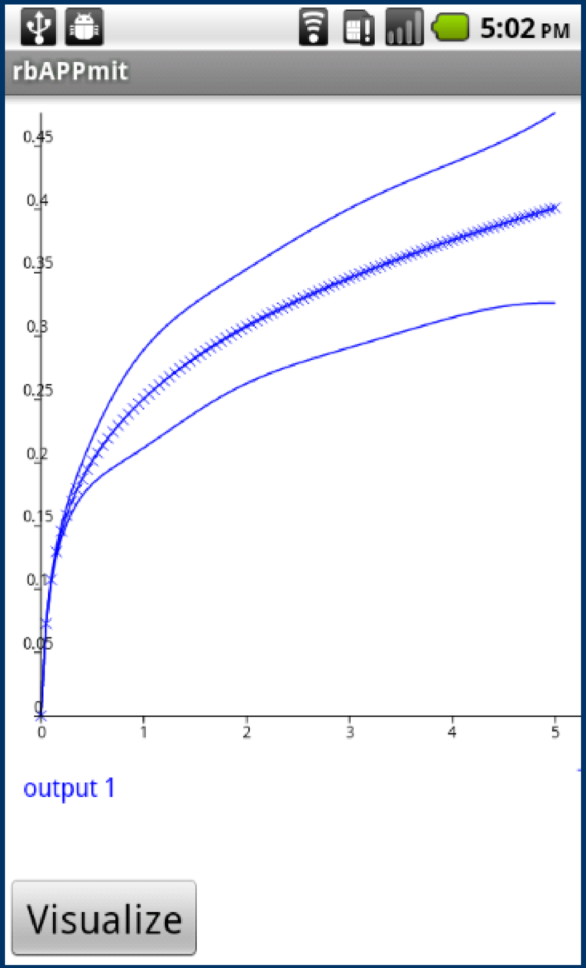
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

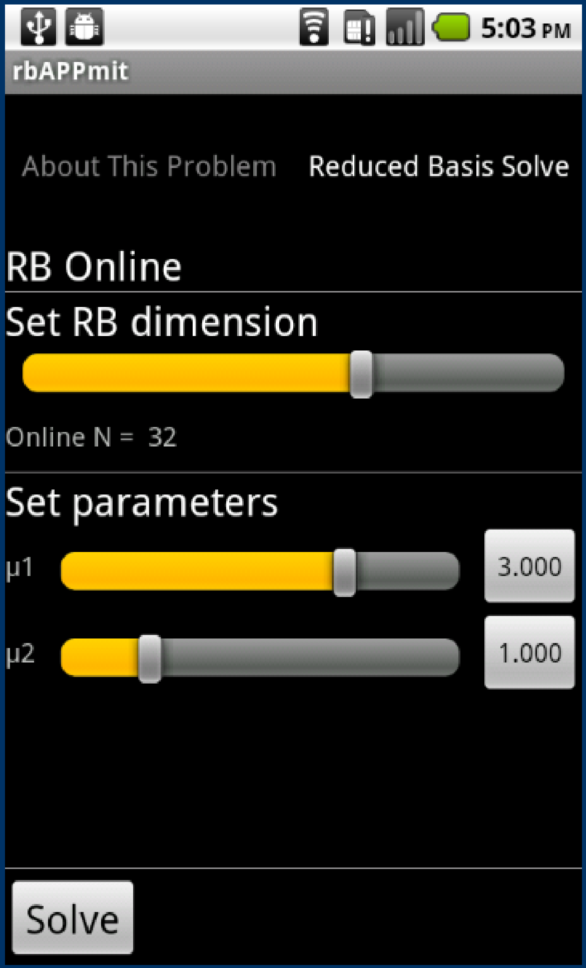
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

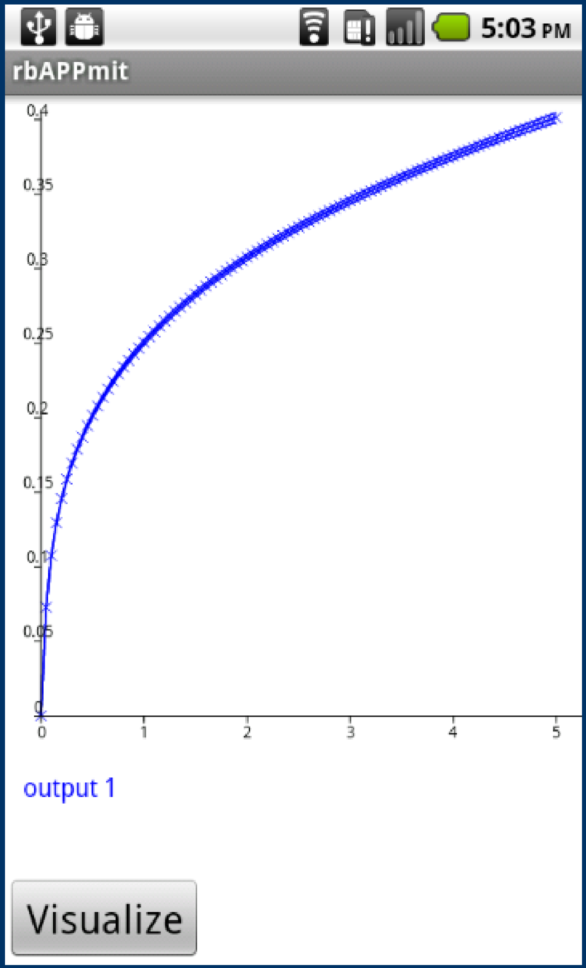
...Convergence...



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

a posteriori Bounds

...Convergence



Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

Offline-Online...

Key requirement:

weak form *affine* in *(functions of) the parameter*.

Key ingredients:

linear approximation space $\boldsymbol{X}_{h,N}$ ($\Rightarrow \boldsymbol{T}^{j}_{h,N}$);

Riesz representation of $\boldsymbol{R}^{j}_{h,N}$ ($\Rightarrow \boldsymbol{\delta}^{j}_{h,N}$, $\boldsymbol{\Delta}^{j}_{h,N}$, $\boldsymbol{T}^{\pm\, j}_{h,N}$).

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online...

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $T^j(\boldsymbol{\kappa}) \in X$ satisfies $T^0(\boldsymbol{\kappa}) = 0$

$$1 \int_\Omega \frac{T^j - T^{j-1}}{\Delta t} v + \sum_{\ell=0}^{2} \kappa_\ell \int_{\Omega_\ell} \nabla T \cdot \nabla v$$

$$= 1 \int_{\Gamma_{\text{in}}} q''_{\text{in}} v, \ \forall\, v \in X, \ j \in \mathbb{J}.$$

Output: $\overline{T}^j(\boldsymbol{\kappa}) = \frac{1}{|\Omega_{\text{me}}|} \int_{\Omega_{\text{me}}} T^j(\boldsymbol{\kappa}), \ j \in \mathbb{J}.$

Affine: $\sum_{q=1}^{Q}$ function$_q$ $(\boldsymbol{\kappa})$ $\times$ (bi)linear form$_q$ (*no* $\boldsymbol{\kappa}$).

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online...

Offline Stage:

$$\mathcal{M}_h \xrightarrow[O(\mathcal{N}_h)\text{ FLOPs}]{} \mathcal{S}_{\text{Online}}[\mathcal{M}_h]\ ;$$

$$\mathcal{S}_{\text{Online}}[\mathcal{M}_h]\text{: } O(N_{\max}^2)\text{ FPNs}\ .$$

Online Stage $(\mathcal{S}_{\text{Online}}[\mathcal{M}_h])$: LTI

$$\kappa, N \xrightarrow[O(N^3+JN^2)\text{ FLOPs}]{} T_{h,N}^{\pm j}(\kappa),\ j \in \mathbb{J}\ .$$

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Computational Strategy

...Offline-Online

Proposition 3.0H. Given

$$\mathcal{S}_{\mathrm{Online}}\left[\mathcal{M}_h\right] \text{ of size } O(N_{\max}^2) \ ,$$

then

$$\kappa, N \longrightarrow T_{h,N}^{\pm j}(\kappa), \ \ j \in \mathbb{J} \ ,$$

may be calculated in $O(N^3 + JN^2)$ FLOPS.

Online operation count *independent* of $\mathcal{N}_h$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

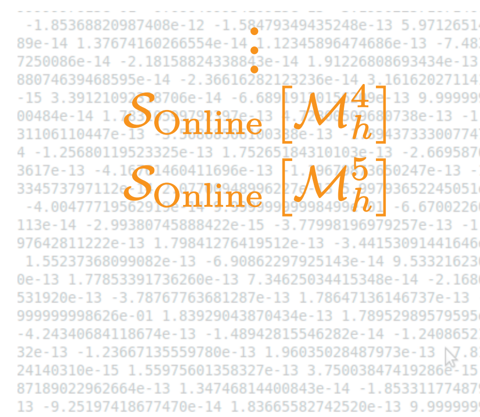
Hierarchical Architecture

"In-the-Lab"

$\vdots$

$\mathcal{M}_h^5$ →

Offline:
Supercomputer†



Library:
www

†Exploit parallelism over Ω and over $\mathcal{D}$.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Hierarchical Architecture

"In-the-Field"...

Library:
www

Online:
Smartphone†

†More generally: any small, lightweight, inexpensive portable or embedded platform.

Parametrized Model $\mathcal{M}_{h,N}$ (RB)

Hierarchical Architecture

...“In-the-Field”

Corollary 1.1H

Smartphone prediction suffices
without appeal to expensive Truth.

In Situ

A Tempo

Observation 2.0H

Smartphone memory suffices
to accommodate $\mathcal{S}_{\text{Online}}[\mathcal{M}_h]$.

Proposition 3.0H

Smartphone processor suffices
to calculate $T^{\pm\,j}_{h,N}(\kappa)$, $j \in \mathbb{J}$.

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\kappa_h^* \,(\mathcal{M}_h \text{ (FE)}) \quad \text{by} \quad \kappa_{h,N}^* \,(\mathcal{M}_{h,N} \text{ (RB)}),$$

$$\Lambda_h \,(\mathcal{M}_h \text{ (FE)}) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \,(\mathcal{M}_{h,N} \text{ (RB)}).$$

Inverse Problem$_h$

Diffusivity Estimate$_h$

Least Squares

Given

$$t^m_{\rm me}, \;\; \overline{T}_{\rm exp}(t^m_{\rm me}), \;\; 1 \le m \le M_{\rm me} \; ,$$

find (any) (no regularization)

$$\kappa^*_h = \arg\min_{\kappa \in \mathcal{D}} \mathcal{E}_h(\kappa) \quad ,$$

$$\mathcal{E}_h(\kappa) \equiv \sum_{m=1}^{M_{\rm me}} \left(\overline{T}_{\rm exp}(t^m_{\rm me}) - \overline{T}_h(t^m_{\rm me}; \kappa) \right)^2 . ^\dagger$$

---

†Note $\overline{T}_h(t^m_{\rm me}; \kappa) = \overline{T}^j_h(\kappa)$ for j: $t^j = t^m_{\rm me}$.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

Approximation

Given

$$t^m_{\rm me},\ \ \overline{T}_{\rm exp}(t^m_{\rm me}),\ \ 1 \le m \le M_{\rm me}\ ,$$

find (any) (no regularization)

$$\kappa^*_{h,N} = \arg\min_{\kappa\in\mathcal{D}} \mathcal{E}_{h,N}(\kappa)\ \ ,$$

$$\mathcal{E}_{h,N}(\kappa) \equiv \sum_{m=1}^{M_{\rm me}} \left(\overline{T}_{\rm exp}(t^m_{\rm me}) - \overline{T}_{h,N}(t^m_{\rm me};\kappa)\right)^2 .^\dagger$$

†Note $\overline{T}_{h,N}(t^m_{\rm me};\kappa) = \overline{T}^j_{h,N}(\kappa)$ for j: $t^j = t^m_{\rm me}$; similarly for $\overline{T}^\pm_{h,N}(t^m_{\rm me};\kappa)$.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

Parametric Derivatives...

Field Sensitivity: $1 \le p \le P\ (= 2)$

$$\partial_p\, T^j_{h,N}(\boldsymbol{x};\boldsymbol{\kappa}) \equiv \frac{\partial T^j_{h,N}}{\partial \kappa_p}(\boldsymbol{x};\boldsymbol{\kappa}),\ \ j \in \mathbb{J}\,.$$

Output Sensitivity: DIRECT APPROACH

$$\partial_p\, \overline{T}^j_{h,N}(\boldsymbol{\kappa}) = \frac{1}{|\Omega_{\mathrm{me}}|}\int_{\Omega_{\mathrm{me}}} \partial_p\, T^j_{h,N}(\boldsymbol{x};\boldsymbol{\kappa}),\ \ j \in \mathbb{J}\,.$$

Jacobian $\mathcal{J}_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^{M_{\mathrm{me}}\times 2}$:

$$\left[\mathcal{J}_{h,N}(\boldsymbol{\kappa})\right]_{m\,p} = \partial_p\, \overline{T}^j_{h,N}(\boldsymbol{\kappa}) \ \text{ for } \ j:\ t^j = t^m_{\mathrm{me}}\,.$$

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Parametric Derivatives...

Given $\boldsymbol{\kappa} \in \mathcal{D}$, $\partial_p\, T^j_{h,N}(\boldsymbol{\kappa}) \in X_{h,N}$ satisfies

$$\int_\Omega \frac{\partial_p\, T^j_{h,N} - \partial_p\, T^{j-1}_{h,N}}{\Delta t}\, v + \sum_{\ell=0}^{2} \int_{\Omega_\ell} \kappa_\ell \nabla \partial_p\, T^j_{h,N} \cdot \nabla v$$

$$= - \int_{\Omega_p} \nabla T^j_{h,N} \cdot \nabla v, \; \forall\, v \in X_{h,N},\;\; j \in \mathbb{J}\,,$$

subject to initial condition $\partial_p\, T^0_{h,N} = 0$.

Note $\partial_p\, T^j_{h,N} \equiv \dfrac{\partial T^j_{h,N}}{\partial \kappa_p} \in X_{h,N} \approx \dfrac{\partial T^j_h}{\partial \kappa_p} \in X_h$.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Parametric Derivatives

Corollary 3.1H. Given $(\boldsymbol{P = 2})$

$$\mathcal{S}_{\text{Online}}[\mathcal{M}_h] \text{ of size } O(N^2_{\max}),$$

then DIRECT APPROACH

$$\boldsymbol{\kappa}, N \to \mathcal{J}_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^{M_{\text{me}} \times 2}$$

may be calculated in $O(N^3 + (P+1)JN^2)$ FLOPs.

Note for large P ADJOINT APPROACH is preferred.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

Levenberg-Marquardt...

Given $\mathcal{J}_{h,N}(\boldsymbol{\kappa}) \in \mathbb{R}^{M_{\mathrm{me}} \times 2}$: $\qquad O(P^2 M_{\mathrm{me}})$

$$\underset{P \times P}{G}(\boldsymbol{\kappa}) \equiv \mathcal{J}^{\mathrm{T}}_{h,N}(\boldsymbol{\kappa})\, \mathcal{J}_{h,N}(\boldsymbol{\kappa}) + \lambda_{\mathrm{L}M}\, \mathrm{diag}\big(\mathcal{J}^{\mathrm{T}}_{h,N}(\boldsymbol{\kappa})\, \mathcal{J}_{h,N}(\boldsymbol{\kappa})\big)\,,$$

and

$$\underset{P \times 1}{b}(\boldsymbol{\kappa}) \equiv \mathcal{J}^{\mathrm{T}}_{h,N}(\boldsymbol{\kappa}) \begin{pmatrix} \overline{T}_{\exp}(t^1_{\mathrm{me}}) - \overline{T}_{h,N}(t^1_{\mathrm{me}}; \boldsymbol{\kappa}) \\ \vdots \\ \overline{T}_{\exp}(t^{M_{\mathrm{me}}}_{\mathrm{me}}) - \overline{T}_{h,N}(t^{M_{\mathrm{me}}}_{\mathrm{me}}; \boldsymbol{\kappa}) \end{pmatrix}.$$

Inverse Problem$_{h,N}$

Diffusity Estimate$_{h,N}$

...Levenberg-Marquardt...

Algorithm Levenberg-Marquardt[†]:

set $\kappa^*_{h,N} = \kappa_{\text{guess}} \in \mathcal{D}$

while $|\nabla \mathcal{E}_{h,N}(\kappa^*_{h,N})| > \text{tol}$

  $G(\kappa^*_{h,N})\,\delta\kappa = b(\kappa^*_{h,N})$; % $N^3 + (P+1)JN^2$

  $\kappa^*_{h,N} \leftarrow \kappa^*_{h,N} + \delta\kappa$;

end while % unconstrained

[†]Apache Math Commons (Java) implementation.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt...

$$\epsilon_{\rm exp} = 0.01$$
$$M_{\rm me} = 20$$

$$\kappa^{**} = (3,1)^{\dagger}$$

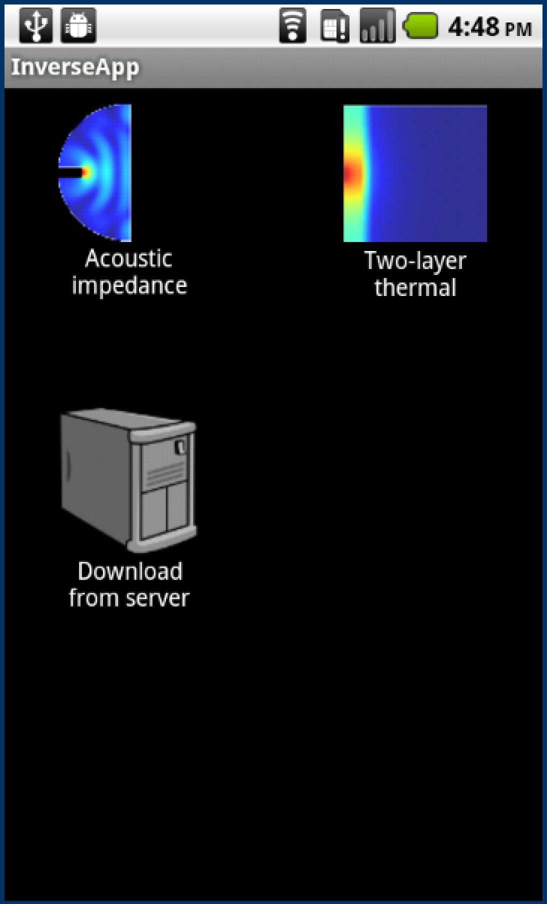
$$N = 50$$
$$\kappa_{\rm guess} = (2,2)$$

†Here $\overline{T}_{\rm exp}(t^m_{\rm me}) = \overline{T}_{h,N_{\rm max}}(t^m_{\rm me};\kappa^{**}) + \epsilon_{\rm exp}\mathcal{N}(0,1)$.

Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt...



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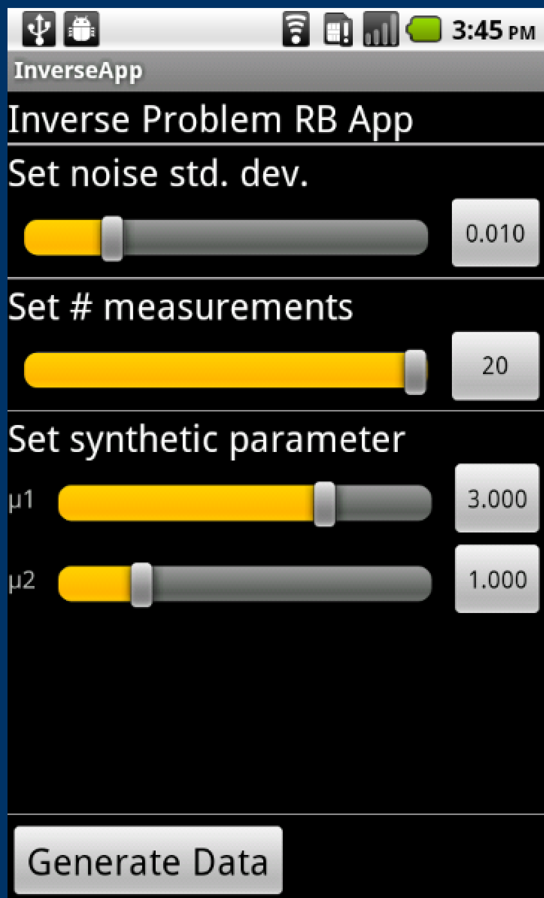
Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt...



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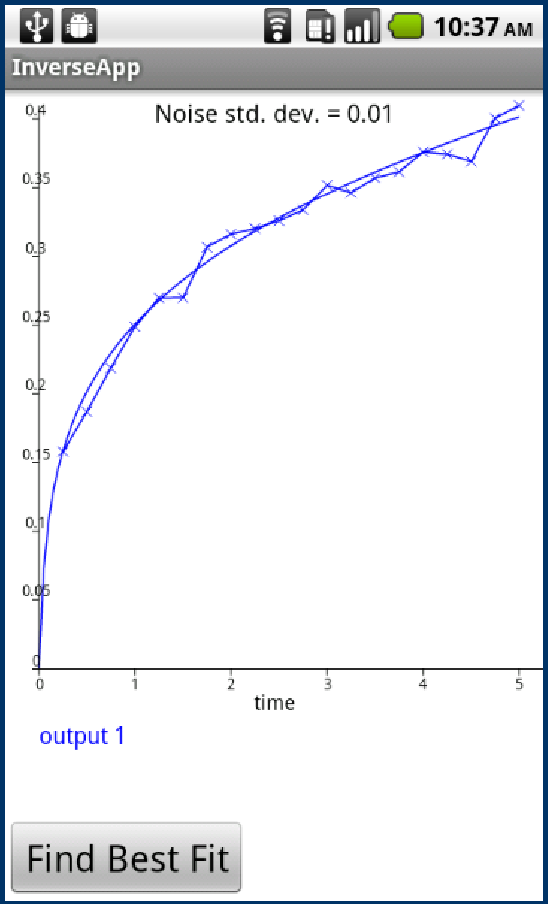
Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt...



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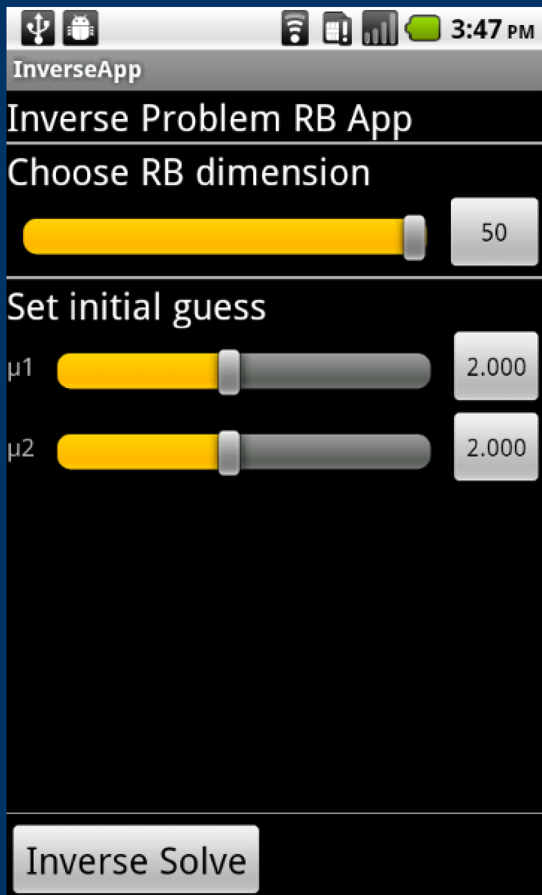
Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt...



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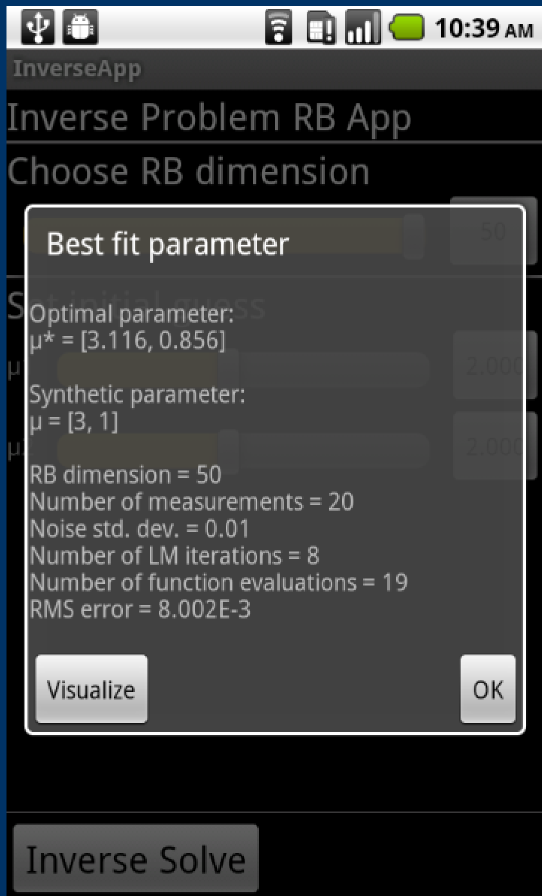
Inverse Problem$_{h,N}$

Diffusivity Estimate$_{h,N}$

...Levenberg-Marquardt



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$$N = 50$$
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†Here $\overline{T}_{\text{exp}}(t^m_{\text{me}}) = \overline{T}_{h,N_{\max}}(t^m_{\text{me}};\kappa^{**}) + \epsilon_{\text{exp}}\mathcal{N}(0,1)$.

Strategy

Replace

$$\mathcal{M}_h \text{ (FE)} \quad \text{by} \quad \mathcal{M}_{h,N} \text{ (RB)}$$

and then

$$\kappa_h^* \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \kappa_{h,N}^* \left(\mathcal{M}_{h,N} \text{ (RB)}\right),$$

$$\Lambda_h \left(\mathcal{M}_h \text{ (FE)}\right) \quad \text{by} \quad \Lambda_{h,N}^{\mathrm{U}} \left(\mathcal{M}_{h,N} \text{ (RB)}\right).$$

Inverse Problem$_h$

Uncertainty Analysis$_h$

Likelihood Ratio: $\Lambda_h(\kappa)$

Given *realization*

$$\overline{T}_{\exp}(t^m_{\mathrm{me}}) = \overline{T}_h(t^m_{\mathrm{me}}; \kappa^{**}) + \epsilon_{\exp}\,\mathcal{N}(0,1)$$

hypothesis

define (pre-Bayesian) $\forall\, \kappa \in \mathcal{D}$

$$\mathcal{L}_h(\kappa) \equiv e^{\left\{-\mathcal{E}_h(\kappa)/2\epsilon^2_{\exp}\right\}}\ ,$$

$$\Lambda_h(\kappa) \equiv \frac{\mathcal{L}_h(\kappa)}{\mathcal{L}_h(\kappa^*_h)}\ .$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Strategy

Given *realization*

$$\overline{T}_{\text{exp}}(t^m_{\text{me}}) = \overline{T}_h(t^m_{\text{me}};\boldsymbol{\kappa}^{**}) + \epsilon_{\text{exp}}\,\mathcal{N}(0,1)$$

hypothesis

form

$$\Lambda^{\text{U}}_{h,N}(\boldsymbol{\kappa})\ \left[\overline{T}^{\pm\,j}_{h,N}\right]_{j\in\mathbb{J}}$$

such that $\forall\ \boldsymbol{\kappa} \in \mathcal{D}$

$$\Lambda_h(\boldsymbol{\kappa}) \le \Lambda^{\text{U}}_{h,N}(\boldsymbol{\kappa})\ .$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Likelihood Bounds...

Define $\mathcal{L}^{\mathrm{L}}_{h,N}(\kappa) \equiv e^{\{-\mathcal{E}^{\mathrm{U}}_{h,N}(\kappa)/2\epsilon^2_{\exp}\}}$,

where

$$\mathcal{E}^{\mathrm{U}}_{h,N}(\kappa) \equiv \sum_{m=1}^{M_{\mathrm{me}}} \left(\overline{T}_{\exp}(t^m_{\mathrm{me}}) - \overline{T}^{\mathrm{U}}_{h,N}(t^m_{\mathrm{me}};\kappa)\right)^2;$$

$$\overline{T}^{\mathrm{U}}_{h,N}(t^m_{\mathrm{me}};\kappa) = \arg \max_{z \in [\overline{T}^{-}_{h,N}(t^m_{\mathrm{me}};\kappa),\, \overline{T}^{+}_{h,N}(t^m_{\mathrm{me}};\kappa)]^{\dagger}} |\overline{T}_{\exp}(t^m_{\mathrm{me}}) - z|.$$

---

†Minimum obtained for $z = \overline{T}^{-}_{h,N}(t^m_{\mathrm{me}};\kappa)$ or $z = \overline{T}^{+}_{h,N}(t^m_{\mathrm{me}};\kappa)$.

Define $$\mathcal{L}^{\mathrm{U}}_{h,N}(\kappa) \equiv e^{\{-\mathcal{E}^{\mathrm{L}}_{h,N}(\kappa)/2\epsilon^2_{\exp}\}},$$

where

$$\mathcal{E}^{\mathrm{L}}_{h,N}(\kappa) \equiv \sum_{m=1}^{M_{\mathrm{me}}} \left(\overline{T}_{\exp}(t^m_{\mathrm{me}}) - \overline{T}^{\mathrm{L}}_{h,N}(t^m_{\mathrm{me}};\kappa)\right)^2;$$

$$\overline{T}^{\mathrm{L}}_{h,N}(t^m_{\mathrm{me}};\kappa) = \arg \min_{z\in[\overline{T}^-_{h,N}(t^m_{\mathrm{me}};\kappa),\overline{T}^+_{h,N}(t^m_{\mathrm{me}};\kappa)]} |\overline{T}_{\exp}(t^m_{\mathrm{me}}) - z|.^\dagger$$

† Now minimum obtained for $z = \overline{T}^-_{h,N}(t^m_{\mathrm{me}};\kappa)$, $\overline{T}^+_{h,N}(t^m_{\mathrm{me}};\kappa)$, or $\overline{T}_{\exp}(t^m_{\mathrm{me}})$.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Bounds

Proposition 4.0H: Given $\{\overline{T}_{\rm exp}(t^m_{\rm me})\}_{1\le m\le M_{\rm me}}$,

$$\mathcal{L}^{\rm L}_{h,N}(\kappa) \le \mathcal{L}_h(\kappa) \le \mathcal{L}^{\rm U}_{h,N}(\kappa), \quad \forall\, \kappa \in \mathcal{D}\ ,$$

for any $N \in \{1,\ldots,N_{\max}\}$.

Likelihood bounds include effects of

approximation error ($\Delta^j_{h,N}(\kappa)$), and

experimental error ($\epsilon_{\rm exp}\,\mathcal{N}(0,1)$).

Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)$...

Define

$$\Lambda^{\mathrm{U}}_{h,N}(\kappa) \equiv \frac{\mathcal{L}^{\mathrm{U}}_{h,N}(\kappa)}{\mathcal{L}^{\mathrm{L}}_{h,N}(\kappa^*_{h,N})} ,$$

for all $\kappa \in \mathcal{D}$.

Similar construction possible for $\Lambda^{\mathrm{L}}_{h,N}(\kappa)$.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\boldsymbol{\Lambda}^{\mathrm{U}}_{h,N}(\boldsymbol{\kappa})$...

Corollary 4.1H: Given $\{\overline{T}_{\exp}(t^m_{\mathrm{me}})\}_{1\le m\le M_{\mathrm{me}}}$,

$$\boldsymbol{\Lambda}_h(\boldsymbol{\kappa}) \le \boldsymbol{\Lambda}^{\mathrm{U}}_{h,N}(\boldsymbol{\kappa}), \quad \forall\, \boldsymbol{\kappa} \in \boldsymbol{\mathcal{D}} \ ,$$

for any $N \in \{1, \ldots, N_{\max}\}$.

Rigorous constructions for parametric uncertainty.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)$

Corollary 3.2H: Given

$$\mathcal{S}_{\mathrm{Online}}\,[\mathcal{M}_h] \text{ of size } O(N^2_{\max})\ ,$$

then given $\kappa^*_{h,N}$

$$\kappa, N \to \Lambda^{\mathrm{U}}_{h,N}(\kappa)$$

may be calculated in

$$O(N^3 + JN^2) \text{ FLOPs } + O(M_{\mathrm{me}}) \text{ exp's.}$$

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^{\dagger}$...

$$\begin{aligned} \epsilon_{\mathrm{exp}} &= 0.01 \\ M_{\mathrm{me}} &= 20 \\ \\ \kappa^{**} &= (3,1) \\ \\ N &= 50 \\ \kappa_{\mathrm{guess}} &= (2,2) \end{aligned}$$

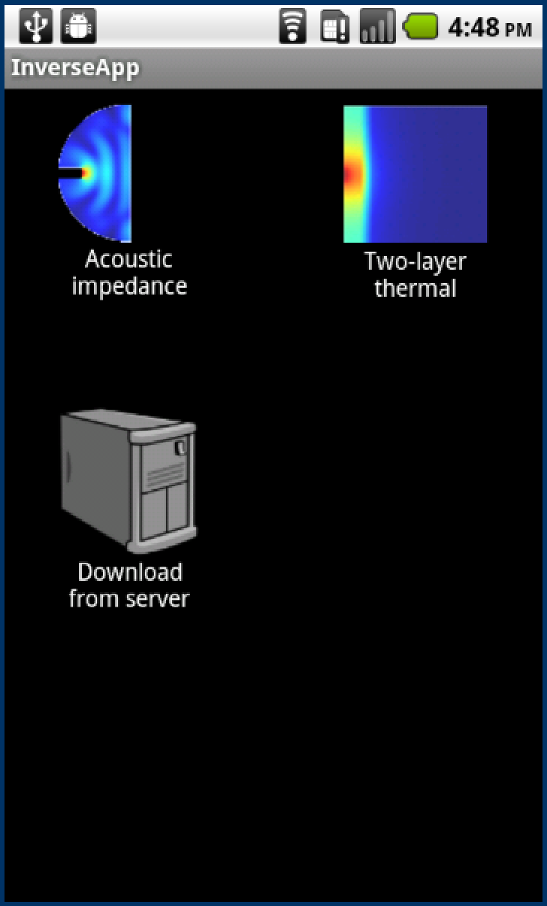
---

† Here $\min(\Lambda^{\mathrm{U}}_{h,N}, 1)$ is plotted near $\kappa^*_{h,N}$ based on 64^2 evaluations.

Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^\dagger$...



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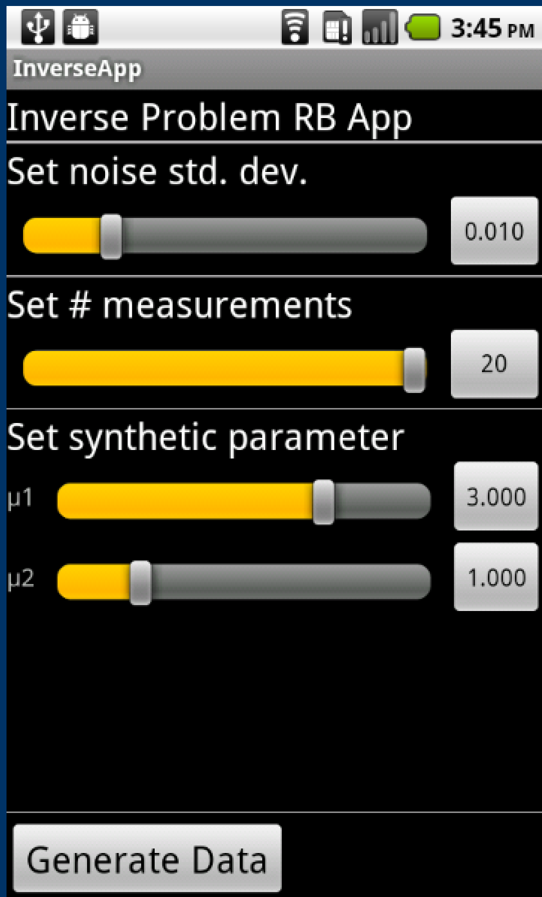
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^{\dagger}$...



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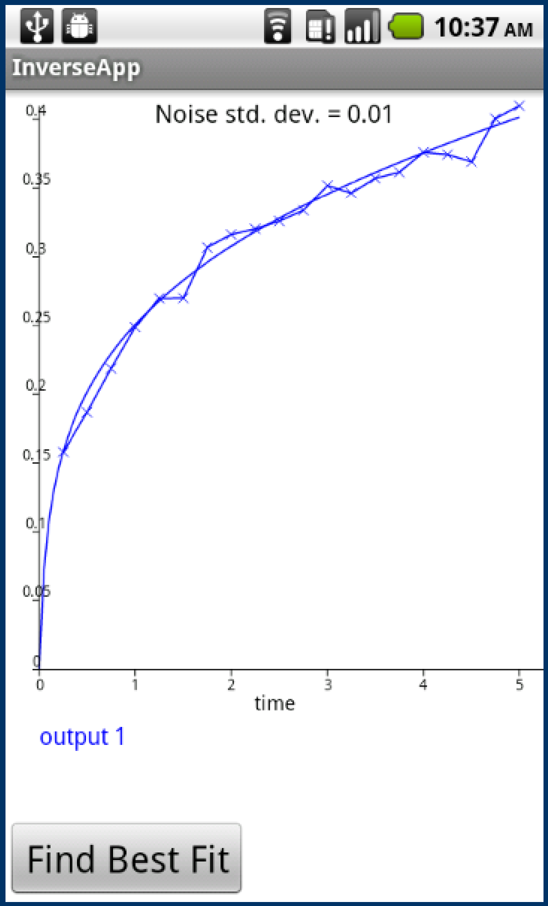
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^{\dagger}$...



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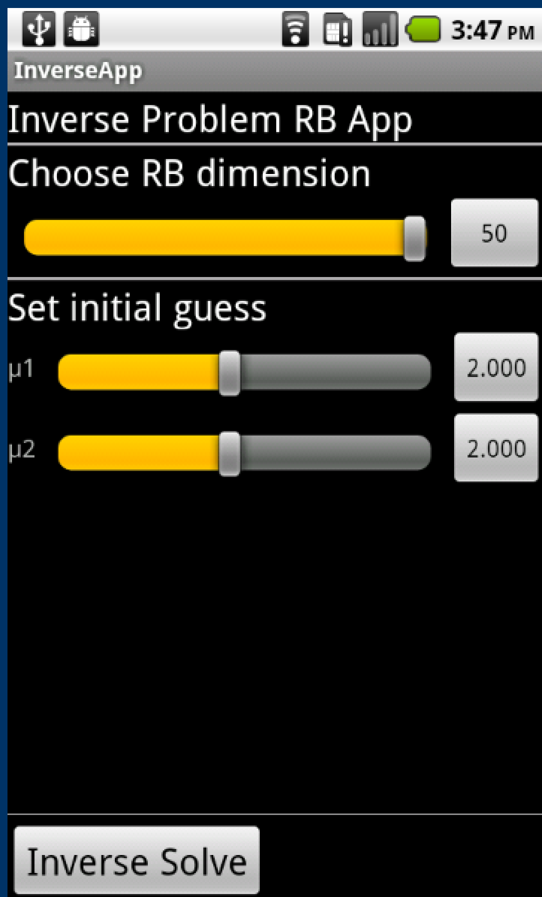
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^{\dagger}$...



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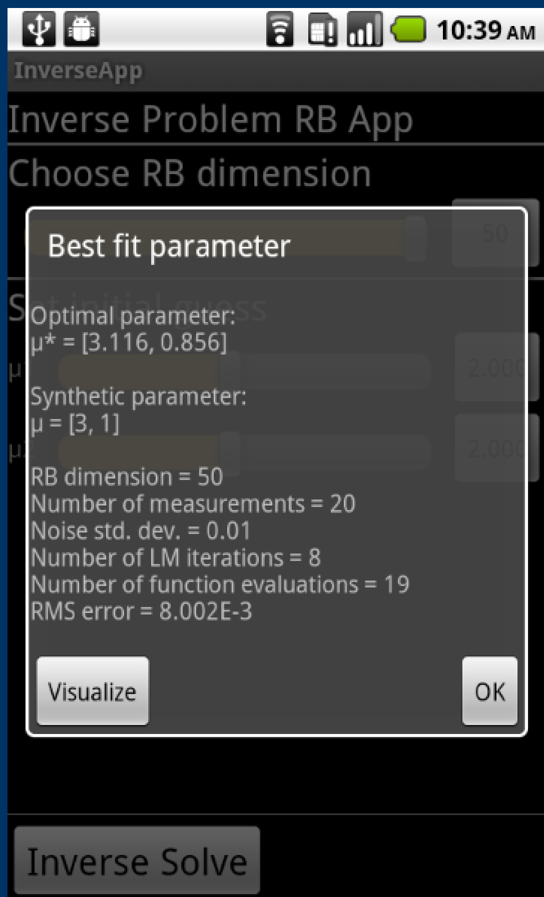
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^{\dagger}$...



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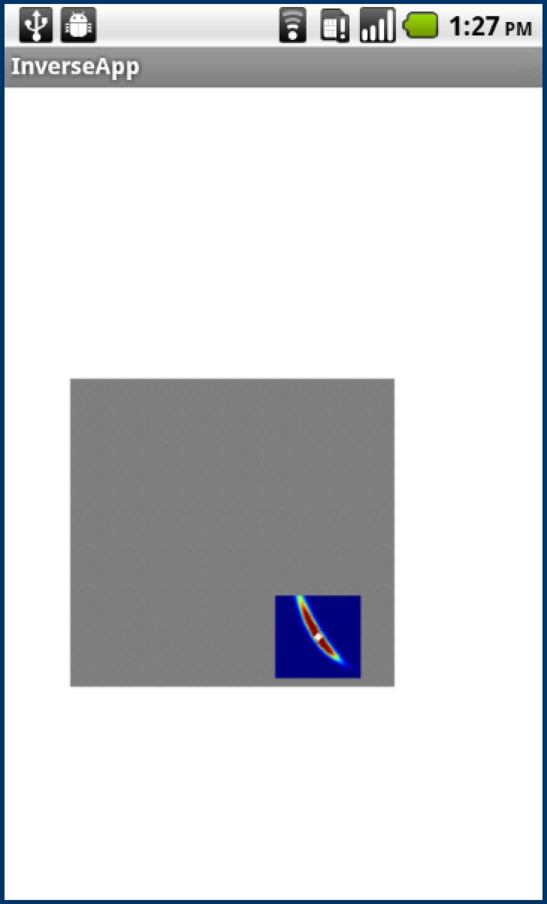
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^\dagger$...



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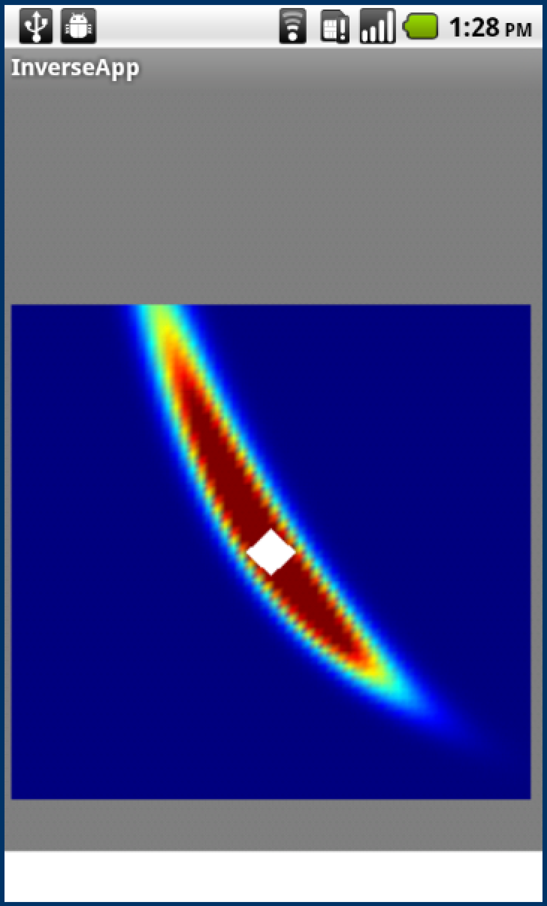
Inverse Problem$_{h,N}$

Uncertainty Analysis$_{h,N}$

...Likelihood Ratio: $\Lambda^{\mathrm{U}}_{h,N}(\kappa)^\dagger$



$$
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\kappa^{**} &= (3, 1) \\
N &= 50 \\
\kappa_{\mathrm{guess}} &= (2, 2)
\end{aligned}
$$

†Here $\min(\Lambda^{\mathrm{U}}_{h,N}, 1)$ is plotted near $\kappa^*_{h,N}$ based on 64^2 evaluations.

Inverse Problem$_{h,N}$

Hierarchical Architecture

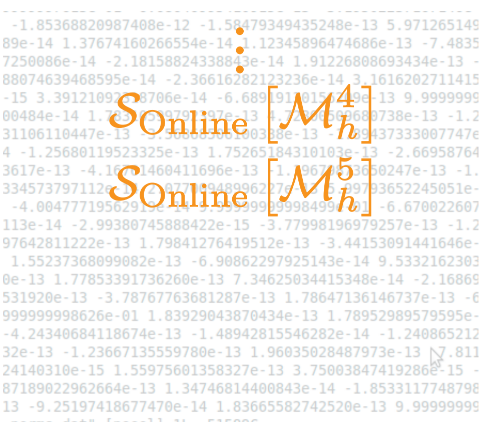
"In-the-Lab"

$\vdots$

$\mathcal{M}_h^5 \longrightarrow$

Offline:
Supercomputer†

$- - - \rightarrow$



Library:
www

†Exploit parallelism over Ω and over $\mathcal{D}$.

Inverse Problem$_{h,N}$

Hierarchical Architecture

"In-the-Field"

$\overline{T}_{\text{exp}}(t^m_{\text{me}}),\ 1 \le m \le M_{\text{me}};\ \ \epsilon_{\text{exp}} \quad N$

$\kappa^*_{h,N};\quad \Lambda^{\text{U}}_{h,N},\ \kappa \in \mathcal{D}$

Library:
www

Online:
Smartphone [†]

[†]More generally: any small, lightweight, inexpensive portable or embedded platform.

Outline

The Big Picture

An Acoustics Example

A Heat Transfer Example

The Big Questions

Many Parameters?

Can we treat problems with many parameters? †

Yes, but . . .

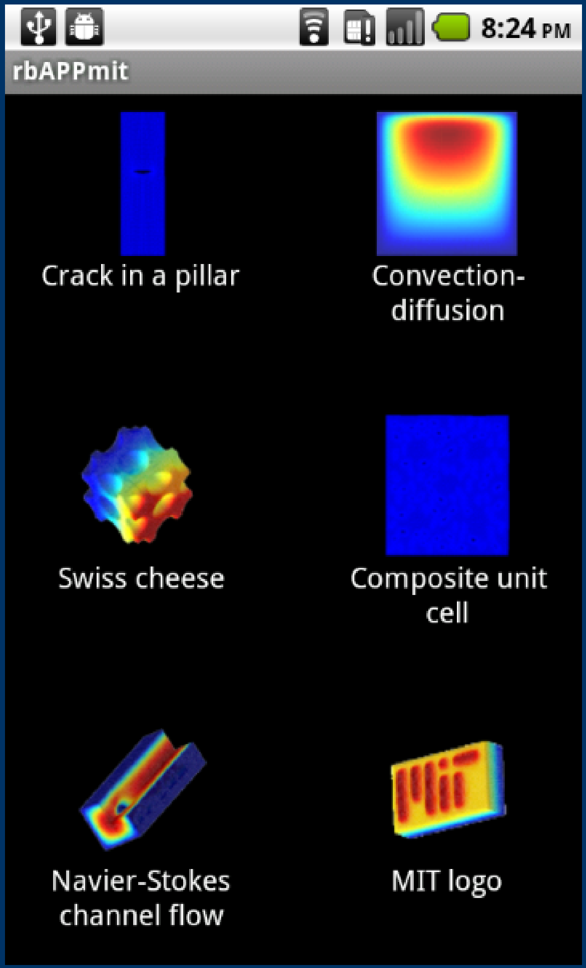
New enablers:

Offline parallel implementation over $\boldsymbol{\Omega}$ and $\mathcal{D}$;

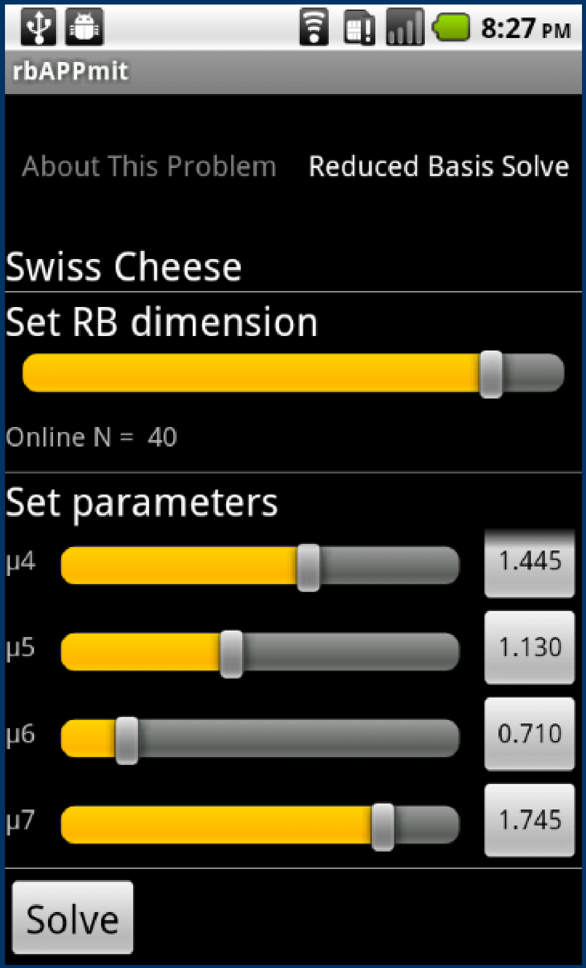
primal-dual approximations.

† . . . and three spatial dimensions — *big* problems?

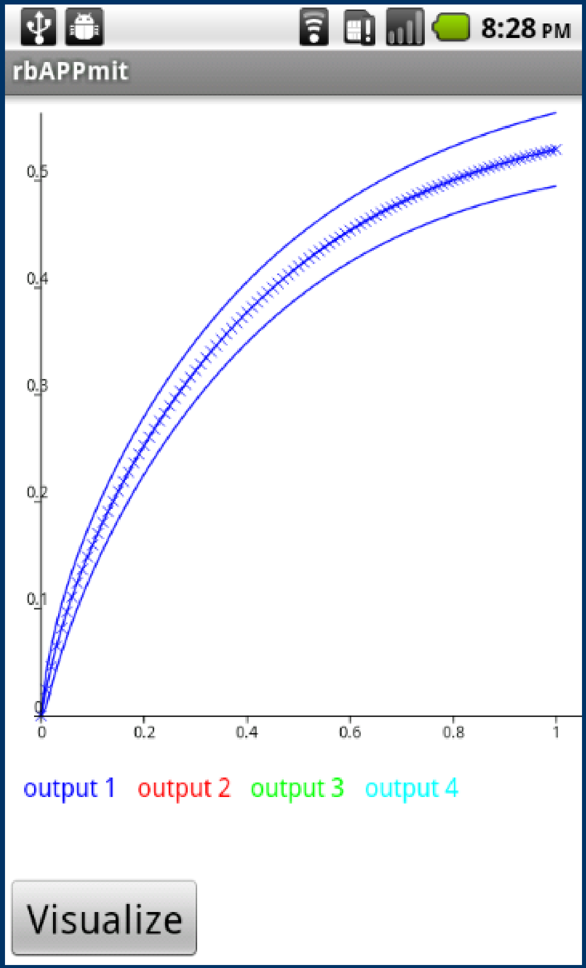
Many Parameters?



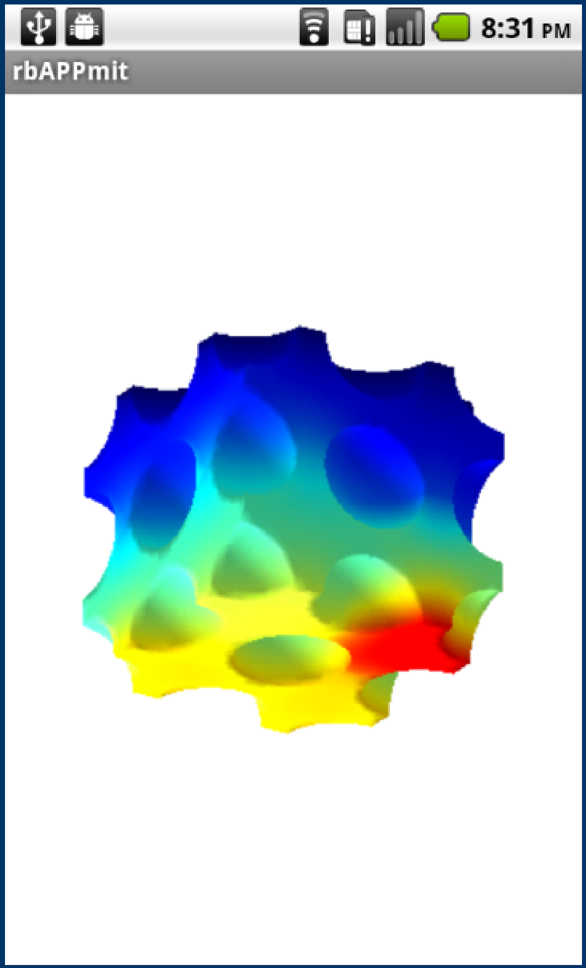
Many Parameters?



Many Parameters?



Many Parameters?



Large Parameter Domains?

Can we treat problems with large parameter domains?

Yes, but . . .

New enablers:

h-p (Greedy) over $\mathcal{D}$;[†]

Unter-Über reduced bases.

[†]We can then also consider the Smartphone memory as "cache" relative to the web Library.

Non-Affine Problems?

Can we treat problems with
non-affine parameter dependence?

Yes, but . . .

New enabler:

Empirical Interpolation Method (EIM).

Geometry?

Can we treat problems with geometric variations?

Yes, but . . .

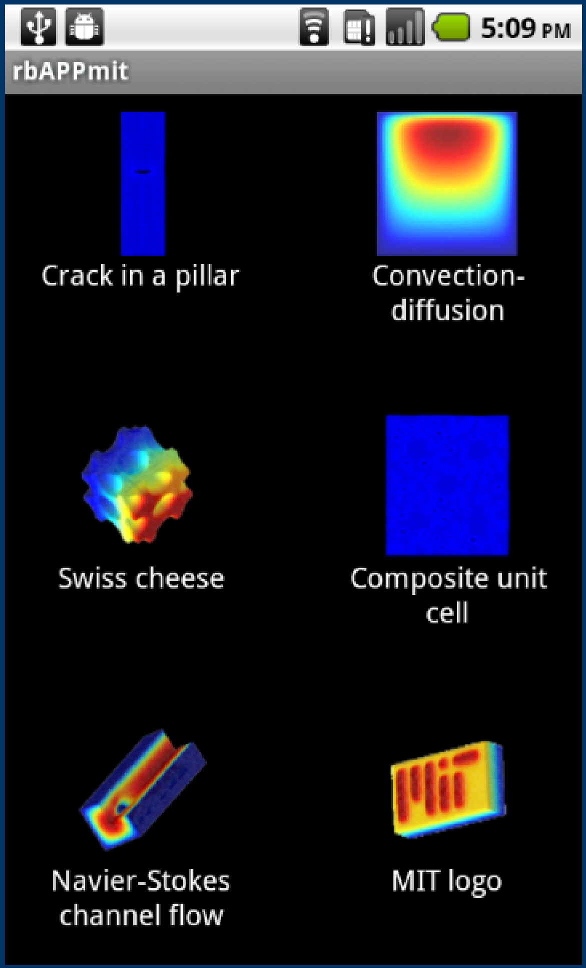
New enablers:

(automated) piecewise-affine transformations;

Empirical Interpolation Method (EIM).

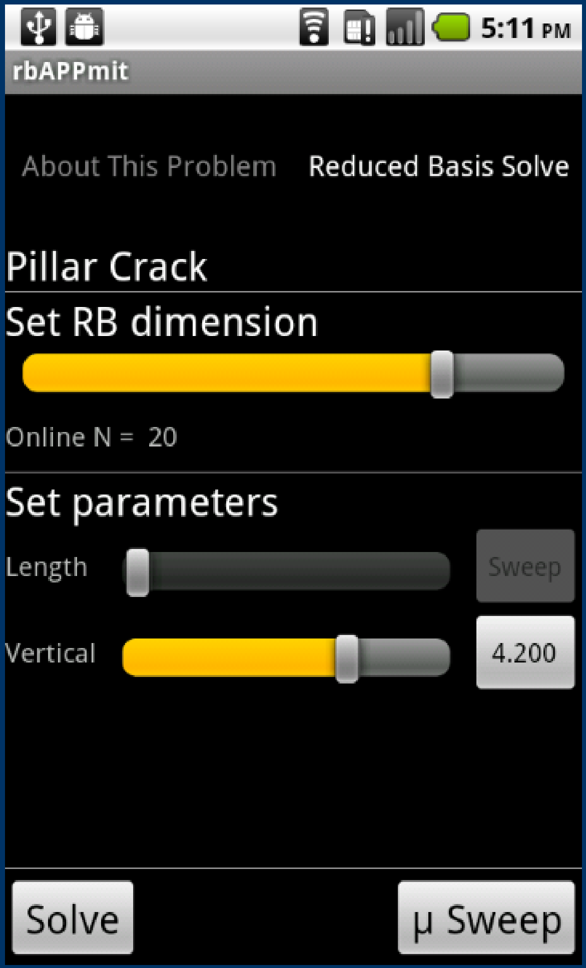
Geometry?

Piecewise-Affine



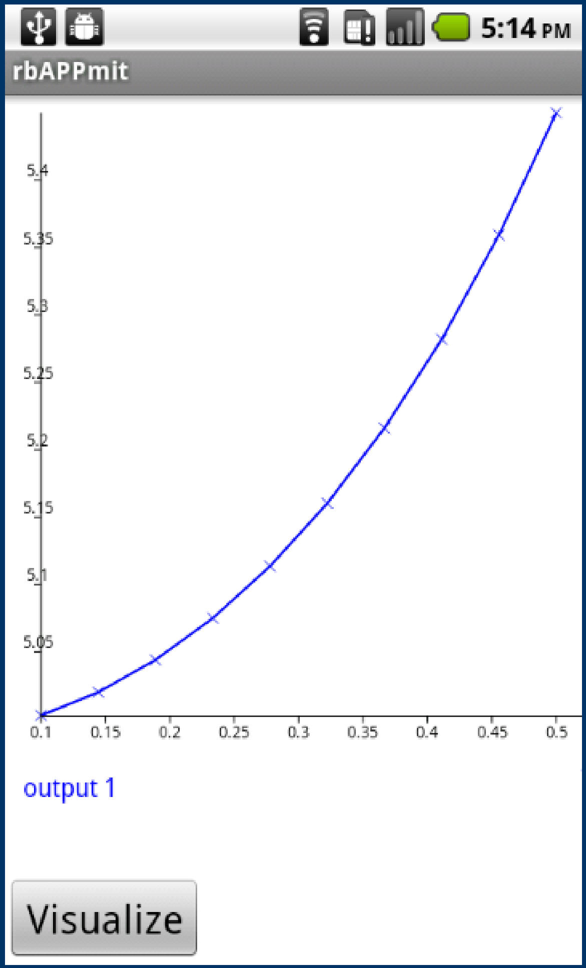
Geometry?

Piecewise-Affine



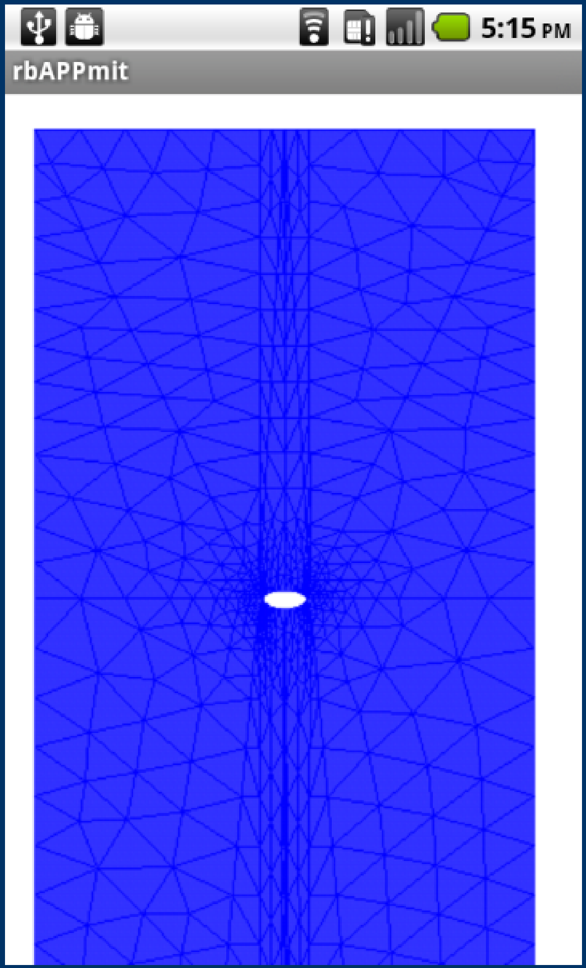
Geometry?

Piecewise-Affine



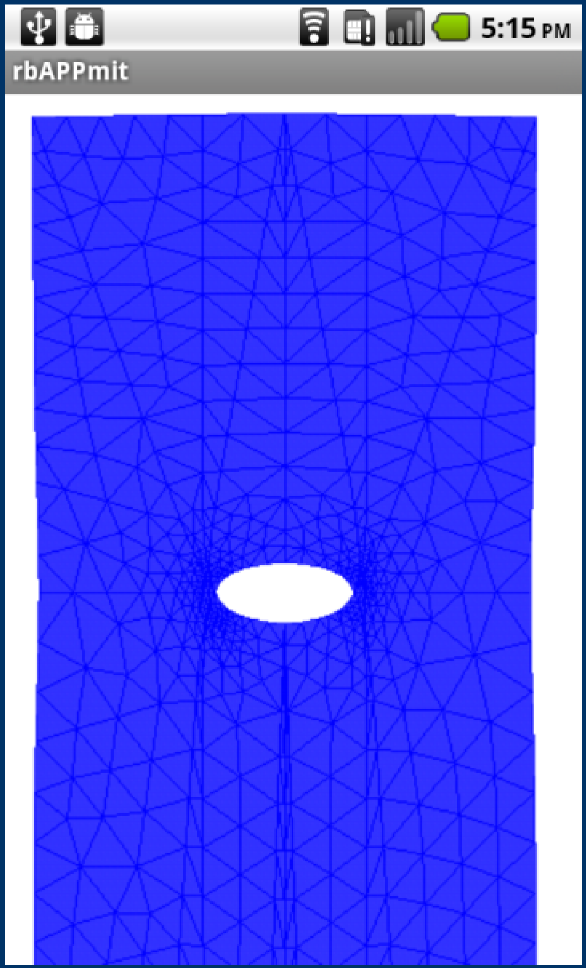
Geometry?

Piecewise-Affine



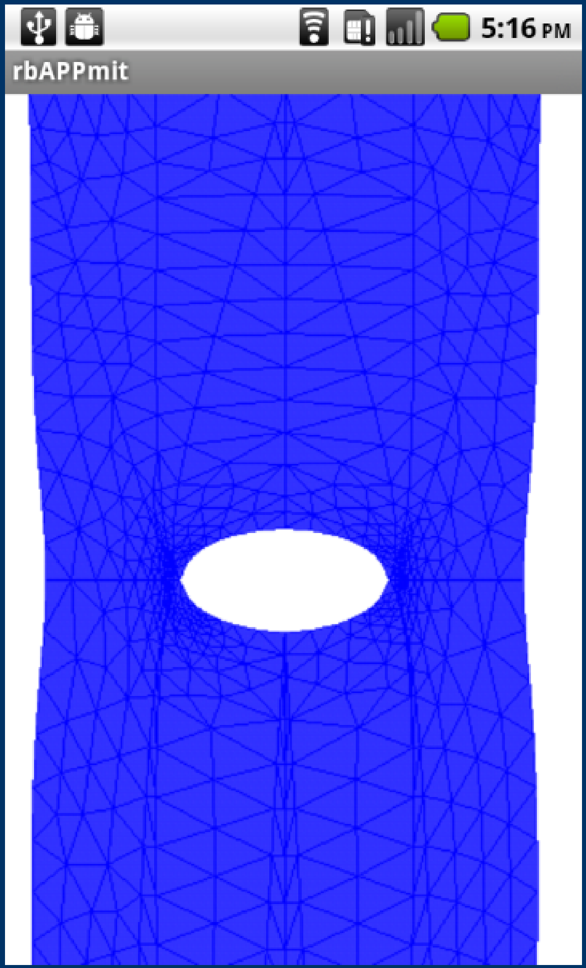
Geometry?

Piecewise-Affine



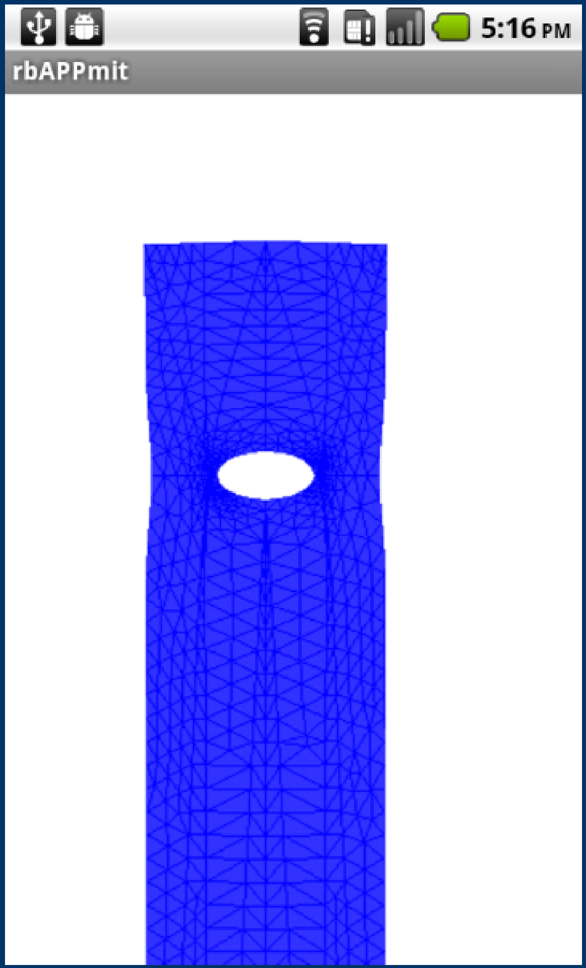
Geometry?

Piecewise-Affine

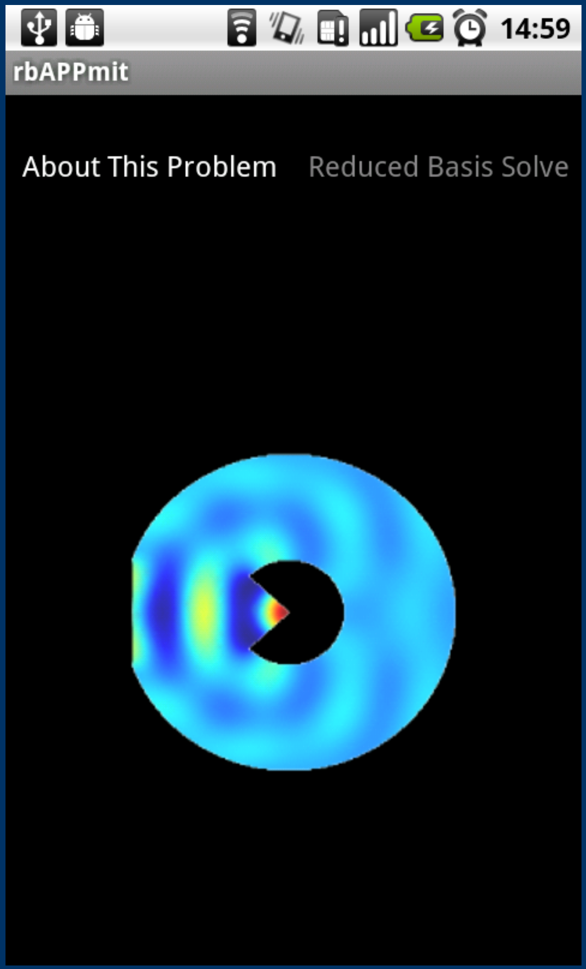


Geometry?

Piecewise-Affine

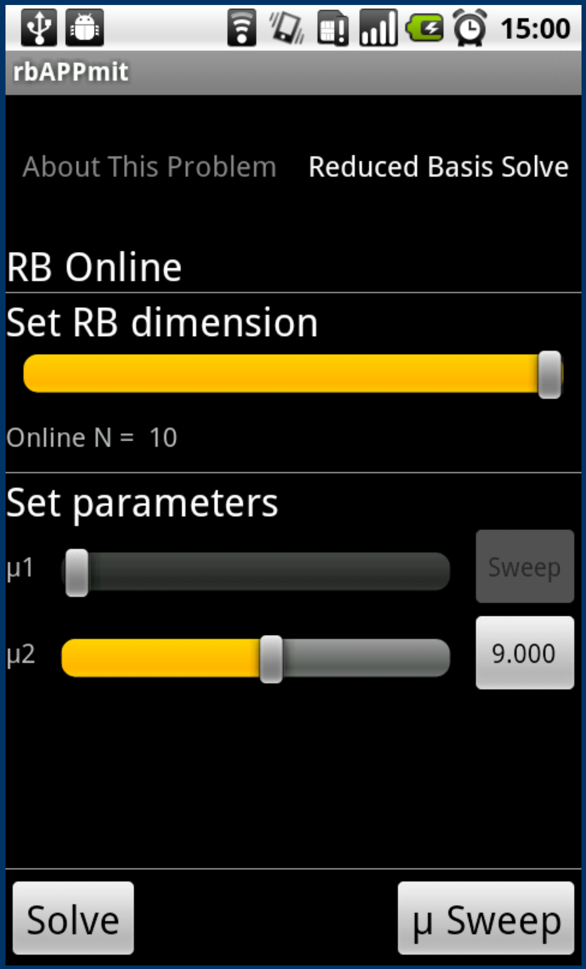


Geometry?



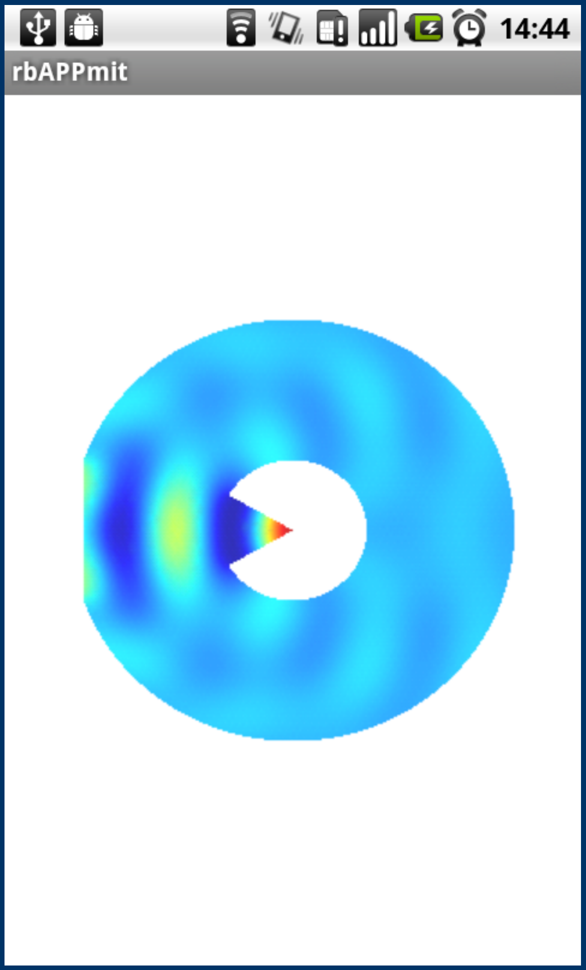
Geometry?

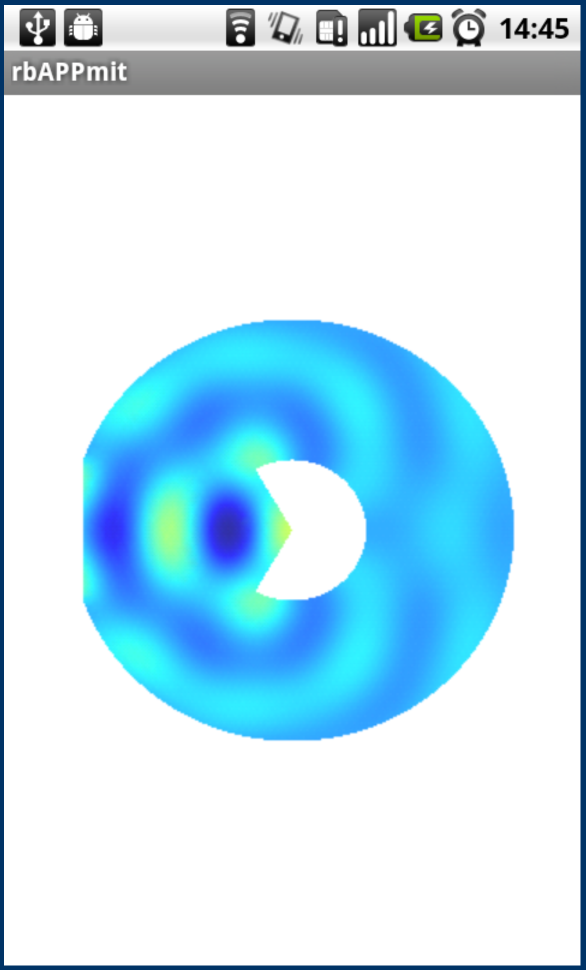
EIM



Geometry?

EIM





Hyperbolic Problems?

Can we treat hyperbolic (time-domain)
partial differential equations?

Yes, but . . .

New enabler:

Laplace Transform modal techniques.

Nonlinear Problems?

Can we treat problems which exhibit

quadratic nonlinearity?	Yes, but
general nonlinearity?	Yes, but but . . .

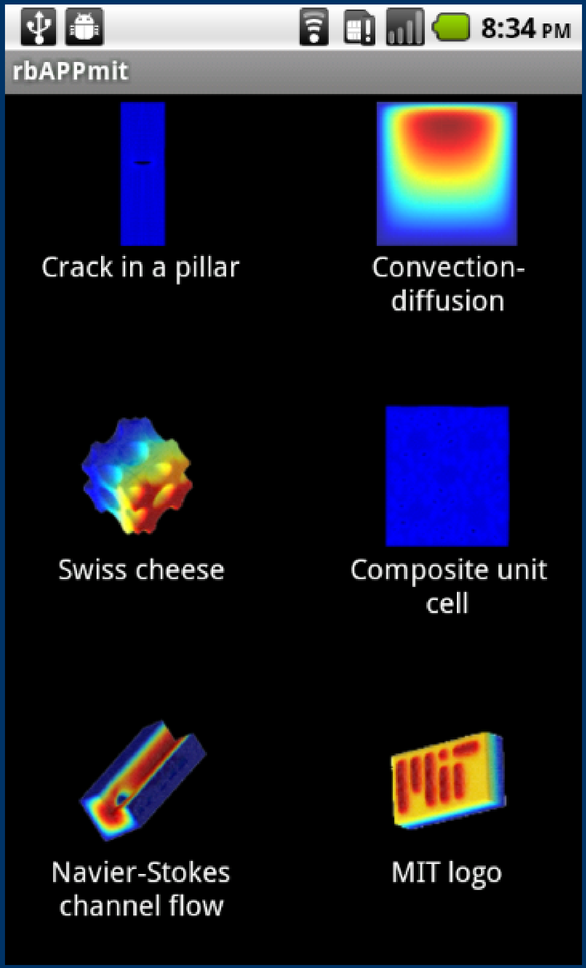
New enablers:

h-p Greedy over $\mathcal{D}$;

Empirical Interpolation Method (EIM).

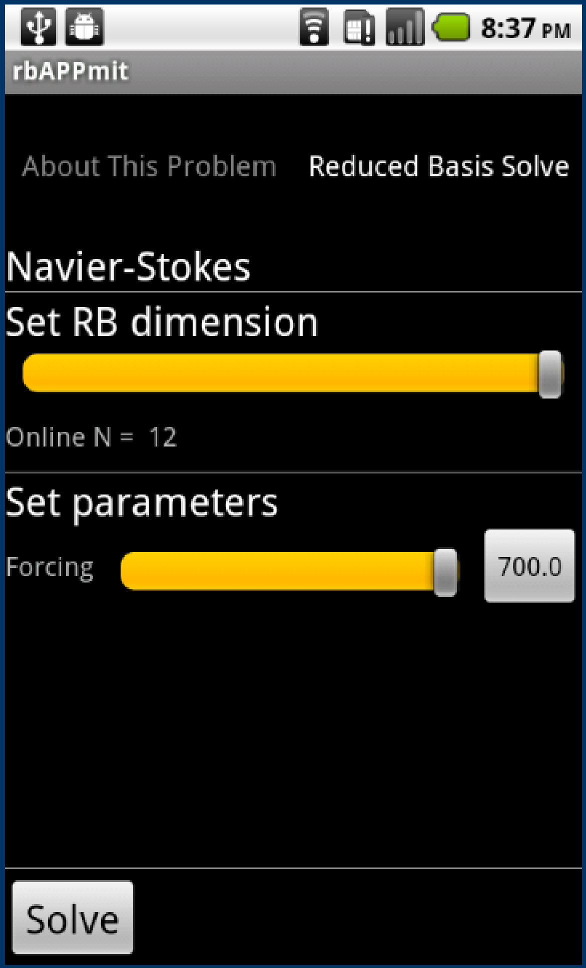
Nonlinear Problems?

Quadratic



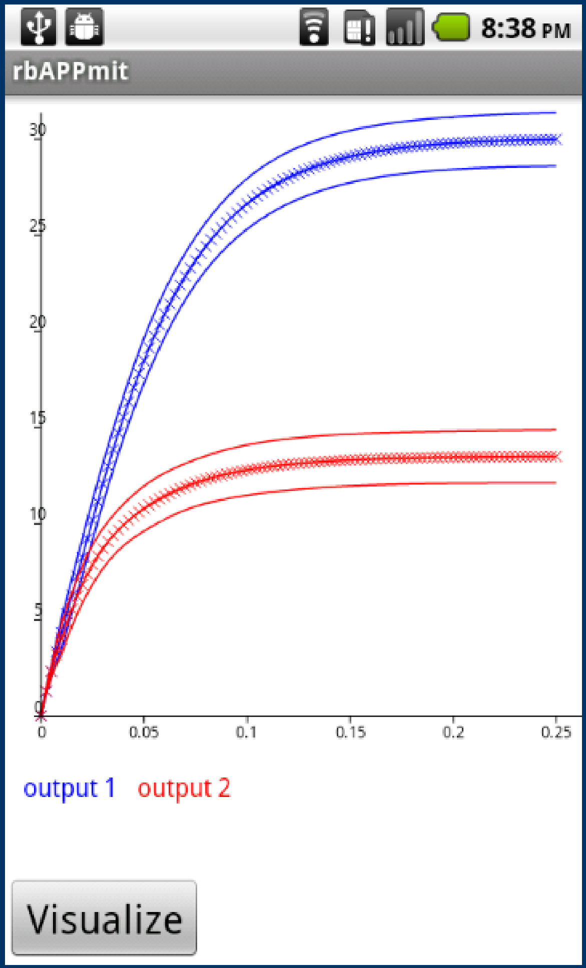
Nonlinear Problems?

Quadratic



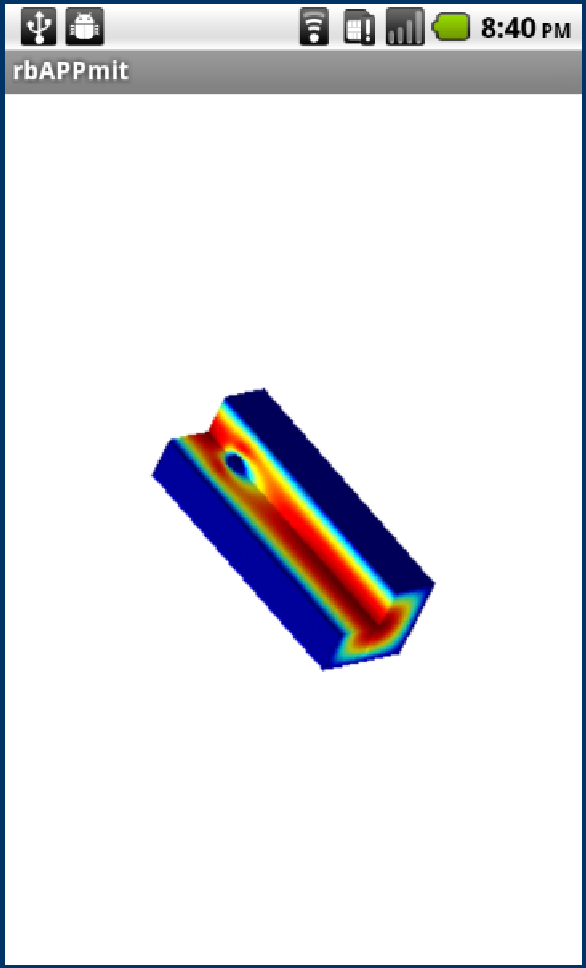
Nonlinear Problems?

Quadratic



Nonlinear Problems?

Quadratic



Inverse Problems

Can we make inferences from inverse analysis?

Yes, but . . .

New enablers:

Uber-Unter reduced bases;

improved sampling methods.

Design Optimization

Can we perform design optimization?

Yes, but . . .

New enabler:

improved optimization procedures.

Design Optimization

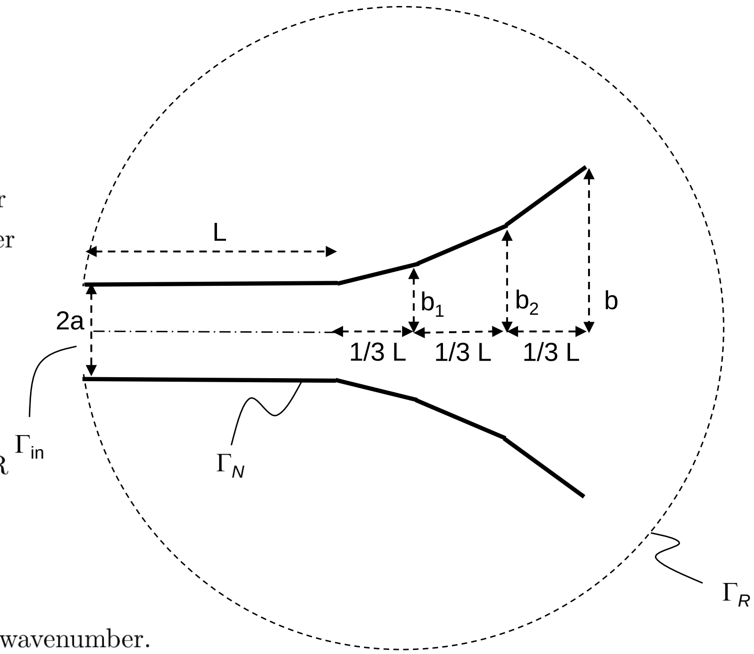
Horn Problem Setup

Geometry Parameters:

L = Length of waveguide and flare
$2a$ = waveguide width
b_1 = height of 1st slice of flare from center
b_2 = height of 2nd slice of flare from center
b = final height of flare from center

Boundaries:

Γ_{in} = waveguide inlet
Γ_N = internal and external horn walls
Γ_R = farfield circular boundary of radius R



Governing Equation: Helmholtz equation

$$\nabla^2 u + k^2 u = 0,$$

where u is amplitude and k is dimensionless wavenumber.

Boundary Conditions:

$$\begin{aligned} iku + \frac{\partial u}{\partial n} &= 2ik \quad \text{on } \Gamma_{\text{in}}, \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \Gamma_N, \\ \frac{\partial u}{\partial n} - \left(ik - \frac{1}{2R} + \frac{1}{8R(1-ikR)} \right) u &= 0 \quad \text{on } \Gamma_R, \end{aligned}$$

where n is the unit normal vector for Γ_N and Γ_R respectively.

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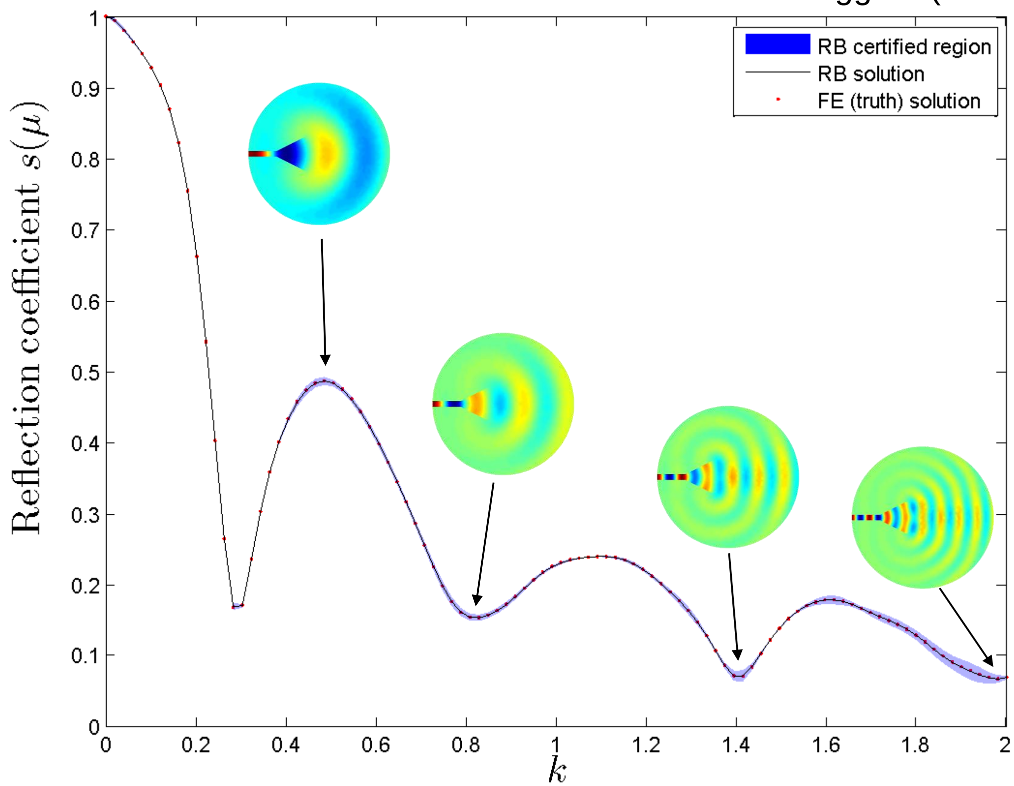
Design Optimization

Horn solutions

Reference geometry, RB model with N=140

Same acoustic model as in Udawapola and Berggren (*IJNME*, 2008).



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Design Optimization

Horn Robust Optimization (Formulation I)

Design for the worst case

Decision Variables: Geometry; assumed to be deterministic

$$\boldsymbol{\mu} = (b_1, b_2)^T$$

Uncontrolled Variable: Wavenumber; assume parametric variability

$$k \sim U[1.3, 1.5]$$

Problem Statement:

$$\min_{\boldsymbol{\mu}} \max_{k} \quad s(\boldsymbol{\mu}; k) = \left| \int_{\Gamma_{\text{in}}} u - 1 \right| \equiv \text{reflection coefficient}$$

s.t. Governing Equation, Boundary Conditions, and Set Constraints.

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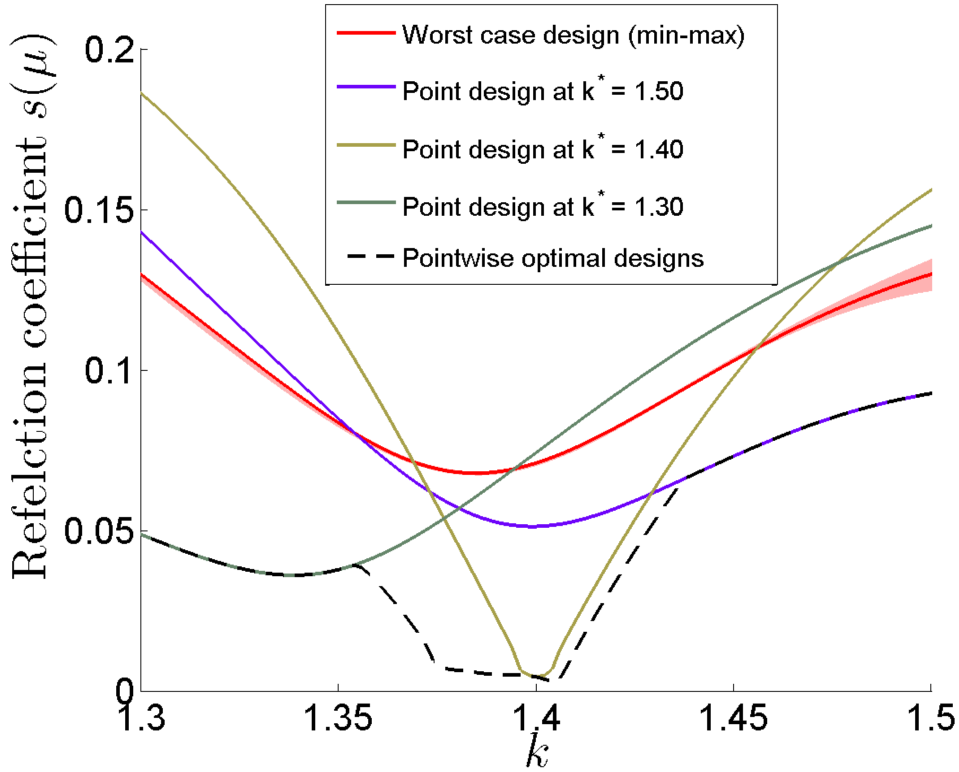
Design Optimization

Formulation I designs for the worst case

Trading performance for robustness



Optimization carried out using RB model with N=85.

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Design Optimization

Horn Robust Optimization (Formulation II)

Weighting between mean and variance trades risk and performance

Decision Variables: Geometry; assumed to be deterministic

$$\boldsymbol{\mu} = (b_1, b_2)^T$$

Uncontrolled Variable: Wavenumber; assume parametric variability

$$k \sim U[1.3, 1.5]$$

Problem Statement:

$$\begin{aligned} \min_{\boldsymbol{\mu}} \quad & \mathbb{E}[s(\boldsymbol{\mu}; k)] + \kappa \mathrm{var}(s(\boldsymbol{\mu}; k)), \text{where } \kappa > 0 \\ \text{s.t.} \quad & \text{Governing Equation, Boundary Conditions, and Set Constraints.} \end{aligned}$$

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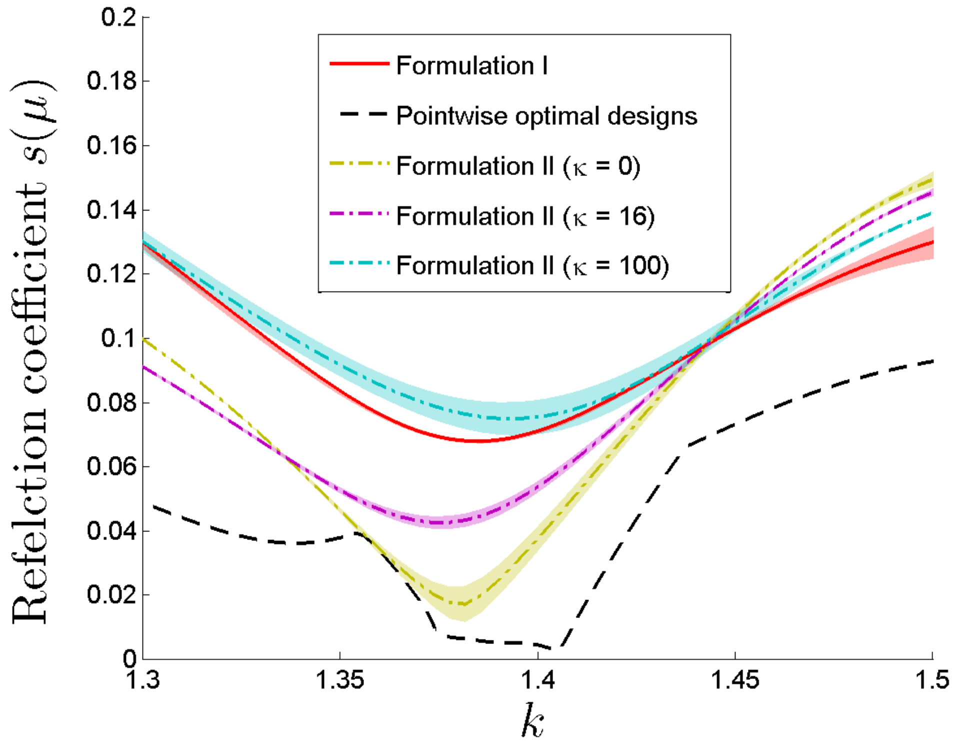
Design Optimization

Formulation II trades risk and performance

Output utility: $\mathbb{E}[s(\boldsymbol{\mu};k)] + \kappa \mathrm{var}(s(\boldsymbol{\mu};k))$



Optimization carried out using RB model with N=85.

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for more information see

`augustine.mit.edu`