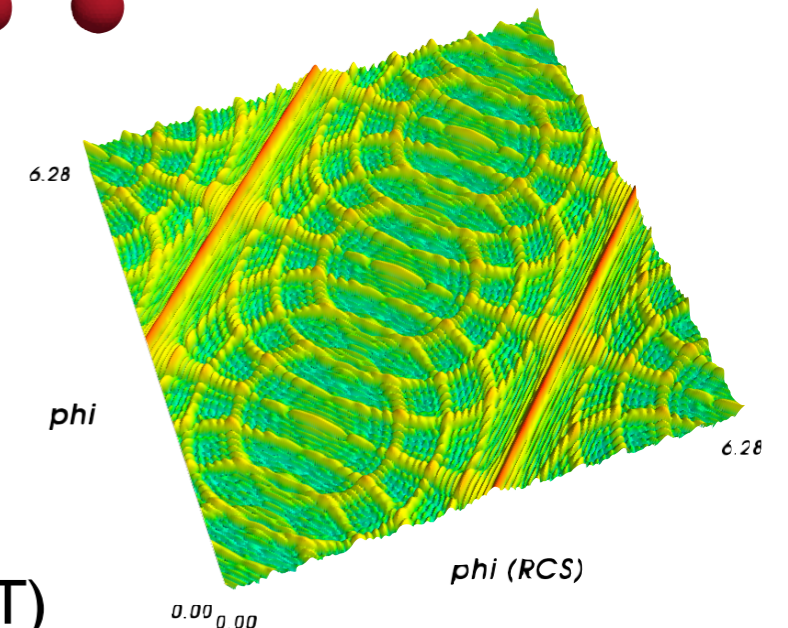
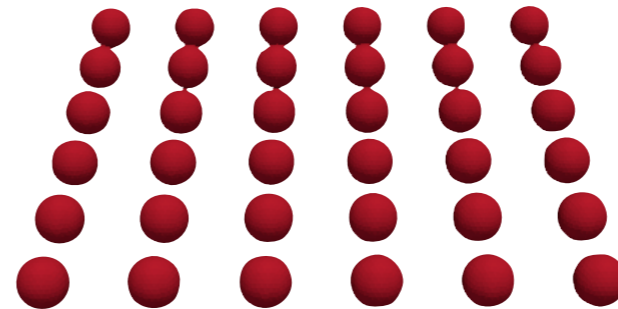


Reduced order models for parameterized problems: Lecture Two

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w/ assistance from B. Stamm (Aachen, D) and G. Rozza (SISSA, IT)

Overview of the lectures

Lecture 1: Introduction, motivation, basics

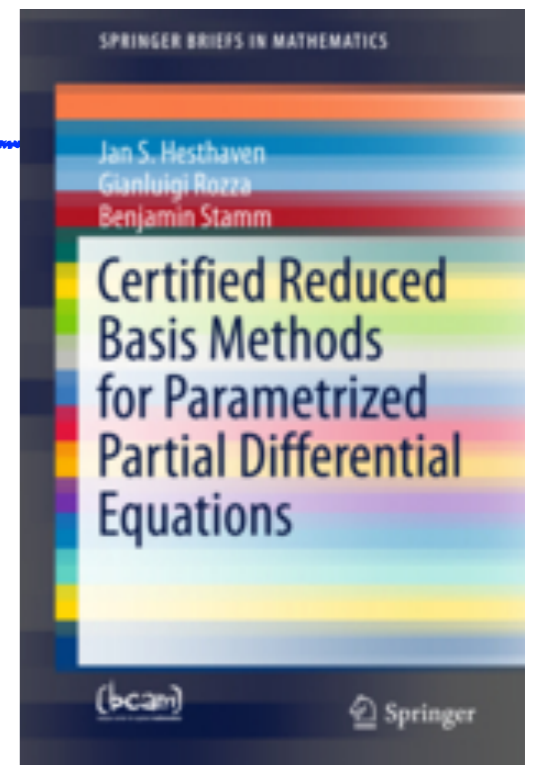
Lecture 2: Certified reduced methods

Lecture 3: The 'non's' etc

Hesthaven, Rozza, Stamm

*Certified Reduced Basis Methods for Parametrized
Partial Differential Equations*

Springer Briefs in Mathematics, 2015



Free: <https://infoscience.epfl.ch/record/213266?ln=en>

Overall goals

Understand Reduced models

Understand Reduced models

WHAT do we mean by 'reduced models' ?

WHY should we care ?

WHEN could it work ?

HOW do we know ?

DOES it work ?

WHAT's next ?



Starting point

We consider physical systems of the form

$$\begin{aligned}\mathcal{L}(\mathbf{x}, \mu)u(\mathbf{x}, \mu) &= f(\mathbf{x}, \mu) & \mathbf{x} \in \Omega \\ u(\mathbf{x}, \mu) &= g(\mathbf{x}, \mu) & \mathbf{x} \in \partial\Omega\end{aligned}$$

where the solutions are implicitly parameterized by

$$\mu \in \mathcal{D} \subset \mathbb{R}^M$$

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where the solutions are implicitly parameterized by

$$\mu \in \mathcal{D} \subset \mathbb{R}^M$$

- ▶ How do we find the basis.
- ▶ How do we ensure accuracy under parameter variation ?
- ▶ How do we ensure efficiency ?

The truth

Let us define:

The **exact solution**: Find $u(\mu) \in X$ such that

$$a(u, \mu, v) = f(\mu, v), \quad \forall v \in X$$

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$$a_h(u_h, \mu, v_h) = f_h(\mu, v_h), \quad \forall v_h \in X_h \quad \dim(X_h) = \mathcal{N}$$

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We always assume that $\mathcal{N} \gg N$

The truth and errors

Solving for the truth is expensive - but we need to be able to trust the RB solution


$$\|u(\mu) - u_{RB}(\mu)\| \leq \|u(\mu) - u_h(\mu)\| + \|u_h(\mu) - u_{RB}(\mu)\|$$

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$$\|u(\mu) - u_h(\mu)\| \leq \varepsilon$$

This is your favorite solver and it is assumed it can be as accurate as you desire - **the truth**

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Bounding we achieve two things

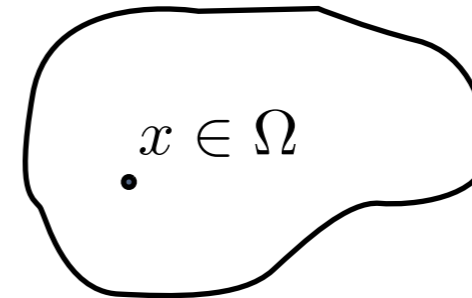
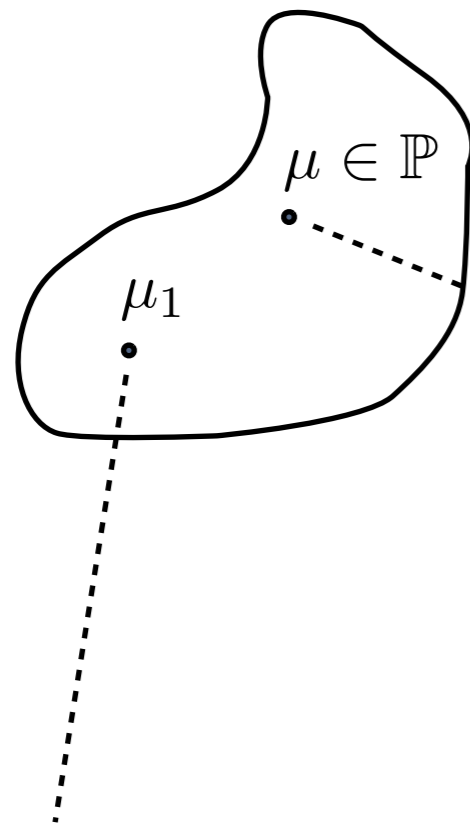
- ▶ Ability to build a basis at minimal cost
- ▶ Certify the quality of the model

Greedy sampling

Notation: a function $v(\cdot; \mu) : \Omega \rightarrow \mathbb{R}$ is often denoted as $v(\mu)$.

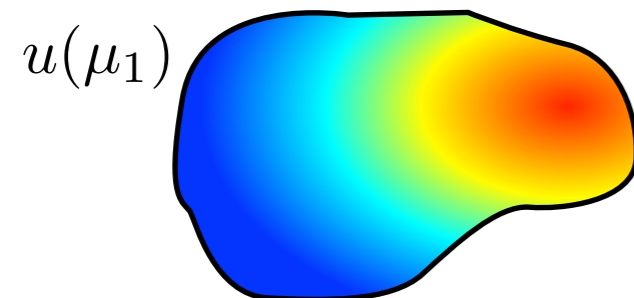
Parameter space \mathbb{P}

Spatial domain Ω



Solution of PDE $u(\mu) \in \mathbb{V}$. That is $u(\mu) : \Omega \rightarrow \mathbb{R}$.

Spatial domain Ω

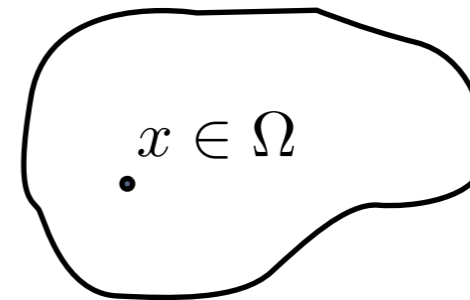
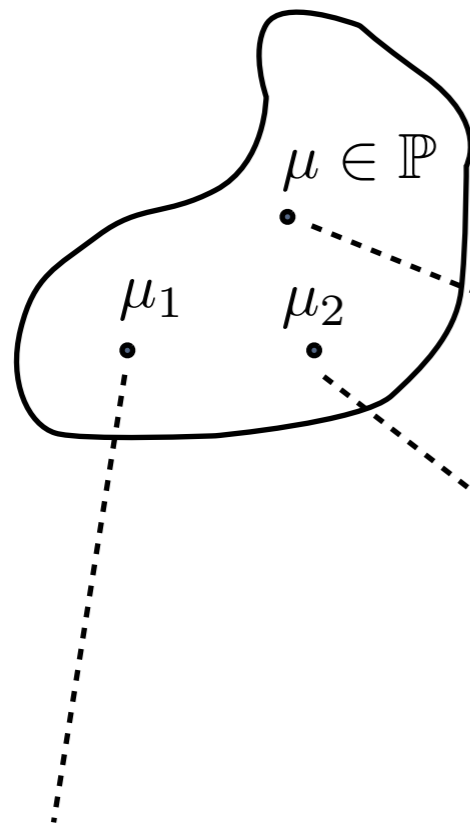


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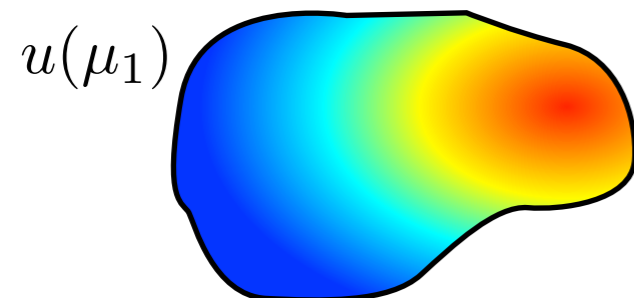
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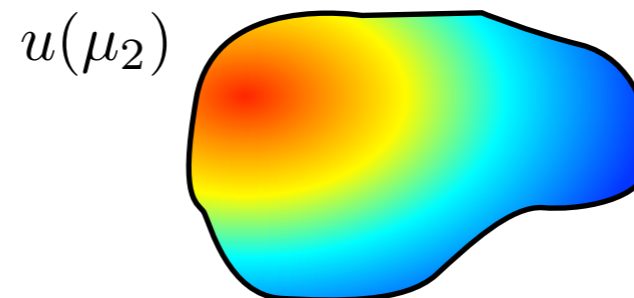


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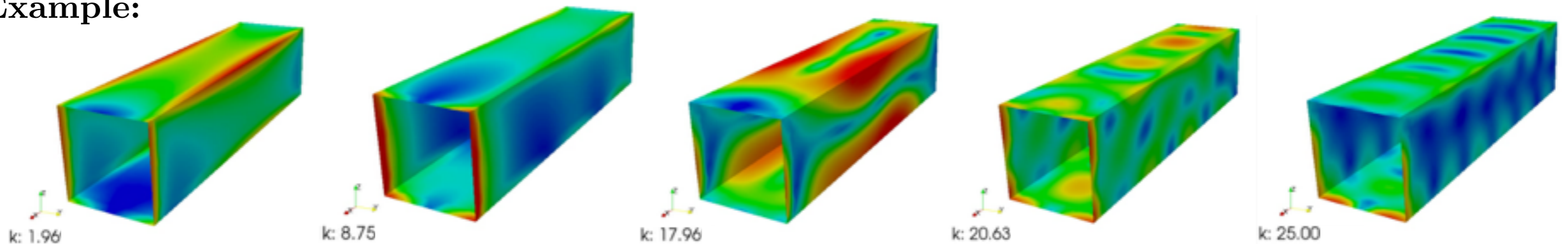
Greedy sampling

Reduced Basis Ansatz:

$$\mathbb{V}_{\text{rb}} = \text{span}\{u_\delta(\mu_1), \dots, u_\delta(\mu_N)\}$$

for some well-chosen sample points μ_1, \dots, μ_N .

Example:



1 parameter: wavenumber k
Different snapshots illustrated

Question: How to find the sample points μ_1, \dots, μ_N such that

$$\mathbb{V}_{\text{rb}} \approx \mathcal{M}_\delta = \{u_\delta(\mu) : \forall \mu \in \mathbb{P}\},$$

i.e. such that

$$E(\mathcal{M}_\delta, \mathbb{V}_{\text{rb}}) = \sup_{u_\delta(\mu) \in \mathcal{M}_\delta} \inf_{v_{\text{rb}} \in \mathbb{V}_{\text{rb}}} \|u_\delta(\mu) - v_{\text{rb}}\|_{\mathbb{V}} < \text{tol}$$

for N as little as possible?

Greedy sampling

Goal: Selection of sample points μ_1, \dots, μ_N such that

$$\mathbb{V}_{\text{rb}} = \text{span}\{u_\delta(\mu_1), \dots, u_\delta(\mu_N)\} \approx \mathcal{M}_\delta$$

Greedy algorithm:

Set $N = 1$, choose $\mu_1 \in \mathbb{P}$ arbitrarily.

1. Compute $u_\delta(\mu_N) \in \mathbb{V}_\delta$ (truth problem: computationally expensive)
2. Set $\mathbb{V}_{\text{rb}} = \text{span}\{\mathbb{V}_{\text{rb}}, u_\delta(\mu_N)\}$
3. Find $\mu_{N+1} = \arg \max_{\mu \in \mathbb{P}} \|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}$
4. Set $N := N + 1$ and goto 1. while $\max_{\mu \in \mathbb{P}} \|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} > \text{Tol}$

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Remarks:

- In order to compute $\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}$, the truth solution $u_\delta(\mu)$ needs to be computed.
- A sequence of hierarchical spaces is generated (which is not the case for the sequence of the best approximation spaces in the sens of Kolmogorov).

Greedy sampling

Key ingredient: (estimated) error feedback: Consider the mapping

$$\mu \mapsto \eta(\mu),$$

where $\eta(\mu)$ is an error estimation for $\|u_{\text{rb}}(\mu) - u_{\delta}(\mu)\|_{\mathbb{V}}$.

Greedy sampling

Key ingredient: (estimated) error feedback: Consider the mapping

$$\mu \mapsto \eta(\mu),$$

where $\eta(\mu)$ is an error estimation for $\|u_{\text{rb}}(\mu) - u_{\delta}(\mu)\|_{\mathbb{V}}$.

Recall that $u_{\delta}(\mu)$ the truth approximation defined by: find $u_{\delta}(\mu) \in \mathbb{V}_{\delta}$ such that

$$a(u_{\delta}(\mu), v_{\delta}; \mu) = f(v_{\delta}; \mu), \quad \forall v_{\delta} \in \mathbb{V}_{\delta},$$

and $u_{\text{rb}}(\mu)$ the reduced basis solution defined by: find $u_{\text{rb}}(\mu) \in \mathbb{V}_{\text{rb}}$ such that

$$a(u_{\text{rb}}(\mu), v_{\text{rb}}; \mu) = f(v_{\text{rb}}; \mu), \quad \forall v_{\text{rb}} \in \mathbb{V}_{\text{rb}}.$$

The Galerkin framework allow for a residual-based a posteriori estimators without computing $u_{\delta}(\mu)$. This will be discussed at a later stage.

Greedy sampling

Greedy algorithm:

Set $N = 1$, choose $\mu_1 \in \mathbb{P}$ arbitrarily.

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$$u_{RM}(\mu) = \sum_{i=1}^N u_N^i(\mu) \xi_i$$

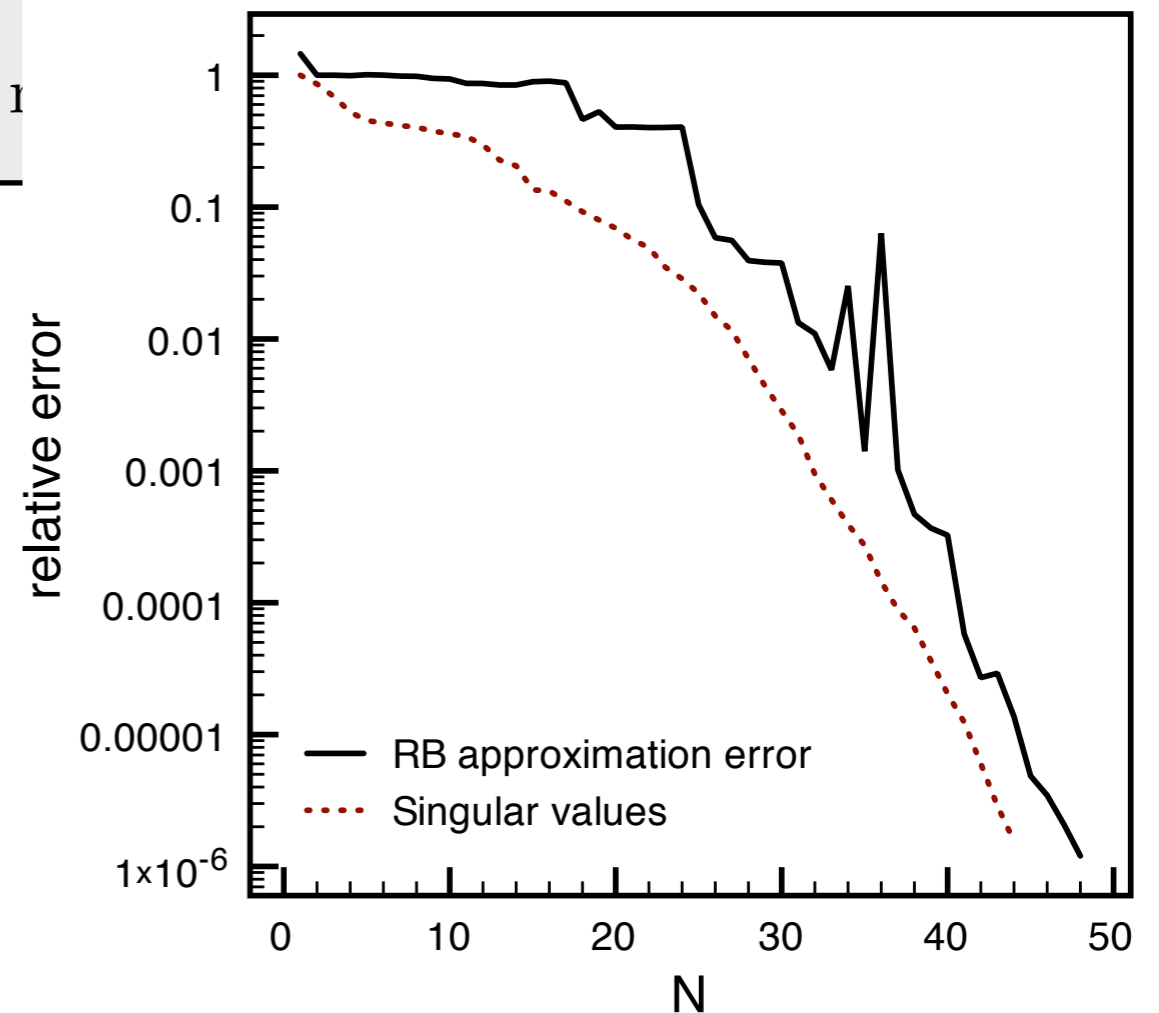
Greedy sampling

Greedy algorithm:

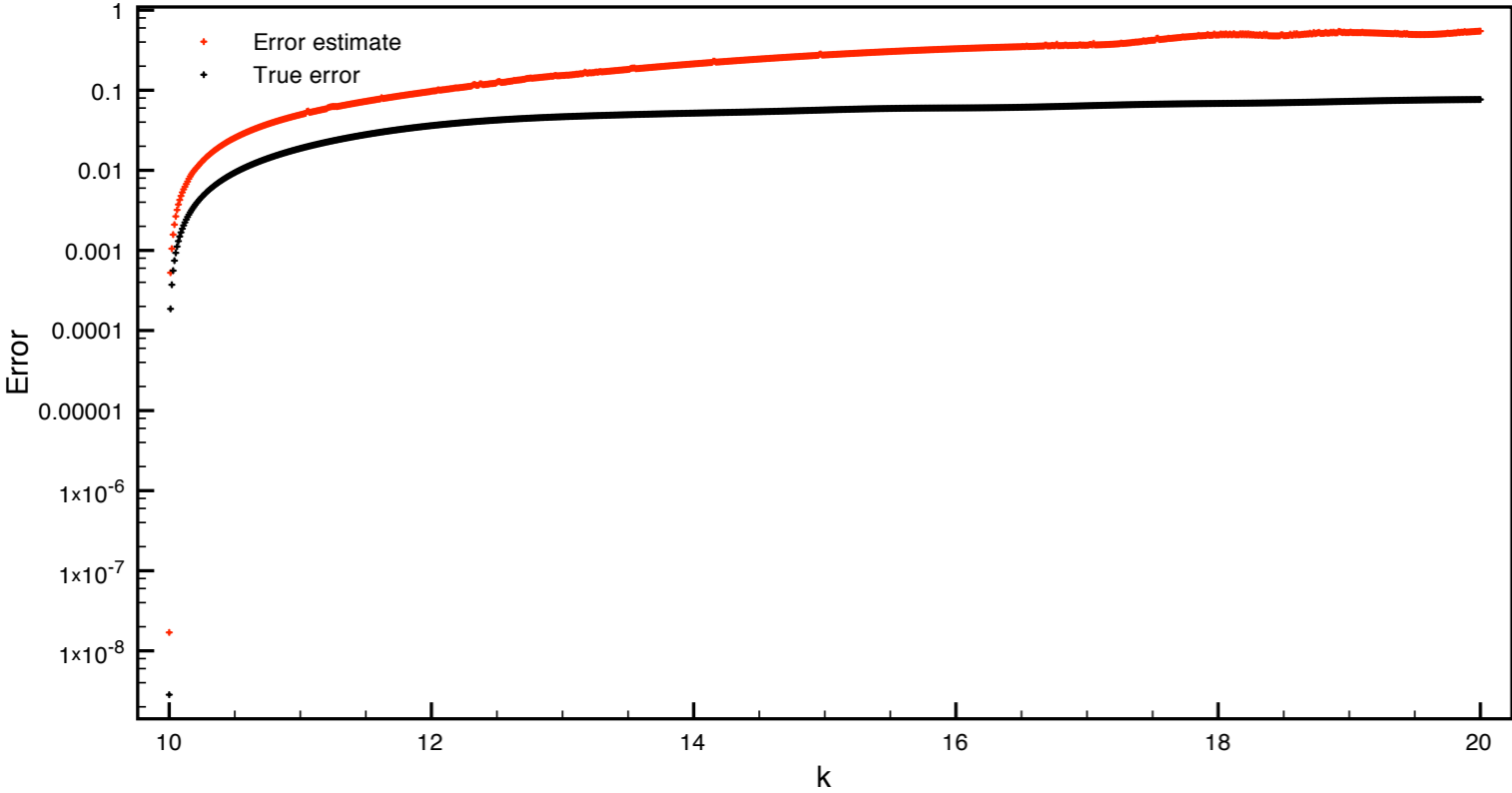
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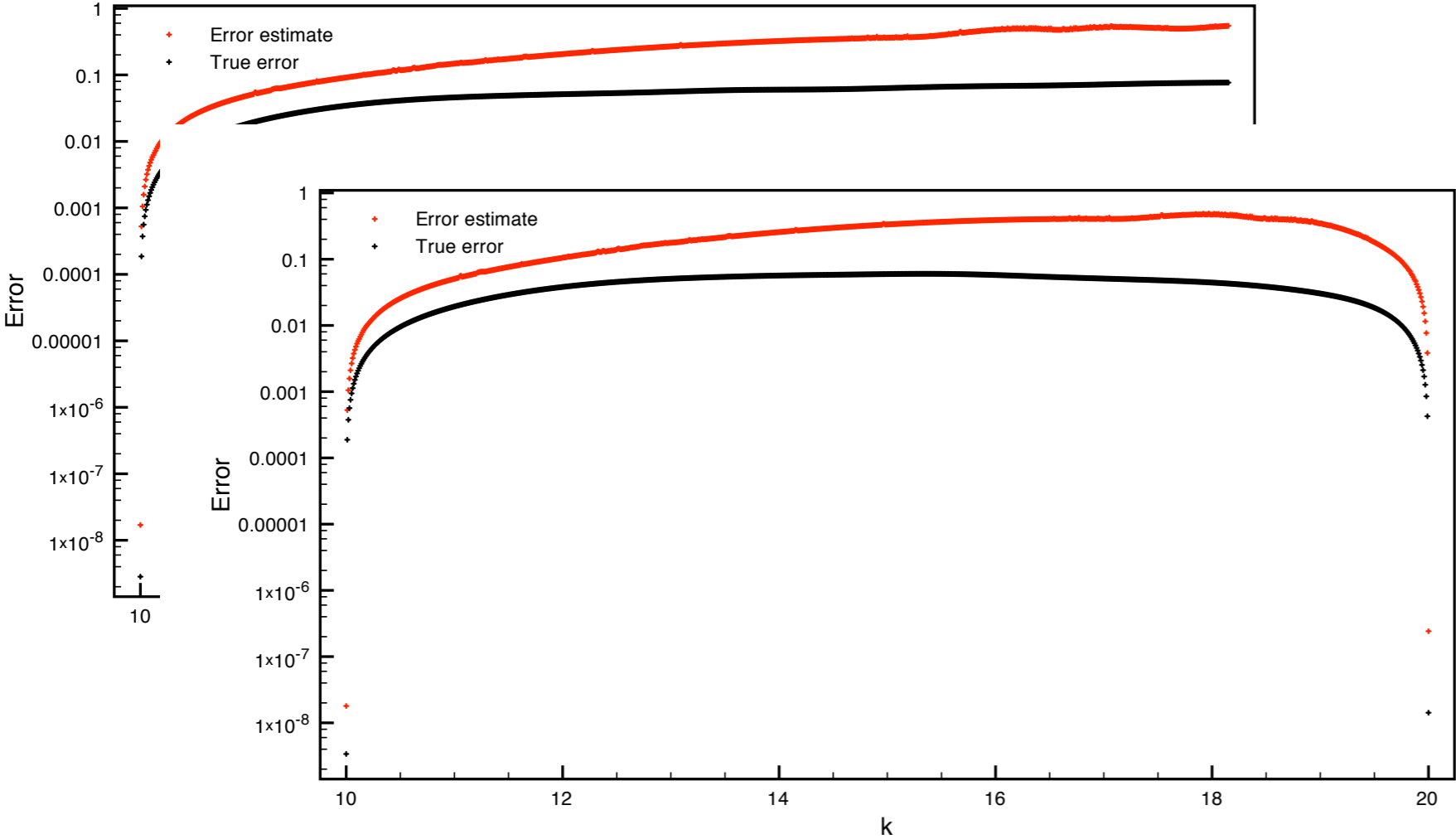
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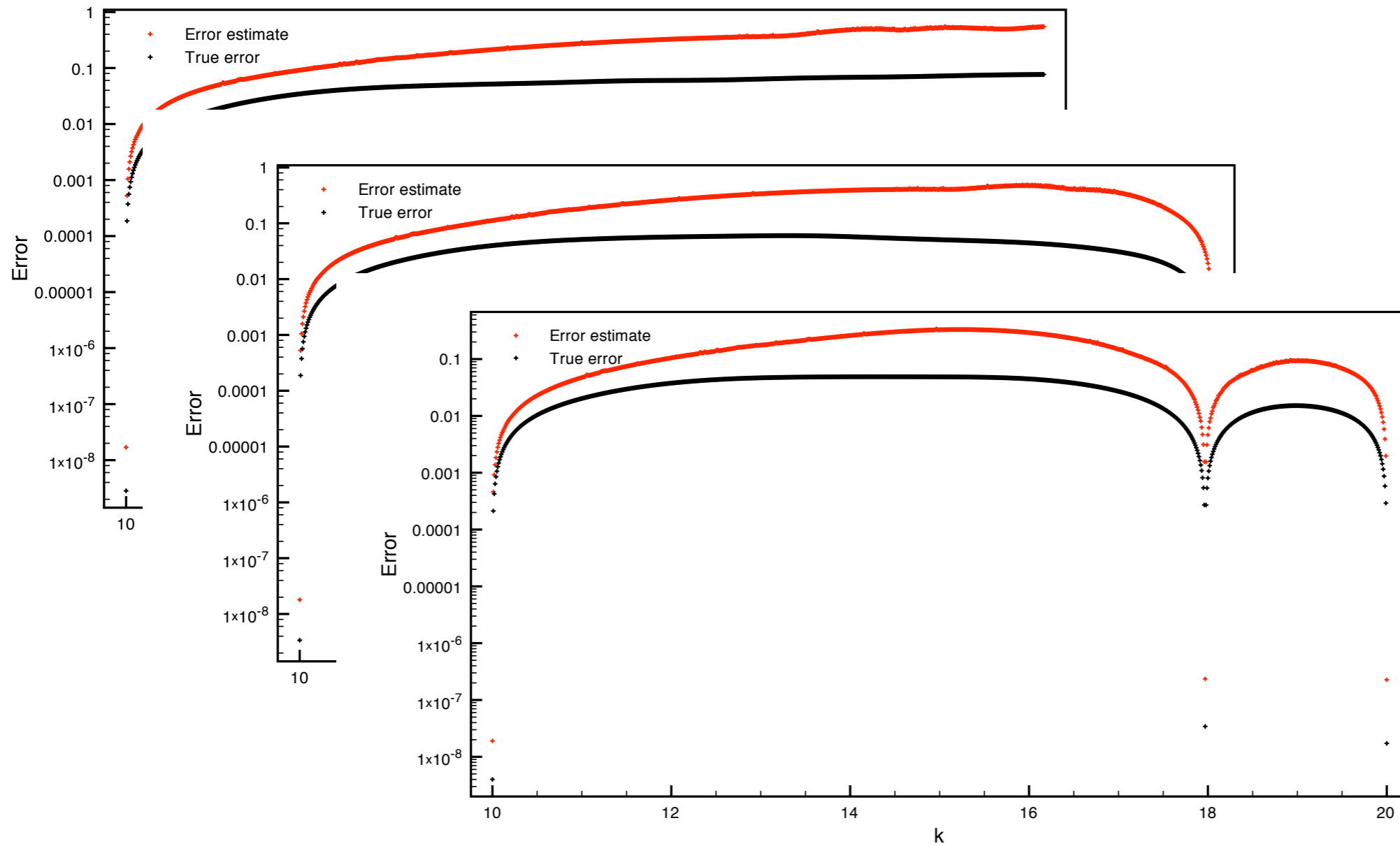
Greedy sampling - example



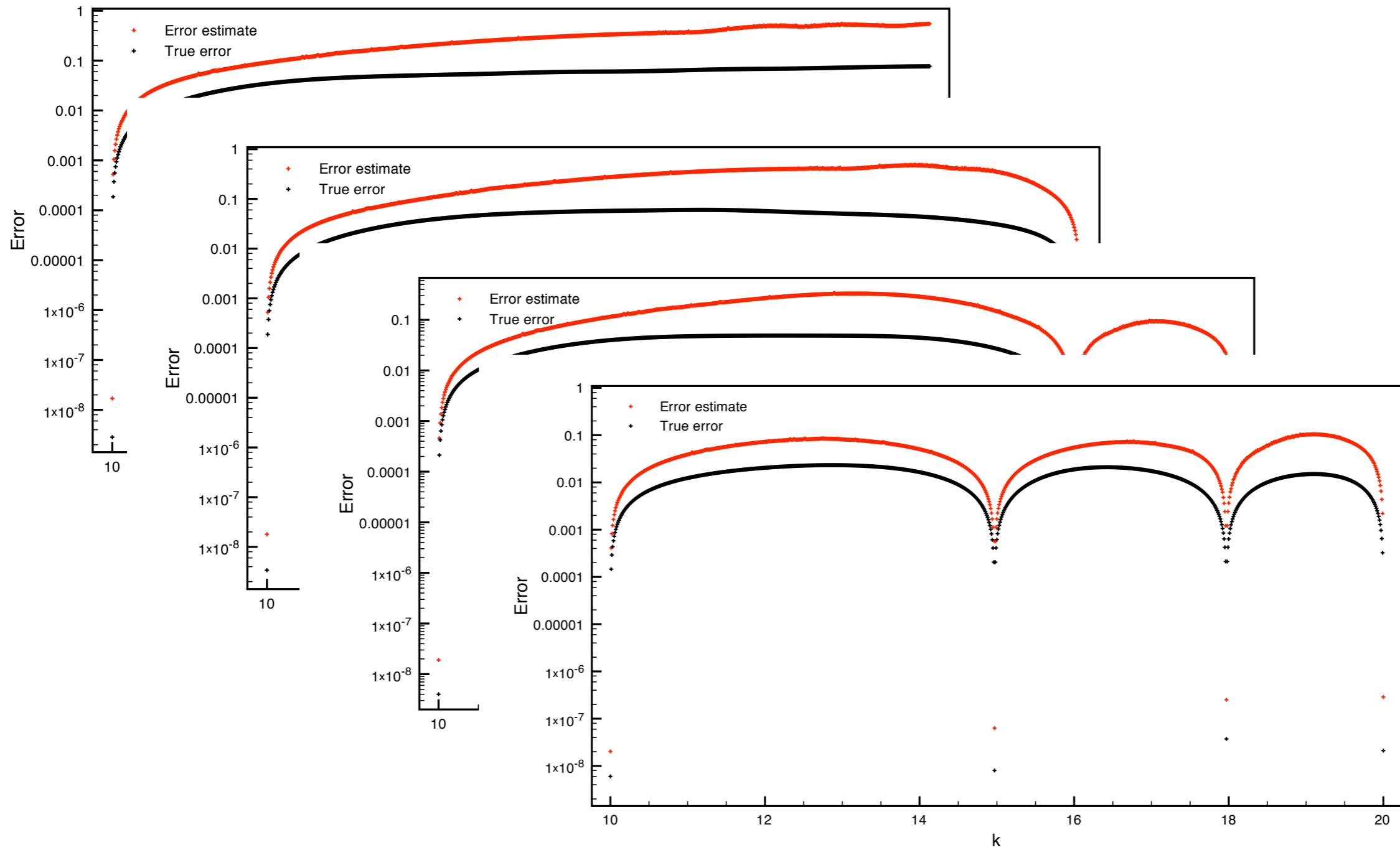
Greedy sampling - example



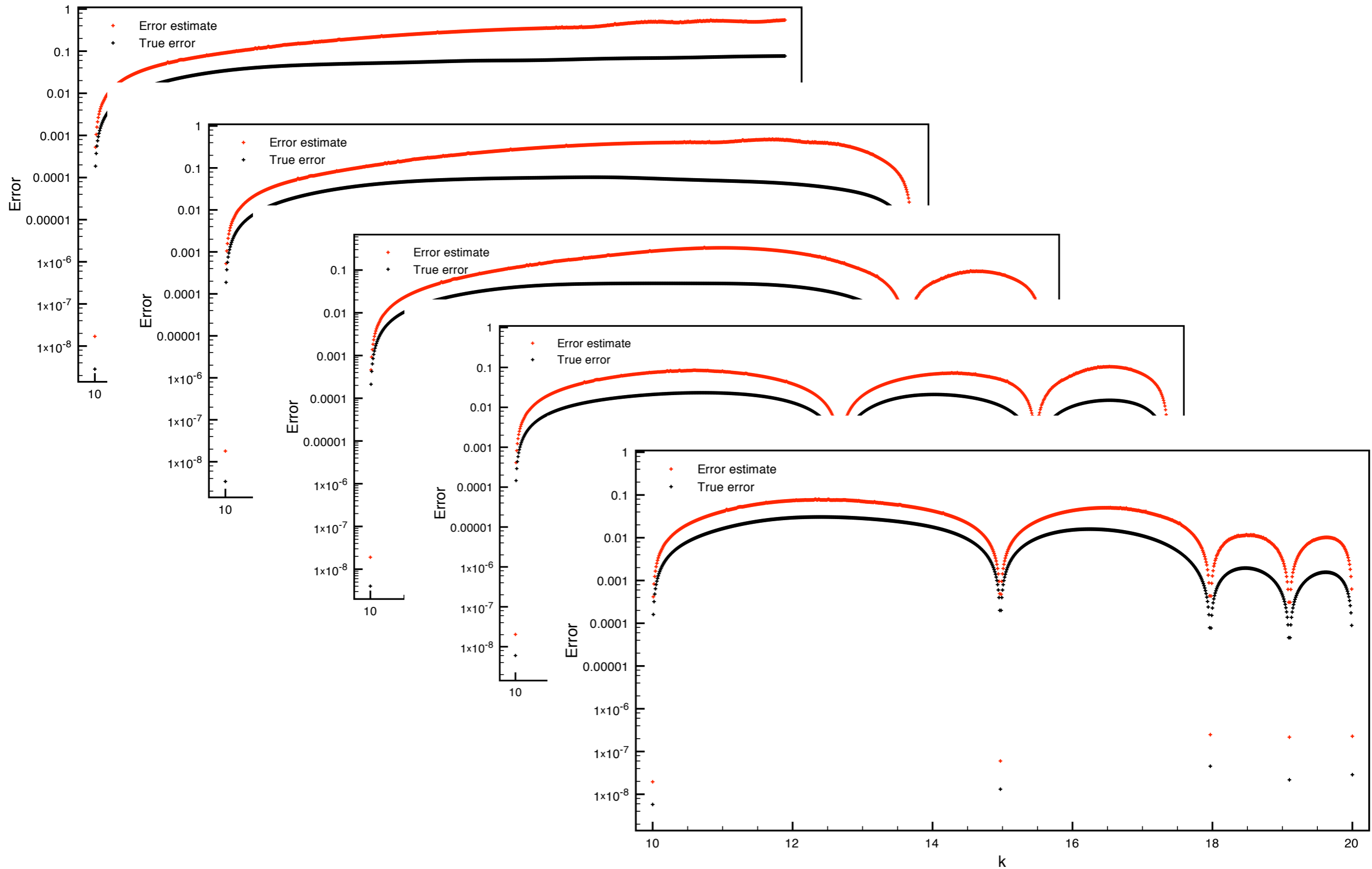
Greedy sampling - example



Greedy sampling - example



Greedy sampling - example



Greedy sampling - theory

Convergence: Is the convergence of the greedy algorithm comparable with the decay of the Kolmogorov N -width? Recall that the Kolmogorov N -width is the error using the best possible N -dimensional space (which is unknown in practice).

Theorem: Assume that the set of all solutions \mathcal{M} has an exponentially small Kolmogorov N -width

$$d_N(\mathcal{M}) \leq ce^{-aN},$$

for an $a > \log(1 + \sqrt{\frac{\gamma}{\alpha}})$, then the reduced basis approximation converges exponentially fast in the sense that there exists a $\beta > 0$ such that

$$\forall \mu \in \mathbb{P} : \|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq Ce^{-\beta N}.$$

Another result exists which says that if the Kolmogorov N -width decays with an algebraic rate, then so does the reduced basis approximation based on the greedy-algorithm. The rates are however different.

Need for speed

How to solve the problem: For $\mu \in \mathbb{P}$, find the solution $u_{\text{rb}}(\mu) \in \mathbb{V}_{\text{rb}}$ of

$$a(u_{\text{rb}}(\mu), v_{\text{rb}}; \mu) = f(v_{\text{rb}}; \mu), \quad \forall v_{\text{rb}} \in \mathbb{V}_{\text{rb}}$$

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It consists of a linear problem with N degrees of freedom, thus results in a N -dimensional linear system

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$$\mathbf{A}_{\text{rb}}^{\mu} \mathbf{u}_{\text{rb}}^{\mu} = \mathbf{f}_{\text{rb}}^{\mu},$$

However: Let the reduced basis space be given by $\mathbb{V}_{\text{rb}} = \text{span}\{\xi_1, \dots, \xi_N\}$, then the N -dimensional matrix

$$(\mathbf{A}_{\text{rb}}^{\mu})_{ij} = a(\xi_j, \xi_i; \mu), \quad 1 \leq i, j \leq N,$$

needs to be reassembled for each new parameter value $\mu \in \mathbb{P}$ and the assembly process depends on $\mathcal{N}_{\delta} = \dim(\mathbb{V}_{\delta})$: $\mathbf{A}_{\text{rb}}^{\mu} = \mathbf{B}^T \mathbf{A}_{\delta}^{\mu} \mathbf{B}$.

The affine assumption

Assumption:

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

$$f(v; \mu) = \sum_{q=1}^{Q_f} \theta_f^q(\mu) f_q(v),$$

$$\ell(v; \mu) = \sum_{q=1}^{Q_1} \theta_1^q(\mu) \ell_q(v),$$

where

$$\theta_a^q, \theta_f^q, \theta_1^q : \mathbb{P} \rightarrow \mathbb{R}$$

$$a_q : \mathbb{V} \times \mathbb{V} \rightarrow \mathbb{R}$$

$$f_q, \ell_q : \mathbb{V} \rightarrow \mathbb{R}$$

μ – dependent functions,

μ – independent forms,

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Example: Convection-diffusion

$$a(u, v; \varepsilon) = \varepsilon \int_0^1 u'(x)v'(x) dx + \int_0^1 u'(x)v(x) dx,$$
$$a_1(u, v; \varepsilon) = \int_0^1 u'(x)v'(x) dx, \quad \theta_a^1(\varepsilon) = \varepsilon,$$
$$a_2(u, v; \varepsilon) = \int_0^1 u'(x)v(x) dx, \quad \theta_a^2(\varepsilon) = 1,$$

Example: Heat conduction on thermal blocks

$$a(w, v; \mu) = \sum_{i=1}^{15} \mu_i \int_{\mathcal{R}_i} \nabla w \cdot \nabla v + \int_{\mathcal{R}_{P+1}} \nabla w \cdot \nabla v,$$
$$a_i(w, v; \mu) = \int_{\mathcal{R}_i} \nabla w \cdot \nabla v, \quad \theta_a^i(\mu) = \mu_i, \quad i = 1, \dots, 15,$$
$$a_{16}(w, v; \mu) = \int_{\mathcal{R}_{16}} \nabla w \cdot \nabla v, \quad \theta_a^{16}(\mu) = 1,$$

Need for speed

Off-line: Given $\mathbb{V}_{\text{rb}} = \text{span}\{\xi_1, \dots, \xi_N\}$ precompute

$$(\mathbf{A}_{\text{rb}}^q)_{ij} = a_q(\xi_j, \xi_i), \quad \forall 1 \leq i, j \leq N,$$

$$(\mathbf{f}_{\text{rb}}^q)_i = f_q(\xi_i), \quad \forall 1 \leq i \leq N,$$

$$(\mathbf{l}_{\text{rb}}^q)_i = \ell_q(\xi_i), \quad \forall 1 \leq i \leq N.$$

Rem. Size of \mathbf{A}_{rb}^q and $\mathbf{f}_{\text{rb}}^q, \mathbf{l}_{\text{rb}}^q$ is $N \times N$ resp. N .

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Rem. The assembling depends on $N_\delta = \dim(\mathbb{V}_\delta)$. Indeed:

$$\mathbf{A}_{\text{rb}}^q = \mathbf{B}^T \mathbf{A}_\delta^q \mathbf{B}, \quad \mathbf{f}_{\text{rb}}^q = \mathbf{B}^T \mathbf{f}_\delta^q, \quad \mathbf{l}_{\text{rb}}^q = \mathbf{B}^T \mathbf{l}_\delta^q,$$

where $(\mathbf{A}_\delta^q)_{ij} = a_q(\varphi_j, \varphi_i)$, $(\mathbf{f}_\delta^q)_j = f_q(\varphi_j)$ and $(\mathbf{l}_\delta^q)_j = \ell_q(\varphi_j)$ for $1 \leq i, j \leq N_\delta$.

Need for speed

On-line: For each new parameter value $\mu \in \mathbb{P}$

1. Assemble (depending on Q_a, Q_f and N , i.e. $\sim Q_a N^2$ resp. $\sim Q_f N$)

$$\mathbf{A}_{\text{rb}}^{\mu} = \sum_{q=1}^{Q_a} \theta_a^q(\mu) \mathbf{A}_{\text{rb}}^q \quad \mathbf{f}_{\text{rb}}^{\mu} = \sum_{q=1}^{Q_f} \theta_f^q(\mu) \mathbf{f}_{\text{rb}}^q$$

2. Solve $\mathbf{A}_{\text{rb}}^{\mu} \mathbf{u}_{\text{rb}}^{\mu} = \mathbf{f}_{\text{rb}}^{\mu}$. (depending on N , i.e. $\sim N^3$ for LU factorization)
3. Compute

$$s_{\text{rb}}(\mu) = \ell(\mathbf{u}_{\text{rb}}(\mu); \mu) = \sum_{q=1}^{Q_1} \theta_1^m(\mu) (\mathbf{u}_{\text{rb}}^{\mu})^T \mathbf{l}_{\text{rb}}^q.$$

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This is independent on N !

Need for speed

Computational costs:

- Off-line procedure: T_{off} .
- One on-line evaluation: T_{on} .
- One truth solve: $T_{\text{tr}} \gg T_{\text{on}}$.

Evaluation for M parameter values:

1. Brute force approach: $M \cdot T_{\text{tr}}$.
2. Reduced basis method: $T_{\text{off}} + M \cdot T_{\text{on}}$.

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Theoretical considerations:

- The parameter space \mathbb{P} is a continuous space (not discrete): M is potentially arbitrarily high.
- Whenever the number M of parameter evaluations is high enough, the reduced basis method is always cheaper.

Need for speed

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- One truth solve: $T_{\text{tr}} \gg T_{\text{on}}$.

Evaluation for M parameter values:

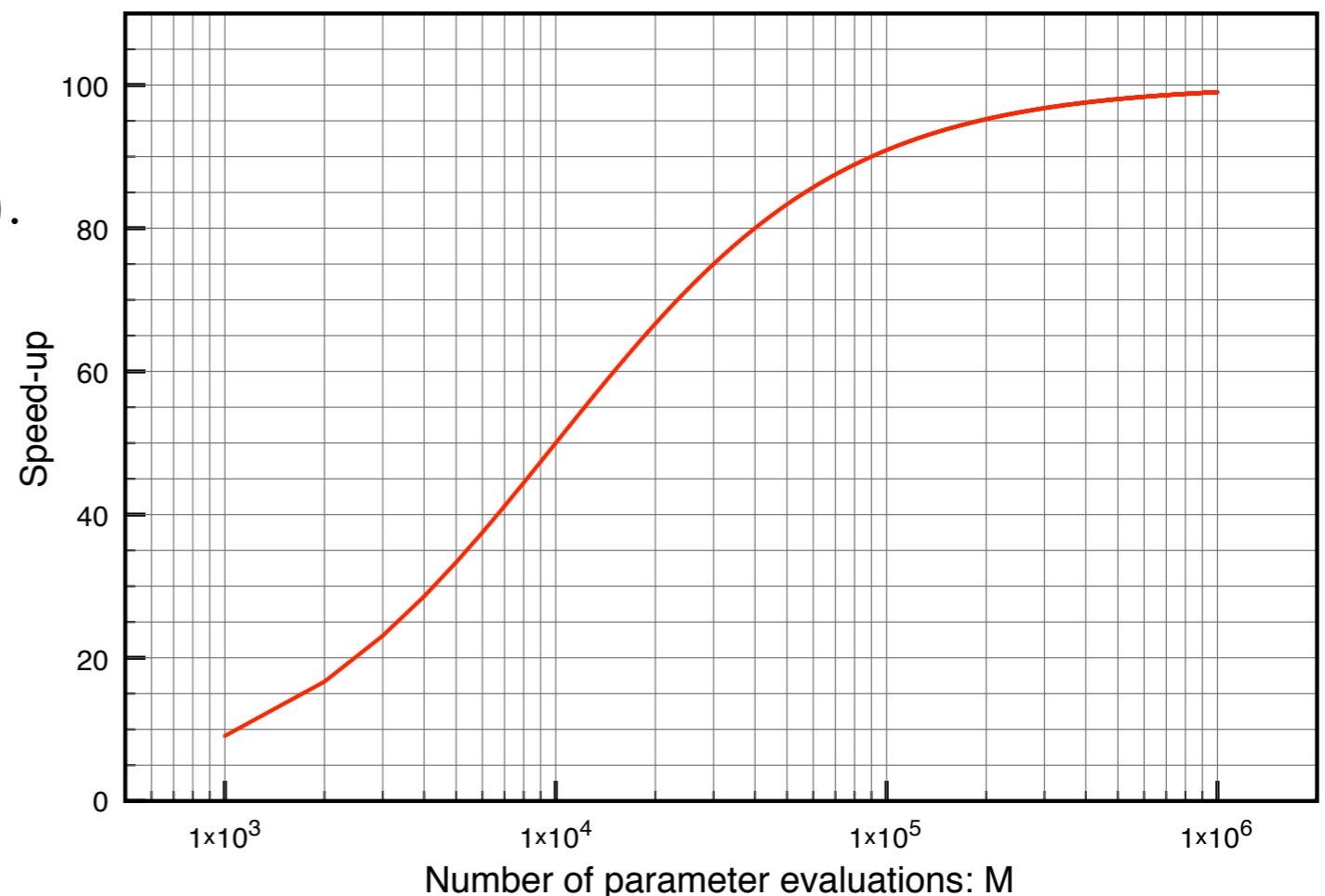
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2. Reduced basis method: $T_{\text{off}} + M \cdot T_{\text{on}}$.

Realistic example:

- $T_{\text{on}} = 1$.
- $T_{\text{tr}} = 10^2$ (realistic speed-up).
- $T_{\text{off}} = 10^4$ ($N = 100$).

Brute force: $M \cdot T_{\text{tr}} = M \cdot 10^2$

RBM: $T_{\text{off}} + M \cdot T_{\text{on}} = 10^4 + M$



The method - so far

Offline procedure:

1. Construct the reduced basis space \mathbb{V}_{rb} empirically based on the weak greedy algorithm using an a posteriori estimator $\eta(\mu)$
2. Precompute the μ -independent matrices \mathbf{A}_{rb}^q and the vectors $\mathbf{f}_{\text{rb}}^q, \mathbf{l}_{\text{rb}}^q$.

Online procedure:

$$\mu \longrightarrow \text{solve for: } u_{\text{rb}}(\mu) \longrightarrow s_{\text{rb}}(\mu) = \ell(u_{\text{rb}}(\mu); \mu)$$

which consists of

1. Assemble

$$\mathbf{A}_{\text{rb}}^{\mu} = \sum_{q=1}^{Q_a} \theta_a^q(\mu) \mathbf{A}_{\text{rb}}^q \quad \mathbf{f}_{\text{rb}}^{\mu} = \sum_{q=1}^{Q_f} \theta_f^q(\mu) \mathbf{f}_{\text{rb}}^q$$

2. Solve $\mathbf{A}_{\text{rb}}^{\mu} u_{\text{rb}}^{\mu} = \mathbf{f}_{\text{rb}}^{\mu}$ (N -dimensional linear system, $N \ll N_{\delta}$)
3. Compute $s_{\text{rb}}(\mu) = \ell(u_{\text{rb}}(\mu); \mu)$
4. Compute the a posteriori error estimator $\eta(\mu)$ to certify the accuracy

$$\|u_{\delta}(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \eta(\mu).$$

Characteristics: Independent of $N_{\delta} = \dim(\mathbb{V}_{\delta})$: cheap. Feasible in a many-query context.

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The a posteriori estimator

So far we assumed the existence of the *a posteriori* estimation process:

$$\mu \longrightarrow \text{solve: } a(u_{\text{rb}}(\mu), v_{\text{rb}}; \mu) = f(v_{\text{rb}}; \mu), \forall v_{\text{rb}} \in \mathbb{V}_{\text{rb}} \longrightarrow \eta(\mu)$$

where $\eta(\mu)$ is an *a posteriori* estimation for $\|u_{\text{rb}}(\mu) - u_{\delta}(\mu)\|_{\mathbb{V}_{\delta}}$.

- o Estimates the discrete error $\|u_{\delta}(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}$ by $\eta(\mu)$: error with respect to the truth approximation $u_{\delta}(\mu)$.
- o Ideal scenario:

$$\|u_{\delta}(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \eta(\mu), \quad \forall \mu \in \mathbb{P}.$$

Certifies the model order reduction error with a computable bound.

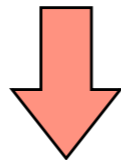
- o Crucial for selection process in weak greedy algorithm. (Off-line)
- o Should be cheap, i.e., independent on $N_{\delta} = \dim(\mathbb{V}_{\delta})$. (Off- and On-line)

Need for speed

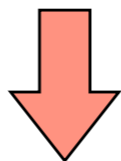
Why only $\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}$?

$$\|u(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \underbrace{\|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}}}_{\text{Error of truth approximation}} + \underbrace{\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}}_{\text{Error of model order reduction}}$$

Error of truth approximation



Given by the approximation space \mathbb{V}_δ

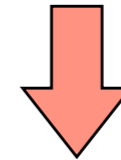


Assumption:

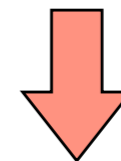
$$\sup_{\mu \in \mathbb{P}} \|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}} \leq \text{tol}$$

by the choice of δ in \mathbb{V}_δ .

Error of model order reduction



Depends on the reduced basis space \mathbb{V}_{rb}



Needs to be estimated

The error estimate

Consider the discrete truth problem

$$A(\mu)u_h(\mu) = f_h(\mu)$$

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Express the solution as

$$u_h = u_N + u_{\perp}$$

$$u_h \in X_h$$

$$u_N \in X_N$$

This results in **the truth problem**

$$\begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \begin{bmatrix} u_N \\ u_{\perp} \end{bmatrix} = \begin{bmatrix} f_{RB} \\ f_{\perp} \end{bmatrix}$$

as well as **the reduced problem**

$$A_{1,1}u_{RB} = f_{RB}$$

The error estimate

This yields the estimate for the error

$$\begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \begin{bmatrix} u_N - u_{RB} \\ u_{\perp} \end{bmatrix} = \begin{bmatrix} 0 \\ f_{\perp} - A_{2,1}u_{RB} \end{bmatrix}$$

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We can recognize the right hand side as

$$\begin{bmatrix} 0 \\ f_{\perp} - A_{2,1}u_{RB} \end{bmatrix} = \begin{bmatrix} f_{RB} - A_{1,1}u_{RB} \\ f_{\perp} - A_{2,1}u_{RB} \end{bmatrix} = f_h - Au_{RB} = R(\mu)$$

and we recover

$$\|u_h(\mu) - u_{RB}(\mu)\| \leq \|A^{-1}(\mu)\| \|R(\mu)\|$$

So with **the residual** and an estimate of **the norm of the inverse of A** we can bound the error

Error estimation

Truth solution: Find $u_\delta(\mu) \in \mathbb{V}_\delta$ such that

$$a(u_\delta(\mu), v_\delta; \mu) = f(v_\delta; \mu), \quad \forall v_\delta \in \mathbb{V}_\delta.$$

RB solution: Find $u_{\text{rb}}(\mu) \in \mathbb{V}_{\text{rb}}$ such that

$$a(u_{\text{rb}}(\mu), v_{\text{rb}}; \mu) = f(v_{\text{rb}}; \mu), \quad \forall v_{\text{rb}} \in \mathbb{V}_{\text{rb}}.$$

Since $\mathbb{V}_{\text{rb}} \subset \mathbb{V}_\delta$, there holds that

$$a(u_\delta(\mu) - u_{\text{rb}}(\mu), v_\delta; \mu) = f(v_\delta; \mu) - a(u_{\text{rb}}(\mu), v_\delta; \mu), \quad \forall v_\delta \in \mathbb{V}_\delta.$$

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Define the error function $e(\mu) \in \mathbb{V}_\delta$ and the residual $r(\cdot; \mu) \in \mathbb{V}'_\delta$ by

$$\begin{aligned} e(\mu) &= u_\delta(\mu) - u_{\text{rb}}(\mu) \in \mathbb{V}_\delta, \\ r(v_\delta; \mu) &= f(v_\delta; \mu) - a(u_{\text{rb}}(\mu), v_\delta; \mu), \quad \forall v_\delta \in \mathbb{V}_\delta. \end{aligned}$$

This establishes the following error equation

$$a(e(\mu), v_\delta; \mu) = r(v_\delta; \mu), \quad \forall v_\delta \in \mathbb{V}_\delta.$$

Error estimation

For coercive problems:

$$\alpha_\delta(\mu) \|v_\delta\|_{\mathbb{V}}^2 \leq a(v_\delta, v_\delta; \mu),$$

with $\alpha_\delta(\mu) \geq \alpha_\delta > 0$.

In consequence

$$\begin{aligned} \underbrace{\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}^2}_{=e(\mu)} &\leq \frac{1}{\alpha_\delta(\mu)} a(e(\mu), e(\mu); \mu) = \frac{1}{\alpha_\delta(\mu)} r(e(\mu); \mu) \\ &= \frac{1}{\alpha_\delta(\mu)} (\hat{r}_\delta(\mu), e(\mu))_{\mathbb{V}} \leq \frac{1}{\alpha_\delta(\mu)} \|\hat{r}_\delta(\mu)\|_{\mathbb{V}} \|e(\mu)\|_{\mathbb{V}} \end{aligned}$$

Thus

$$\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}}{\alpha_\delta(\mu)}$$

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Thus

$$\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}}{\alpha_\delta(\mu)}$$

Computing the stability constant

In the coercive case $\alpha_\delta(\mu)$ is defined by

$$\alpha_\delta(\mu) = \inf_{v_\delta \in \mathbb{V}_\delta} \frac{a(v_\delta, v_\delta; \mu)}{\|v_\delta\|_{\mathbb{V}}^2} = \inf_{v_\delta \in \mathbb{V}_\delta} \frac{a(v_\delta, v_\delta; \mu)}{(v_\delta, v_\delta)_{\mathbb{V}}}.$$

Thus $\alpha_\delta(\mu)$ is the smallest eigenvalue of: find $(\lambda, w_\delta) \in \mathbb{R}^+ \times \mathbb{V}_\delta$ such that

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This can be translated to find the smallest eigenvalue of the generalised eigenvalue problem

$$\mathbf{A}_\delta^\mu \mathbf{v}_\delta = \lambda \mathbf{M}_\delta \mathbf{v}_\delta,$$

where $(\mathbf{A}_\delta^\mu)_{ij} = a(\varphi_j, \varphi_i; \mu)$, $(\mathbf{M}_\delta)_{ij} = (\varphi_j, \varphi_i)_{\mathbb{V}}$ and recall that $\{\varphi_i\}_{i=1}^{N_\delta}$ is a basis of \mathbb{V}_δ .

Depends on N

Computing the stability constant

How to compute $\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}$?

Let

$$\mathbf{r}_\delta^\mu = \mathbf{f}_\delta^\mu - \mathbf{A}_\delta^\mu \mathbf{B} \mathbf{u}_{\text{rb}}^\mu \in \mathbb{R}^{N_\delta},$$

be the residual vector of the N_δ -dimensional linear system

$$\mathbf{A}_\delta^\mu \mathbf{u}_\delta^\mu = \mathbf{f}_\delta^\mu$$

for the truth solution for a particular μ . The quantity $\mathbf{B} \mathbf{u}_{\text{rb}}^\mu$ is the representation of $u_{\text{rb}}(\mu)$ in the basis $\{\varphi_i\}_{i=1}^{N_\delta}$.

Then

$$\|\hat{r}_\delta(\mu)\|_{\mathbb{V}} = \sqrt{(\mathbf{r}_\delta^\mu)^T \mathbf{M}_\delta^{-1} \mathbf{r}_\delta^\mu}.$$

The quantity $\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}$ can thus be computed but the costs depends on N_δ .

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The quantity $\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}$ can thus be computed but the costs depends on N_δ .

Strategy: Use the affine decomposition in combination with pre-computations that are μ -independent.

Computing the stability constant

Let us thus define

$$\eta(\mu) = \frac{\|\hat{r}_\delta(\mu)\|_{\mathbb{V}}}{\alpha_{\text{LB}}(\mu)}$$

Theorem: We just proved that there holds

$$\|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}} \leq \eta(\mu).$$

Theorem: The estimator is efficient

$$\eta(\mu) \leq \frac{\gamma_\delta(\mu)}{\alpha_{\text{LB}}(\mu)} \|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mathbb{V}}.$$

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Proposition. In the compliant case, i.e. $\ell(\cdot; \mu) = f(\cdot; \mu)$ and a symmetric, there holds that

$$s_\delta(\mu) - s_{\text{rb}}(\mu) = \|u_\delta(\mu) - u_{\text{rb}}(\mu)\|_{\mu}^2,$$

for all $\mu \in \mathbb{P}$.

Computing the stability constant

Recall:

$$\alpha_\delta(\mu) := \inf_{v_\delta \in \mathbb{V}_\delta} \frac{a(v_\delta, v_\delta; \mu)}{\|v_\delta\|_{\mathbb{V}}^2}.$$

Goal: Design an off-line/on-line procedure where the on-line part consists of

$$\mu \rightarrow \alpha_{\text{LB}}(\mu)$$

such that $0 < \alpha_{\text{LB}}(\mu) \leq \alpha_\delta(\mu)$ and in a fashion that is independent of N_δ .

$\alpha_\delta(\mu)$ is the smallest eigenvalue of: find $(\lambda, w_\delta) \in \mathbb{R}^+ \times \mathbb{V}_\delta$ such that

$$a(w_\delta, v_\delta; \mu) = \lambda (w_\delta, v_\delta)_{\mathbb{V}}, \quad \forall v_\delta \in \mathbb{V}_\delta.$$

which can be translated to find the smallest eigenvalue of the generalised eigenvalue problem

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where $(\mathbf{A}_\delta^\mu)_{ij} = a(\varphi_j, \varphi_i; \mu)$, $(\mathbf{M}_\delta)_{ij} = (\varphi_j, \varphi_i)_{\mathbb{V}}$ and recall that $\{\varphi_i\}_{i=1}^{N_\delta}$ is a basis of \mathbb{V}_δ .

Computing the stability constant

Special case: If the decomposition

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

is such that

$$\begin{aligned} \theta_a^q(\mu) &> 0, & \forall \mu \in \mathbb{P}, \quad q = 1, \dots, Q_a, \\ a_q(v_\delta, v_\delta) &\geq 0, & \forall v_\delta \in \mathbb{V}_\delta, \quad q = 1, \dots, Q_a. \end{aligned}$$

we call the bilinear form $a(\cdot, \cdot; \mu)$ to be **parametrically coercive**.

Example: Heat conduction on thermal blocks

$$\begin{aligned} a(w, v; \mu) &= \sum_{q=1}^{15} \mu_q \int_{\mathcal{R}_q} \nabla w \cdot \nabla v + \int_{\mathcal{R}_{16}} \nabla w \cdot \nabla v, \\ a_q(w, v; \mu) &= \int_{\mathcal{R}_q} \nabla w \cdot \nabla v, & \theta_a^q(\mu) &= \mu_q, & q &= 1, \dots, 15, \\ a_{16}(w, v; \mu) &= \int_{\mathcal{R}_{16}} \nabla w \cdot \nabla v, & \theta_a^{16}(\mu) &= 1, \end{aligned}$$

Computing the stability constant

Develop

$$\begin{aligned}\alpha_\delta(\mu) &= \inf_{v_\delta \in \mathbb{V}_\delta} \frac{a(v_\delta, v_\delta; \mu)}{\|v_\delta\|_{\mathbb{V}}^2} \\ &= \inf_{v_\delta \in \mathbb{V}_\delta} \sum_{q=1}^{Q_a} \theta_a^q(\mu) \frac{a_q(v_\delta, v_\delta)}{\|v_\delta\|_{\mathbb{V}}^2} \\ &= \inf_{v_\delta \in \mathbb{V}_\delta} \sum_{q=1}^{Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')} \theta_a^m(\mu') \frac{a_q(v_\delta, v_\delta)}{\|v_\delta\|_{\mathbb{V}}^2} \\ &\geq \inf_{v_\delta \in \mathbb{V}_\delta} \min_{q=1, \dots, Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')} \sum_{q=1}^{Q_a} \theta_a^q(\mu') \frac{a_q(v_\delta, v_\delta)}{\|v_\delta\|^2} \\ &= \min_{q=1, \dots, Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')} \inf_{v_\delta \in \mathbb{V}_\delta} \sum_{q=1}^{Q_a} \theta_a^q(\mu') \frac{a_q(v_\delta, v_\delta)}{\|v_\delta\|_{\mathbb{V}}^2} \\ &= \alpha_\delta(\mu') \min_{q=1, \dots, Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')} := \alpha_{\text{LB}}(\mu).\end{aligned}$$

Then

$$\alpha_{\text{LB}}(\mu) := \underbrace{\alpha_\delta(\mu') \min_{q=1, \dots, Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')}}_{\in (0, \infty)} \leq \alpha_\delta(\mu).$$

Computing the stability constant

Min- Θ approach

$$\alpha_{\text{LB}}(\mu) := \underbrace{\alpha_{\delta}(\mu') \min_{q=1, \dots, Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu')}}_{\in (0, \infty)} \leq \alpha_{\delta}(\mu).$$

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Multiple anchor points

$$\alpha_{\text{LB}}(\mu) = \max_{k=1,\dots,K} \left(\alpha_{\delta}(\mu_k) \min_{q=1,\dots,Q_a} \frac{\theta_a^q(\mu)}{\theta_a^q(\mu_k)} \right).$$

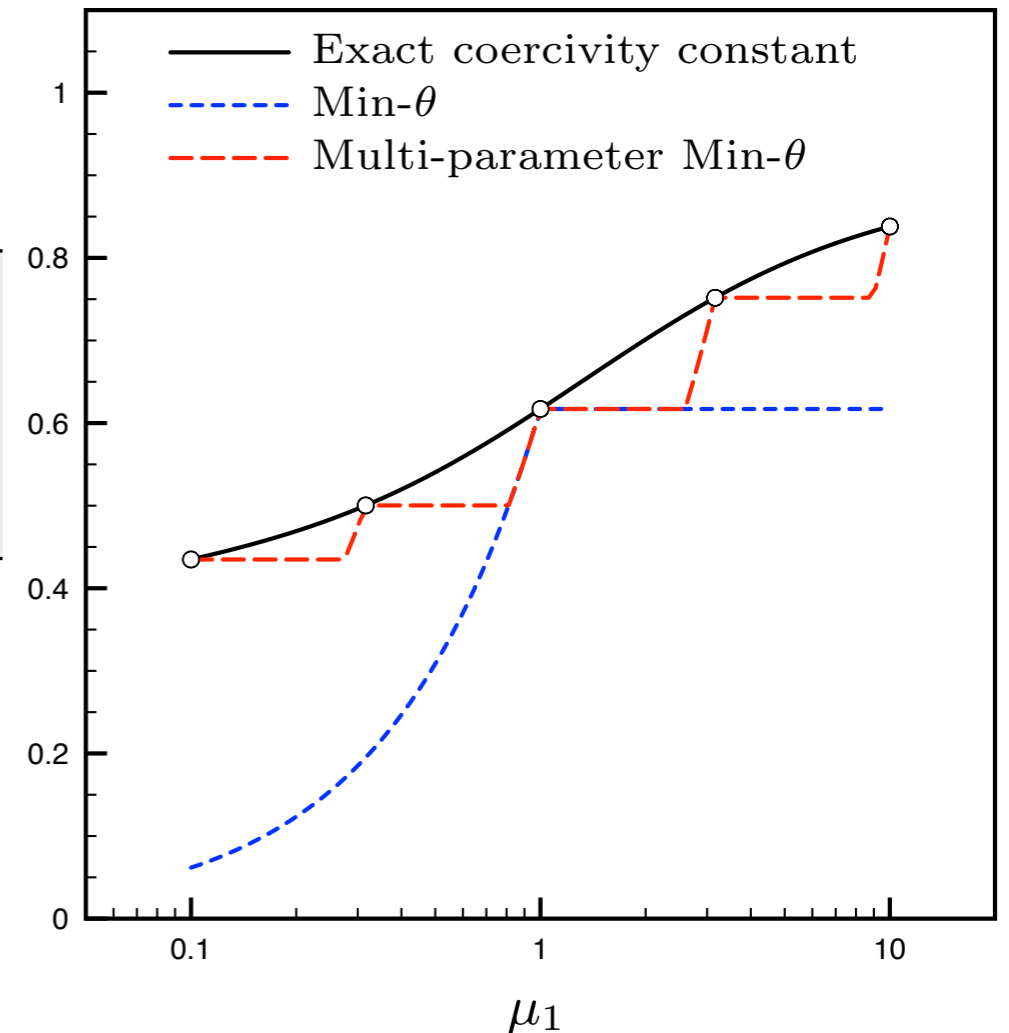
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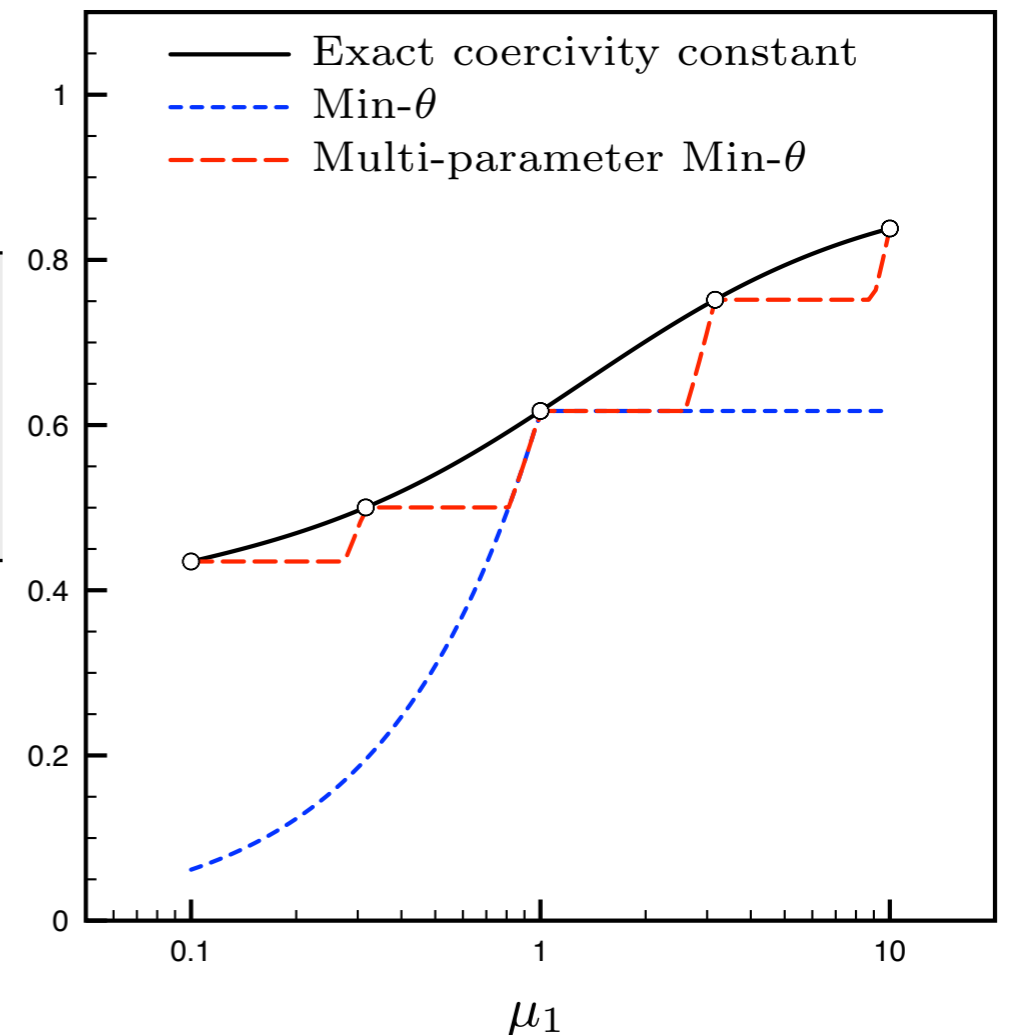
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Limited and not very accurate

Computing the stability constant (SCM)

Consider the coercive case (for simplicity)

$$\alpha(\mu) = \inf_{v_h \in X_h} \frac{a_h(v_h, \mu, v_h)}{\|v_h\|^2} = \inf_{v_h \in X_h} \sum_{k=1}^{Q_a} \Theta_k^a(\mu) \frac{a_k(v_h, v_h)}{\|v_h\|^2}$$

and define

$$\mathcal{Y} = \left\{ y \in \mathbb{R}^{Q_a} \mid \exists w_h \in X_h; y_k = \frac{a_k(w_h, w_h)}{\|w_h\|^2} \right\}$$

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If we have

$$\mathcal{J} : \mathbb{R}^{Q_a} \times \mathcal{D} \rightarrow \mathbb{R} \quad \mathcal{J}(y, \mu) = \sum_{k=1}^{Q_a} Q_k^a(\mu) y_k$$

then

$$\alpha(\mu) = \min_{y \in \mathcal{Y}} \mathcal{J}(y, \mu)$$

Computing the stability constant (SCM)

Strategy: Find upper and lower bounds such that

$$\mathcal{Y}_{UB} \subset \mathcal{Y} \subset \mathcal{Y}_{LB}$$

and define

$$\alpha_{LB}(\boldsymbol{\mu}) = \min_{\boldsymbol{y} \in \mathcal{Y}_{LB}} \mathcal{I}(\boldsymbol{\mu}; \boldsymbol{u}) \quad \alpha_{UB}(\boldsymbol{\mu}) = \min_{\boldsymbol{y} \in \mathcal{Y}_{UB}} \mathcal{I}(\boldsymbol{\mu}; \boldsymbol{u}),$$

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Introduce

$$1 \leq k \leq Q_a \quad \sigma_k^- = \inf_{v_h \in X_h} \frac{a_k(v_h, v_h)}{\|v_h\|^2}$$
$$\sigma_k^+ = \sup_{v_h \in X_h} \frac{a_k(v_h, v_h)}{\|v_h\|^2}$$

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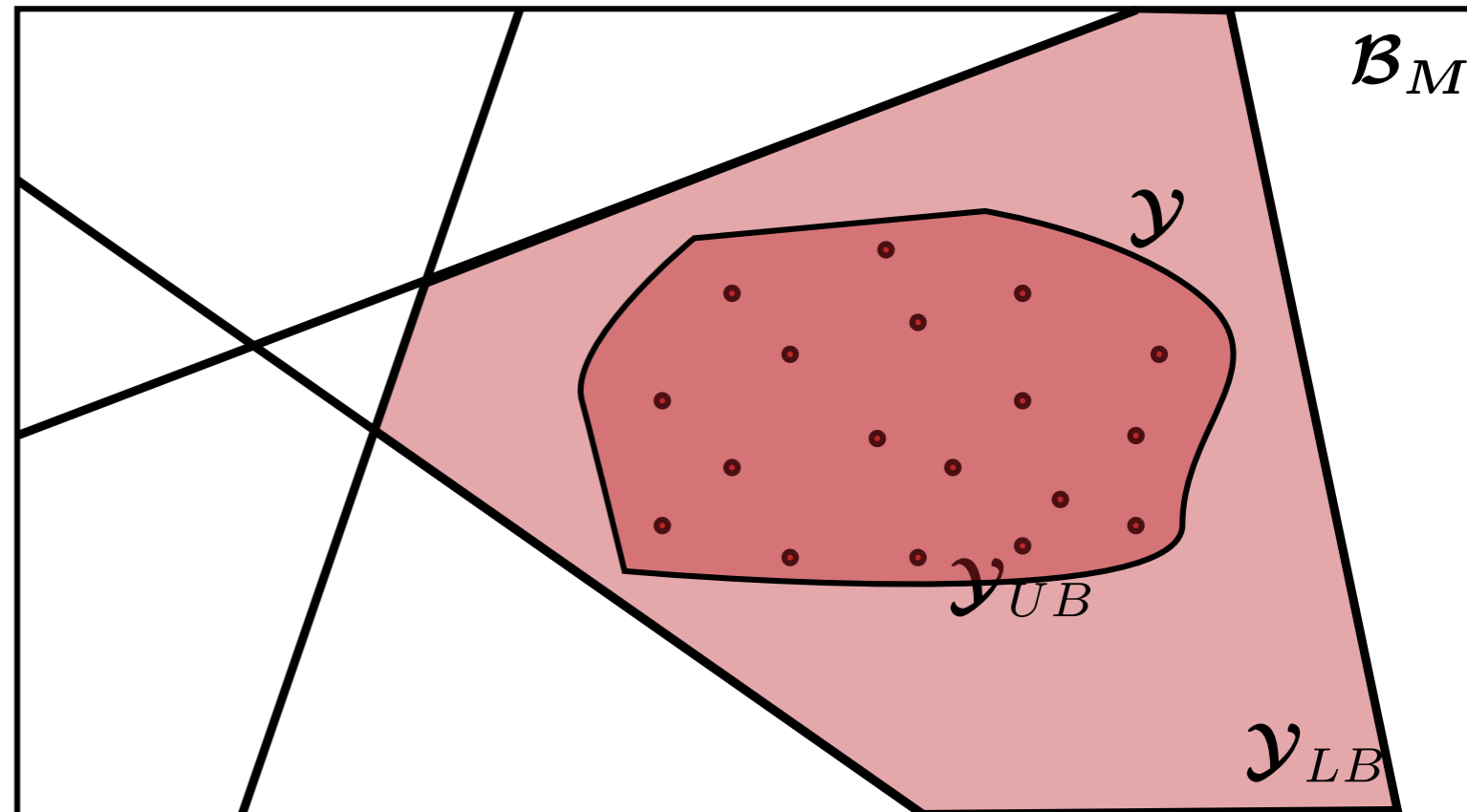
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Introduce

$$1 \leq k \leq Q_a \quad \sigma_k^- = \inf_{v_h \in X_h} \frac{a_k(v_h, v_h)}{\|v_h\|^2}$$

$$\sigma_k^+ = \sup_{v_h \in X_h} \frac{a_k(v_h, v_h)}{\|v_h\|^2}$$

$$\mathcal{B} = \prod_{k=1}^{Q_a} [\sigma_k^-, \sigma_k^+]$$



Computing the stability constant (SCM)

Algorithm: Offline-procedure of the SCM

Input: An error tolerance Tol , some initial set $\mathbb{C}_1 = \{\mu_1\}$ and $n = 1$

Output: The sample points $\mathbb{C}_N = \{\mu_1, \dots, \mu_N\}$, the corresponding coercivity constants $\alpha_\delta(\mu_n)$ and vectors y^n , $n = 1, \dots, N$, as well as the lower bounds $\alpha_{\text{LB}}^N(\mu)$ for all $\mu \in \Xi_a$.

1. For each $\mu \in \Xi_a$:
 - a. Compute the upper bound $\alpha_{\text{UB}}^n(\mu) = \min_{y \in \mathcal{Y}_{\text{UB}}^n} \mathbf{S}(\mu, y)$.
 - b. Compute the lower bound $\alpha_{\text{LB}}^n(\mu) = \min_{y \in \mathcal{Y}_{\text{LB}}^n(\mu)} \mathbf{S}(\mu, y)$.
 - c. Define the error estimate $\eta(\mu; \mathbb{C}_n) = 1 - \frac{\alpha_{\text{LB}}^n(\mu)}{\alpha_{\text{UB}}^n(\mu)}$.
2. Select $\mu_{n+1} = \operatorname{argmax}_{\mu \in \mathbb{P}} \eta(\mu; \mathbb{C}_n)$ and set $\mathbb{C}_{n+1} = \mathbb{C}_n \cup \{\mu_{n+1}\}$.
3. If $\max_{\mu \in \mathbb{P}} \eta(\mu; \mathbb{C}_n) \leq \text{Tol}$, **terminate**.
4. Solve the generalized eigenvalue problem (4.26) associated with μ_{n+1} , store $\alpha_\delta(\mu_{n+1})$, y^{n+1} .
5. Set $n := n + 1$ and **goto 1**.

Online part

$$\alpha_{\text{LB}}(\mu) = \min_{y \in \mathcal{Y}_{\text{LB}}(\mu)} \mathbf{S}(\mu, y),$$

Computing the stability constant (SCM)

The upper bound

Assumption: We know the coercivity constant $\alpha(\omega_i)$ for a given point set $C_K = \{\omega_1, \dots, \omega_K\}$

Then define

$$\mathcal{Y}_{UB}(C_K) = \{y^*(\omega_k) | 1 \leq k \leq K\}, \quad y^*(\mu) = \arg \inf_{y \in \mathcal{Y}} \mathcal{I}(\mu, y)$$

Greedy by

$$1 - \frac{\alpha_{LB}(\mu)}{\alpha_{UB}(\mu)},$$

Computing the stability constant (SCM)

The upper bound

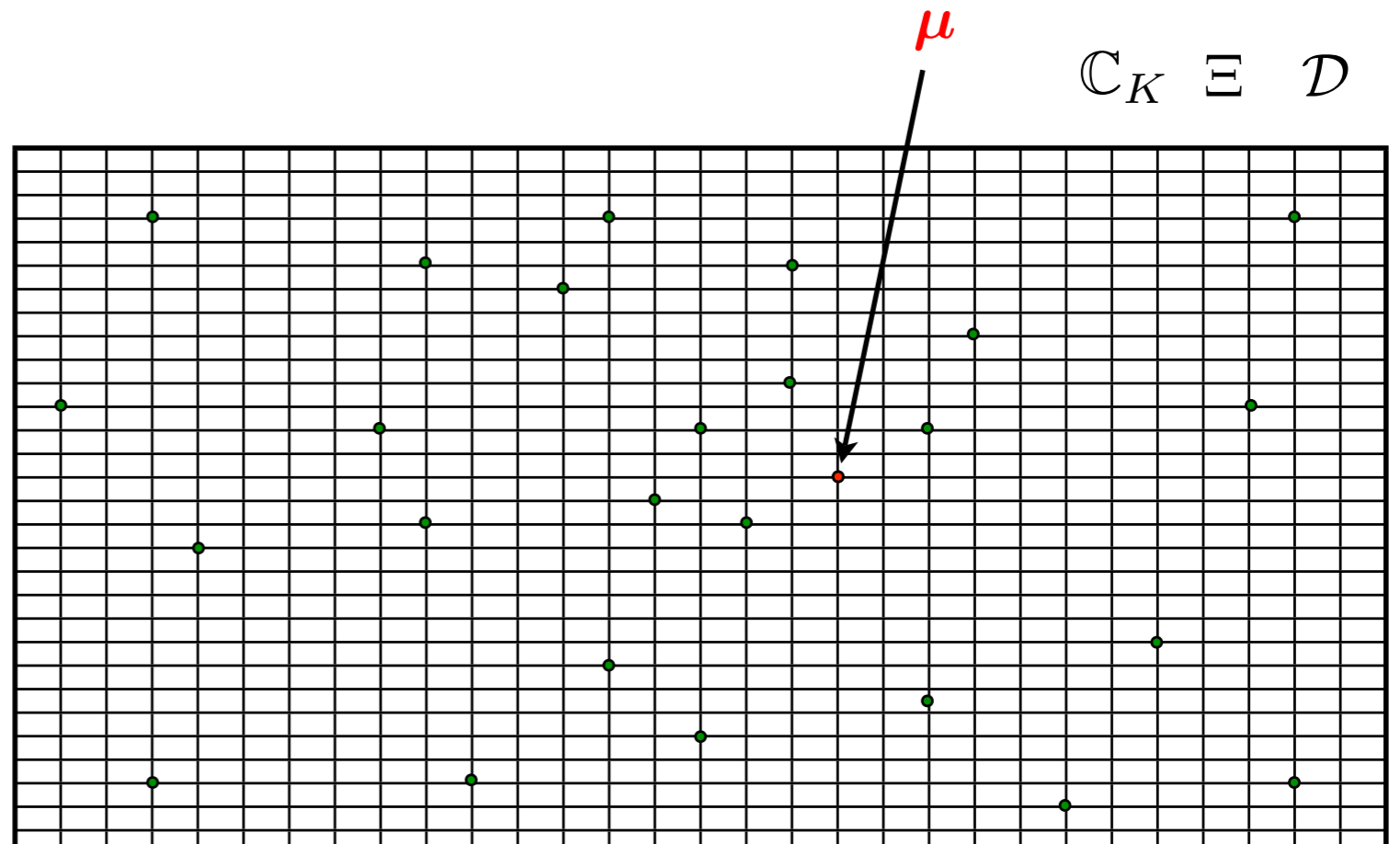
Assumption: We know the coercivity constant $\alpha(\omega_i)$ for a given point set $C_K = \{\omega_1, \dots, \omega_K\}$

Then define

$$\mathcal{Y}_{UB}(C_K) = \{y^*(\omega_k) \mid 1 \leq k \leq K\}, \quad y^*(\mu) = \arg \inf_{y \in \mathcal{Y}} \mathcal{I}(\mu, y)$$

Greedy by

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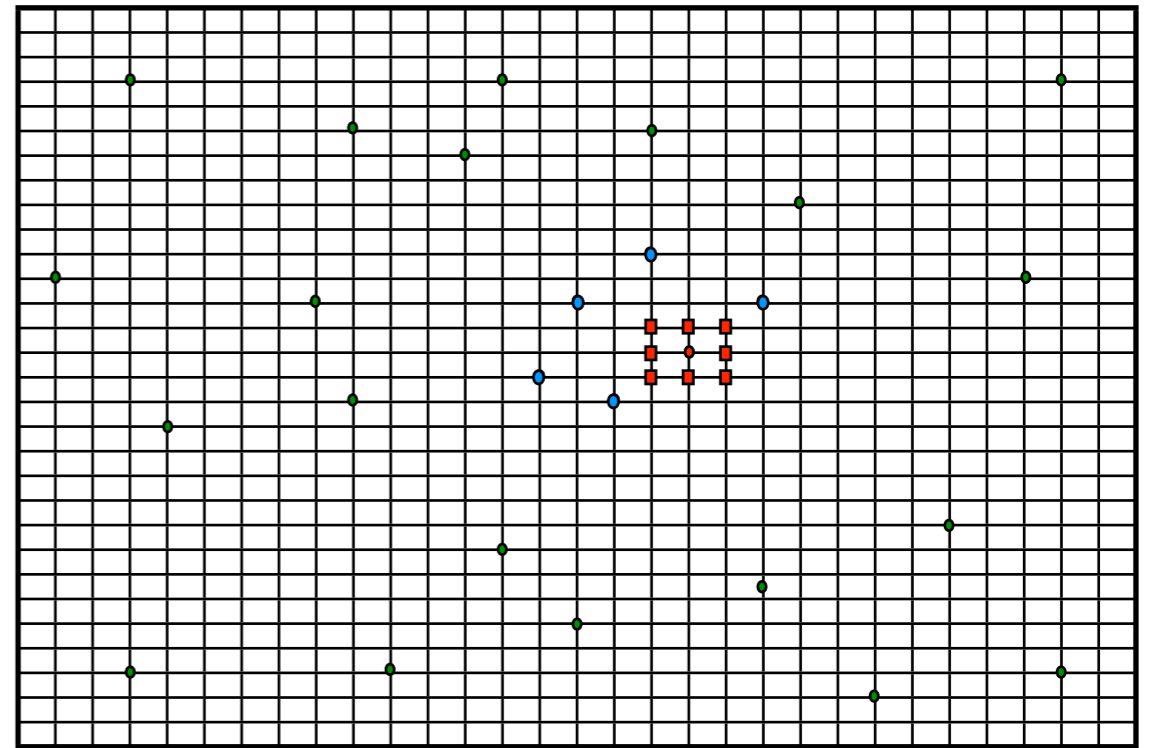
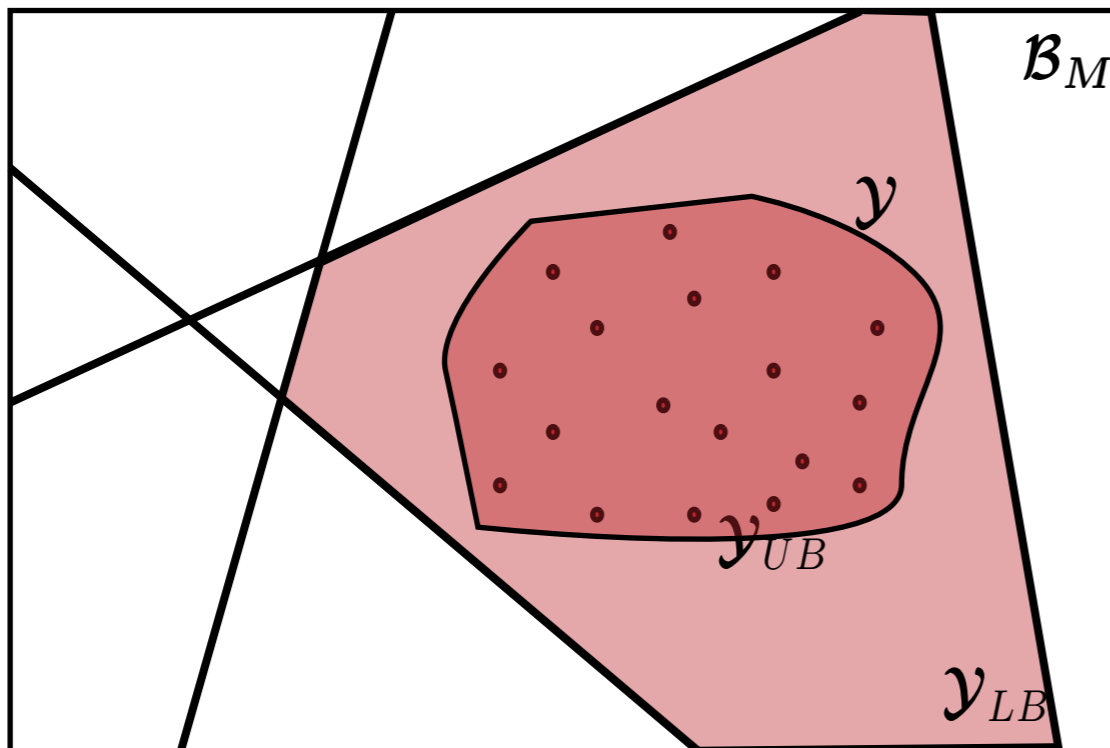


Computing the stability constant (SCM)

The lower bound is found through

$$\mathcal{Y}_{LB}(\mu; \mathbb{C}_K) = \left\{ \mathbf{y} \in \mathcal{B}_M \left| \begin{array}{l} \sum_{m=1}^M \Theta^m(\mu') \mathbf{y}_m \geq \alpha_h(\mu'), \quad \forall \mu' \in \mathbb{P}_{M_\alpha}(\mu; \mathbb{C}_K) \\ \sum_{m=1}^M \Theta^m(\mu') \mathbf{y}_m \geq 0, \quad \forall \mu' \in \mathbb{P}_{M_+}(\mu; \Xi) \end{array} \right. \right\}$$

$\mathbb{C}_K \quad \Xi \quad \mathcal{D}$



Computing the stability constant (SCM)

The upper and lower bound computation requires

- ✓ Local minimization to compute upper bound
- ✓ Linear programming problem to compute lower bound

Computing the stability constant (SCM)

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Complexity is independent of \mathcal{N}

Computing the stability constant (SCM)

The upper and lower bound computation requires

- ✓ Local minimization to compute upper bound
- ✓ Linear programming problem to compute lower bound

Complexity is independent of \mathcal{N}

Set \mathbb{C}_K is computed through greedy approach by minimizing difference between upper and lower bound estimate

$$\text{Find } \Omega_{K+1} = \arg \max_{\mu \in \Xi} \frac{\alpha_{UB}(\mu; \mathbb{C}_K) - \alpha_{LB}(\mu; \mathbb{C}_K)}{\alpha_{UB}(\mu; \mathbb{C}_K)}.$$

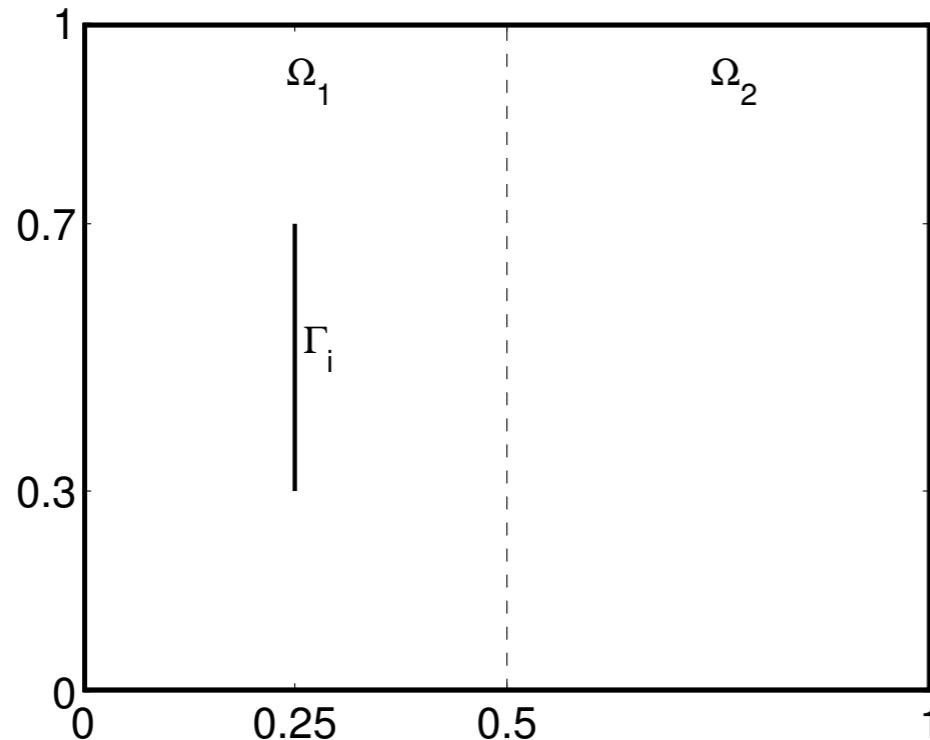
$$\text{Update } \mathbb{C}_{K+1} = \mathbb{C}_K \cup \omega_{K+1}$$

Lets see if it works

In the first examples, the lower bound on the stability does not play an essential role.

Lets see if it works

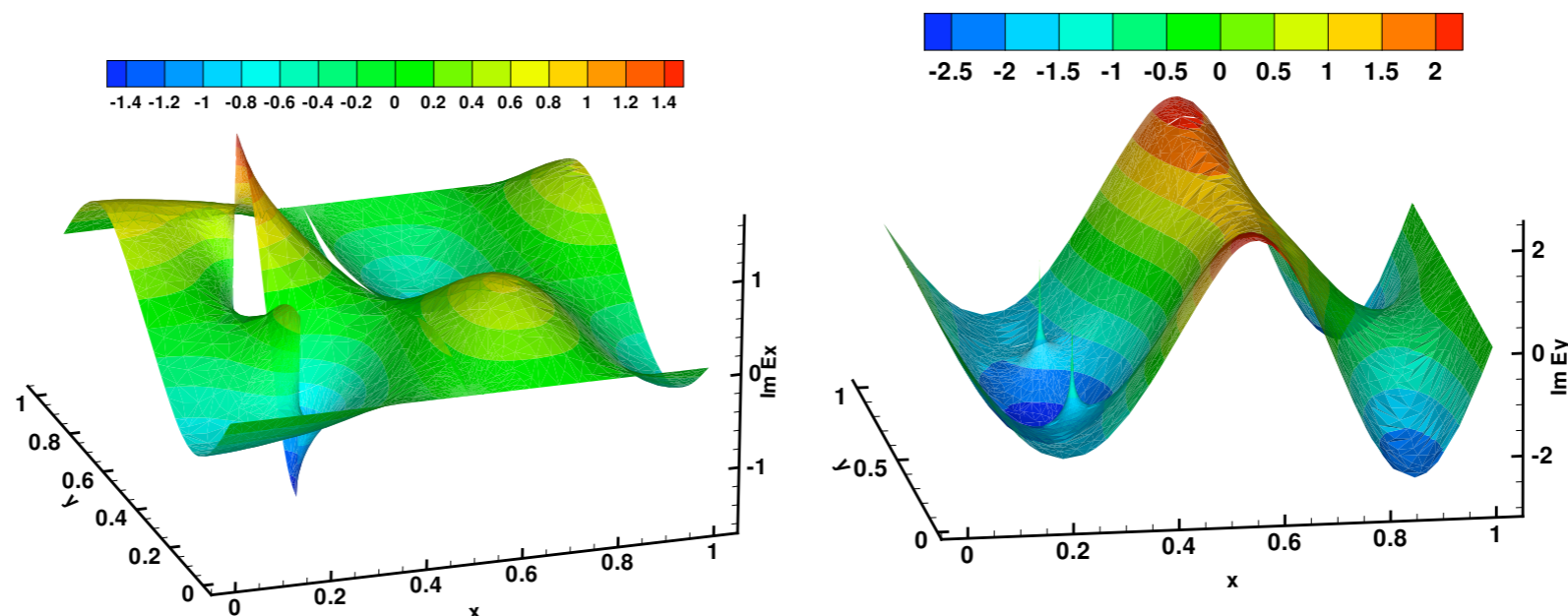
In the first examples, the lower bound on the stability does not play an essential role.



2D EM problem

Parameters are material properties in right half

$$s = \int_{\Omega_2} E_x + E_y dx$$

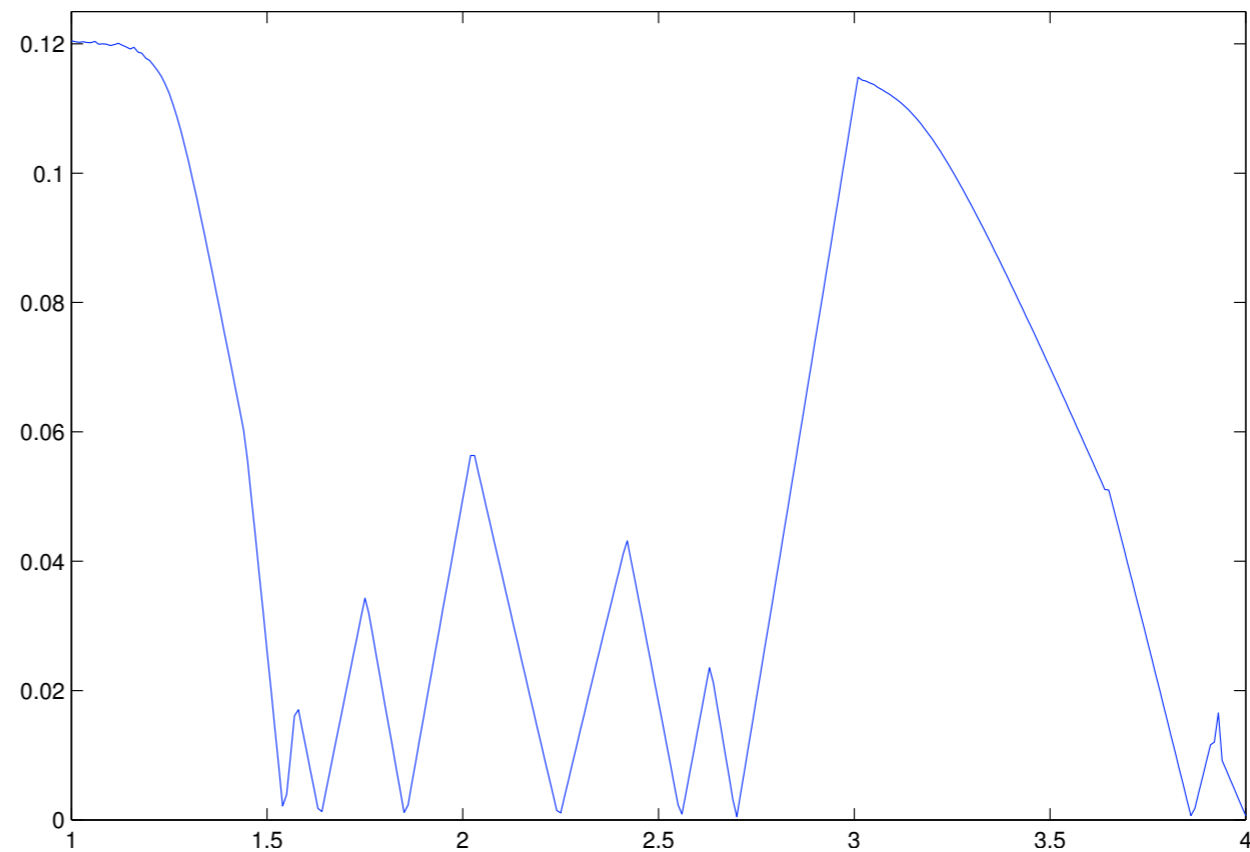


Lets see if it works

This is in fact a hard problem

$\varepsilon_2 : \omega = 5\pi/2$ is a resonance
1.5434
1.6357
1.8532
2.2456
2.5569
2.6983
3.8615
4.0033

(a) Resonances.



(b) $\beta^{pd}(\mu)$.

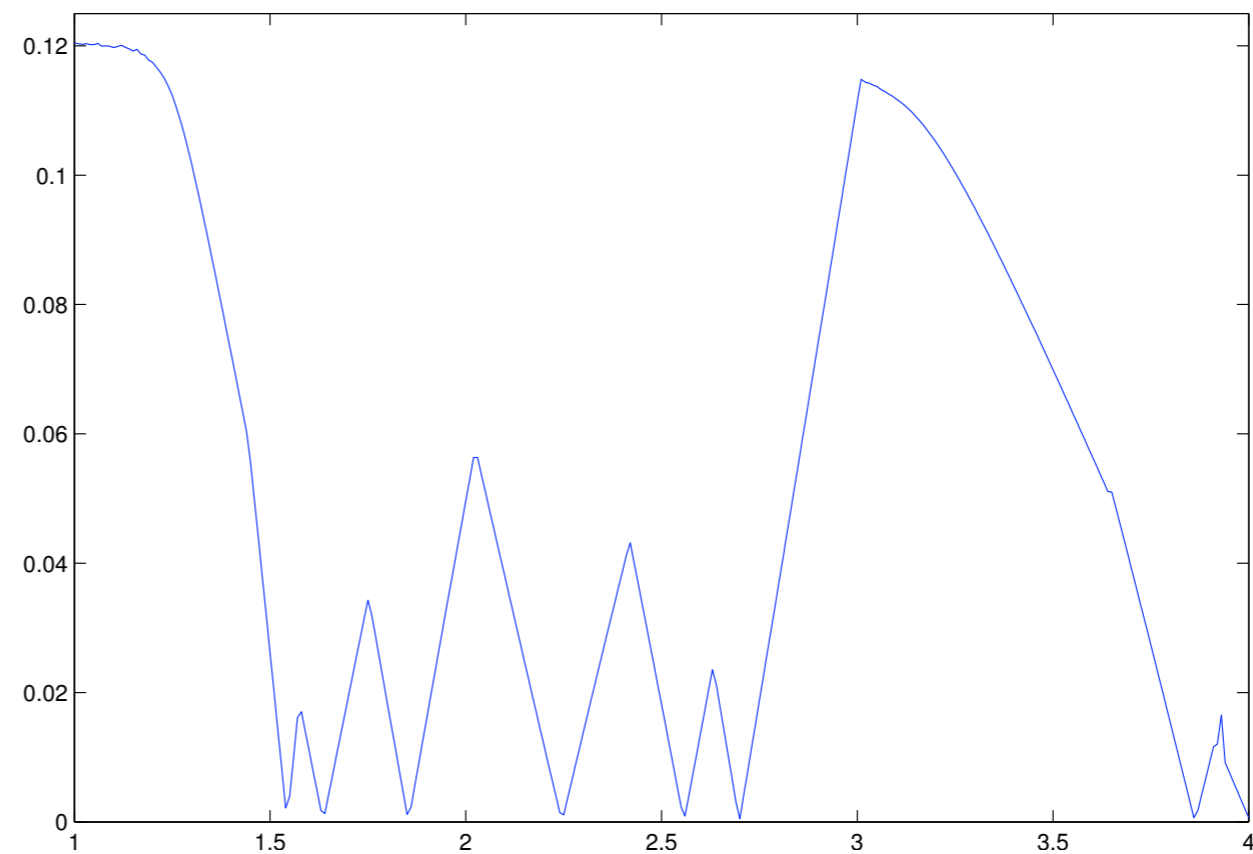
$\mathcal{N} = 11884$, 4th order, 282 elements

Lets see if it works

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1.5434
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(a) Resonances.



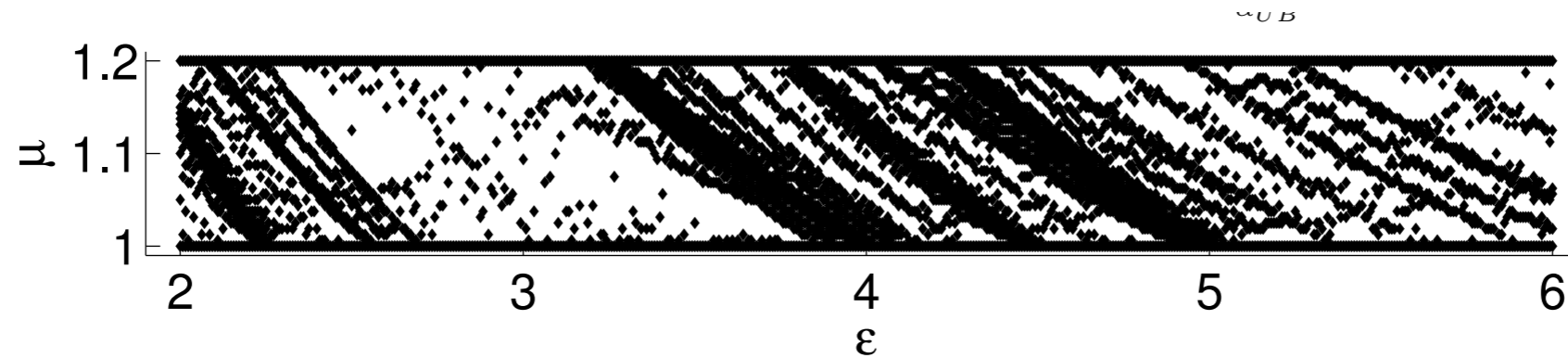
(b) $\beta^{pd}(\mu)$.

$\mathcal{N} = 11884$, 4th order, 282 elements

In this case the stability constant is important

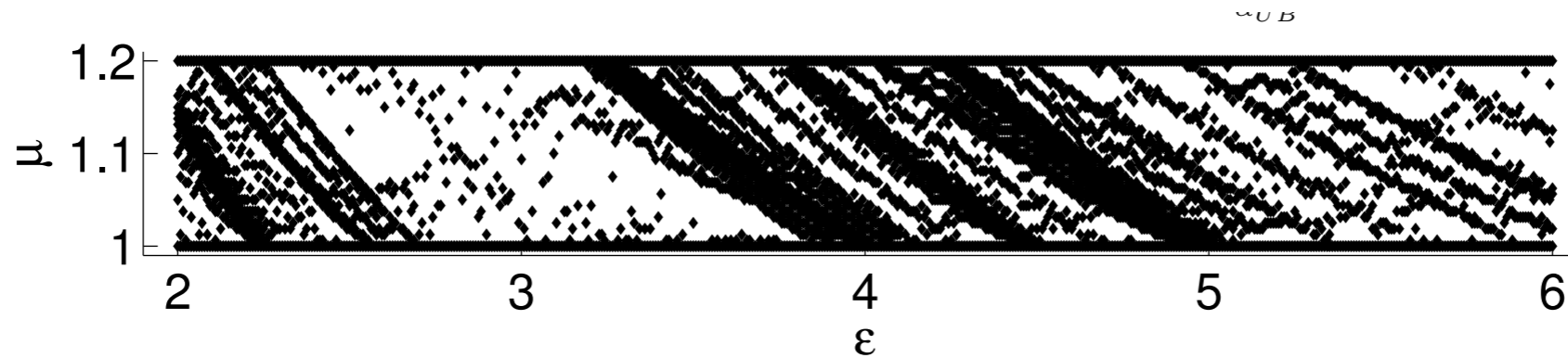
Lets see if it works

Point sets computed for lower-bound computation

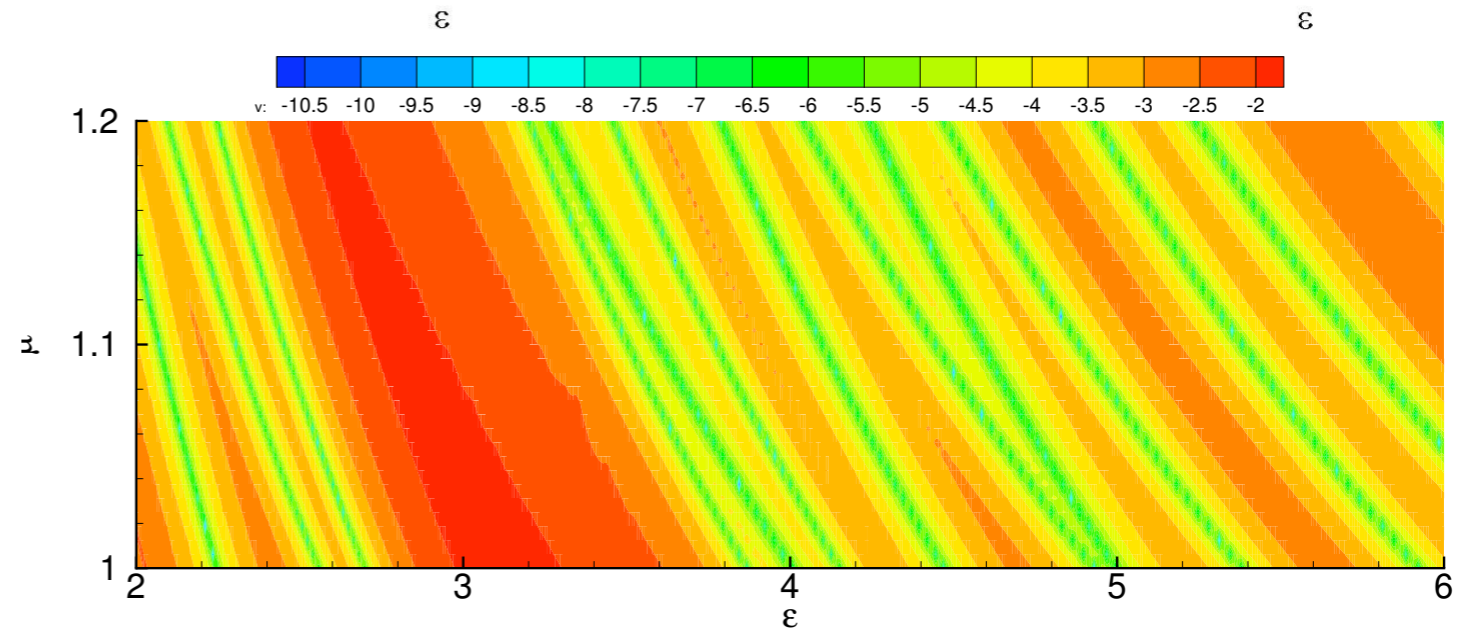


Lets see if it works

Point sets computed for lower-bound computation

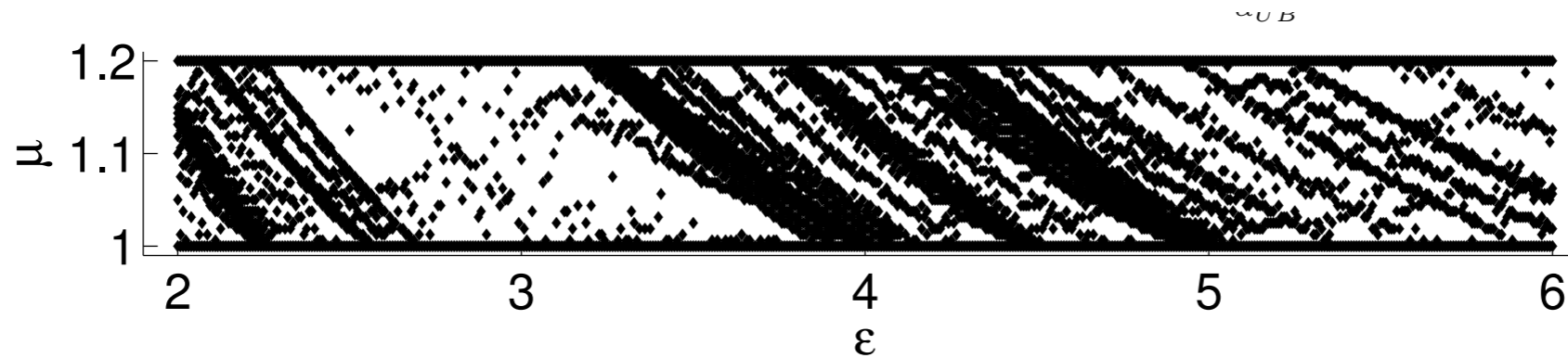


Lower bound
approximation

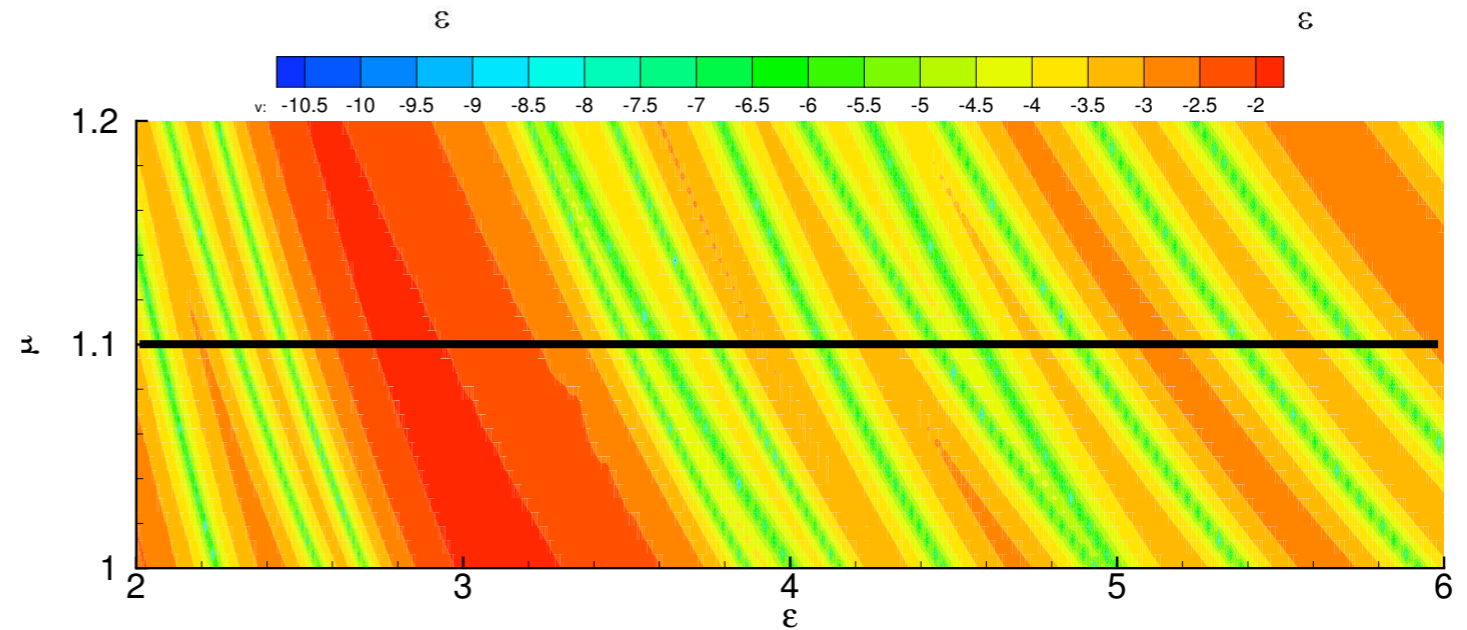


Lets see if it works

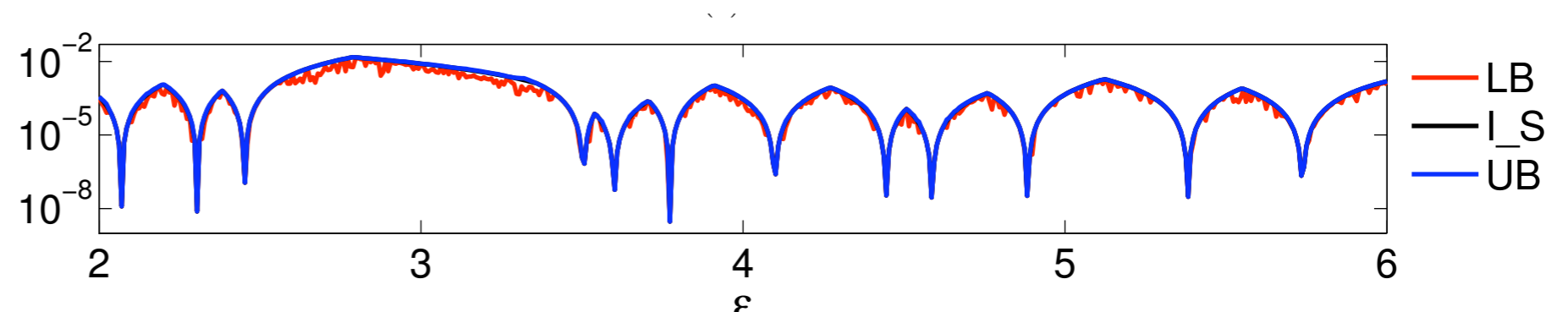
Point sets computed for lower-bound computation



Lower bound approximation

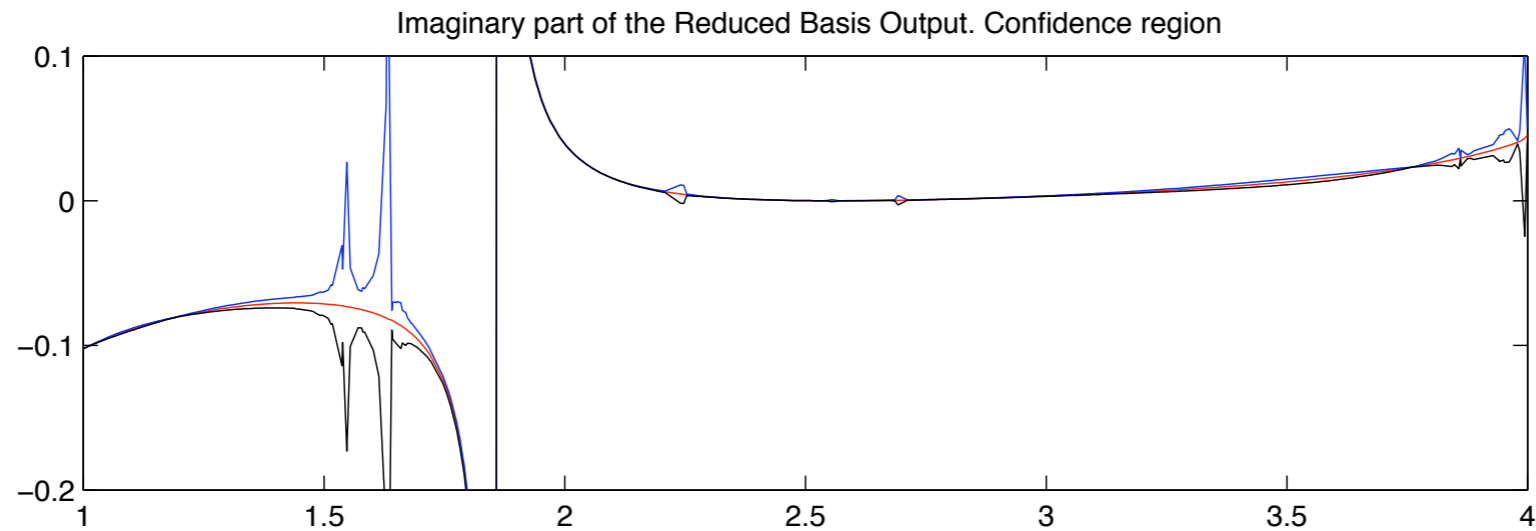


Accuracy

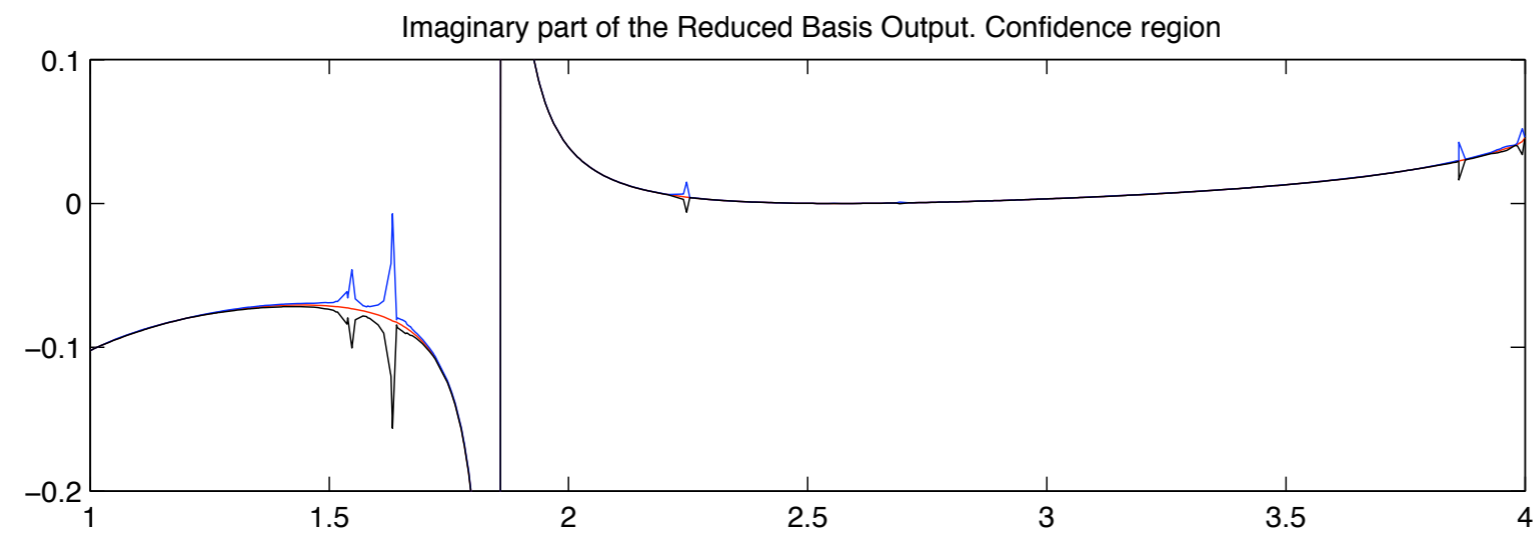


Lets see if it works

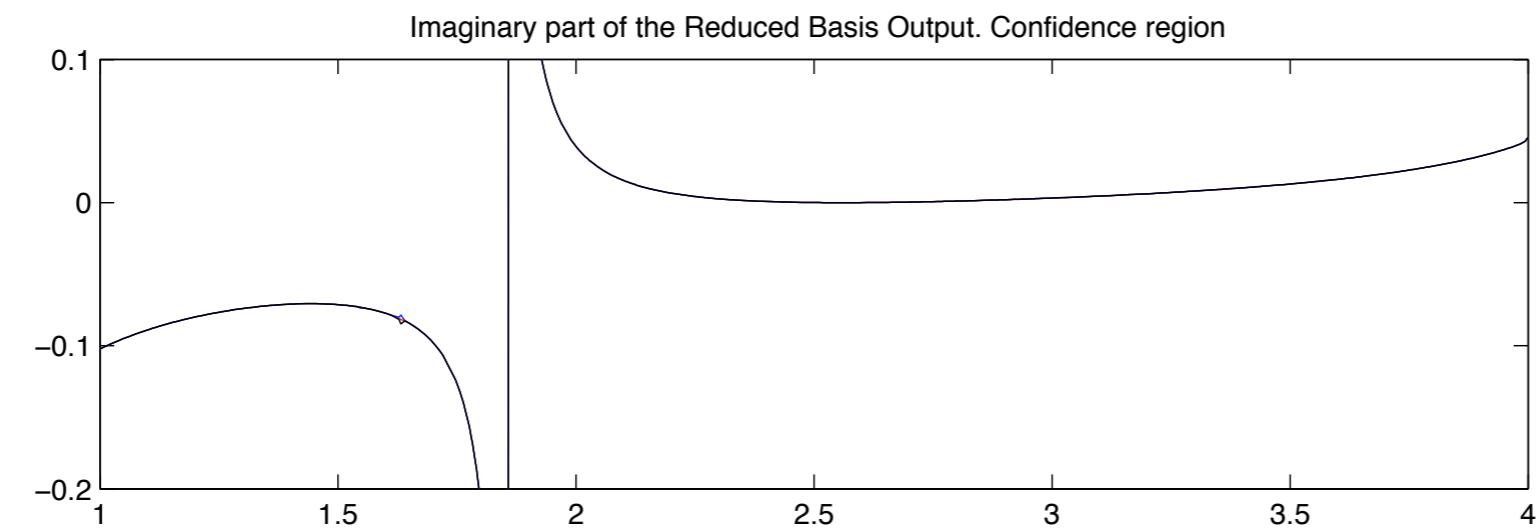
N=10



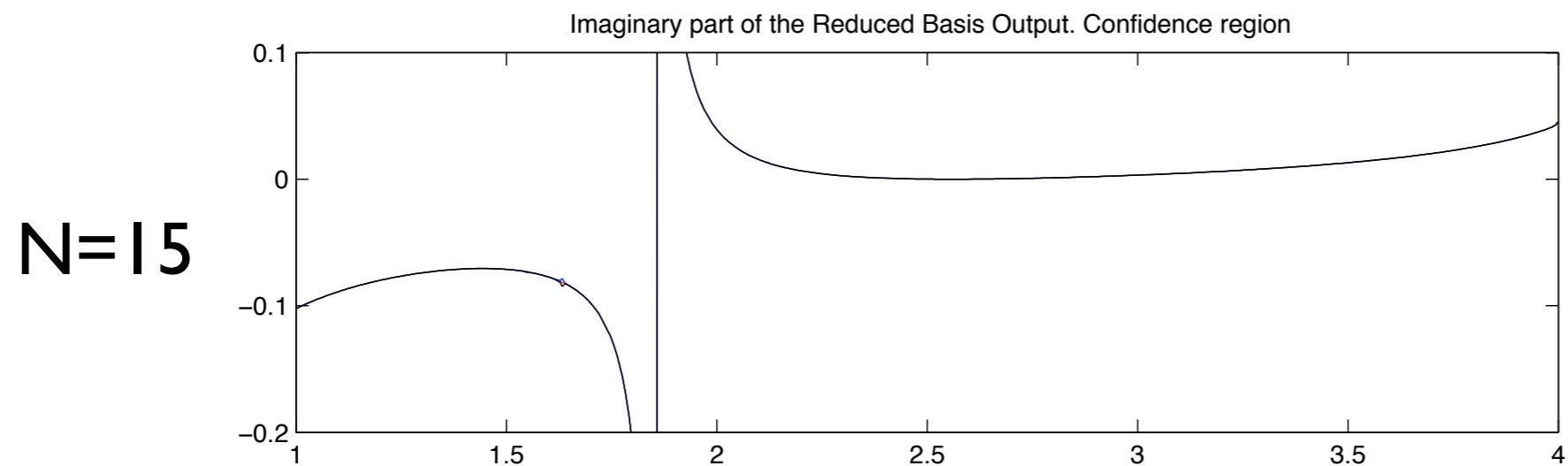
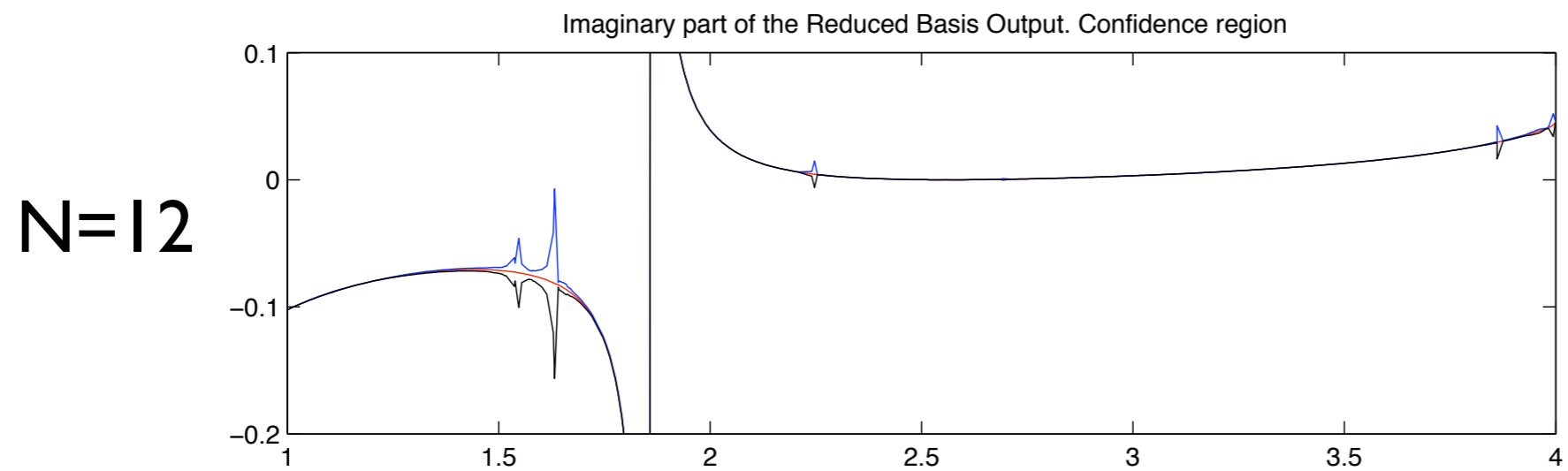
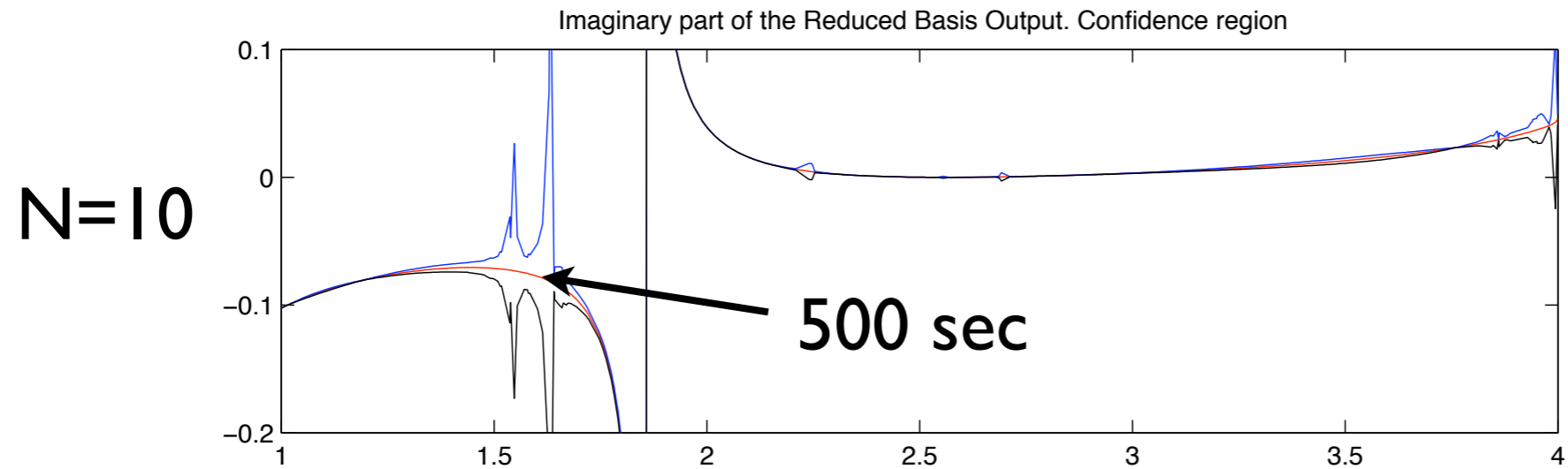
N=12



N=15

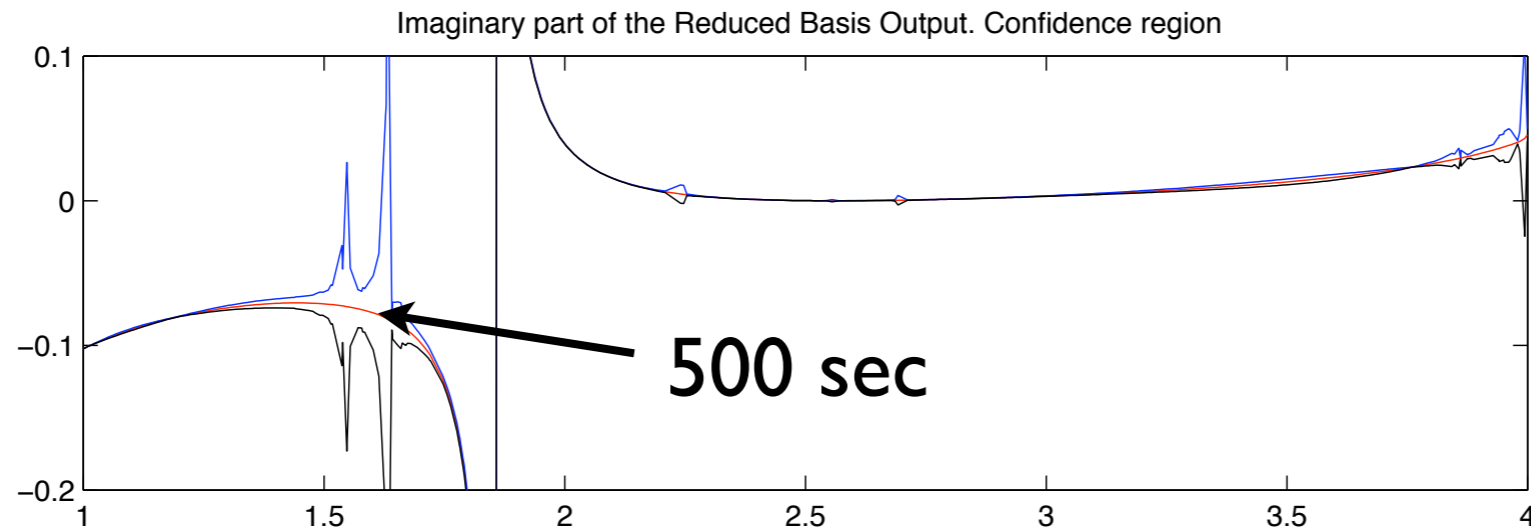


Lets see if it works



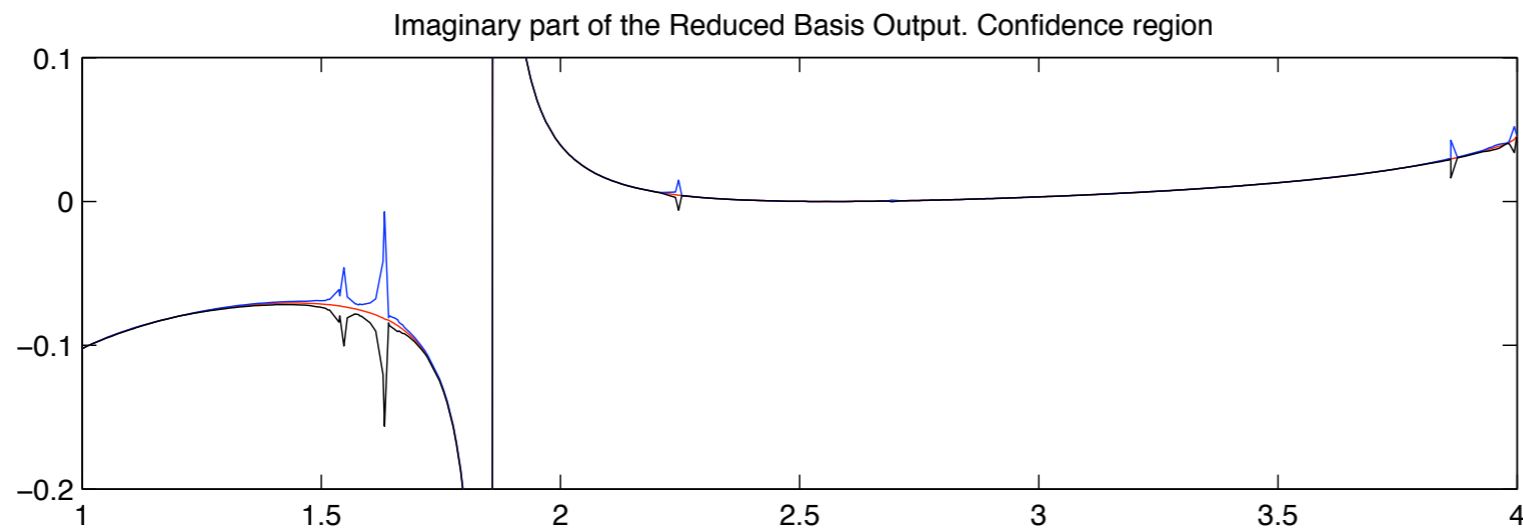
Lets see if it works

N=10

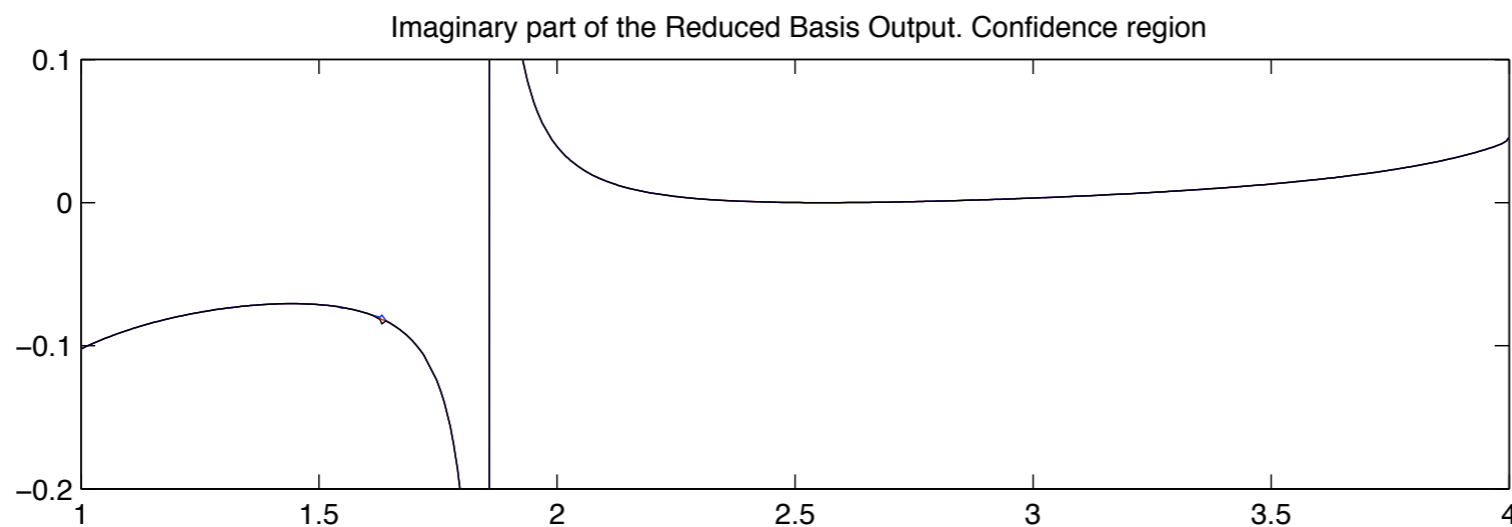


0.25 sec

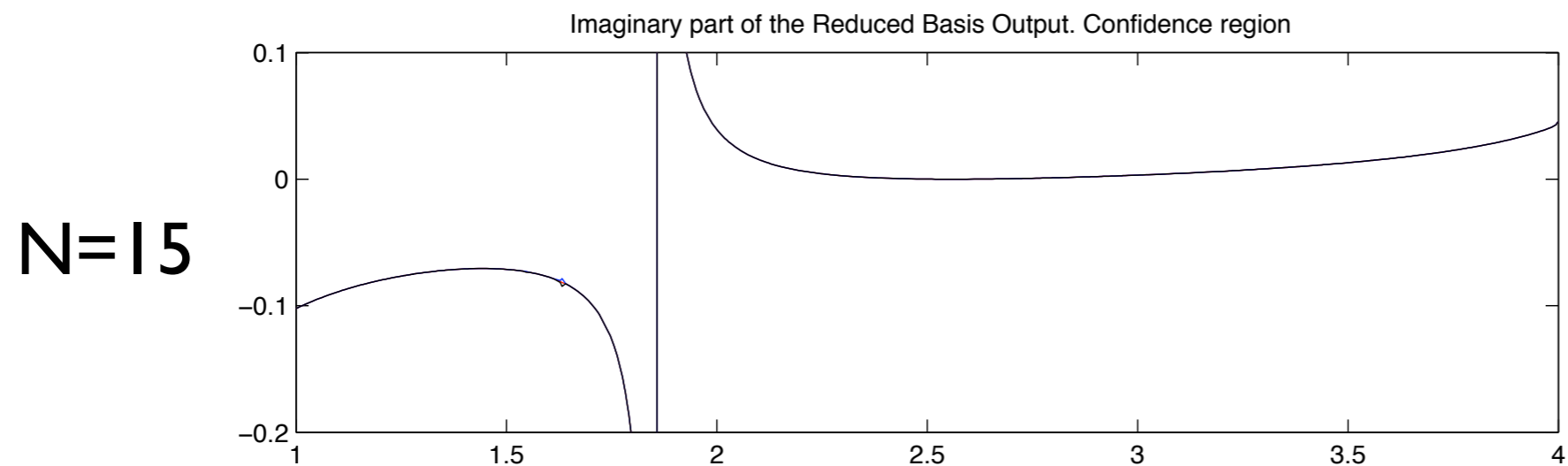
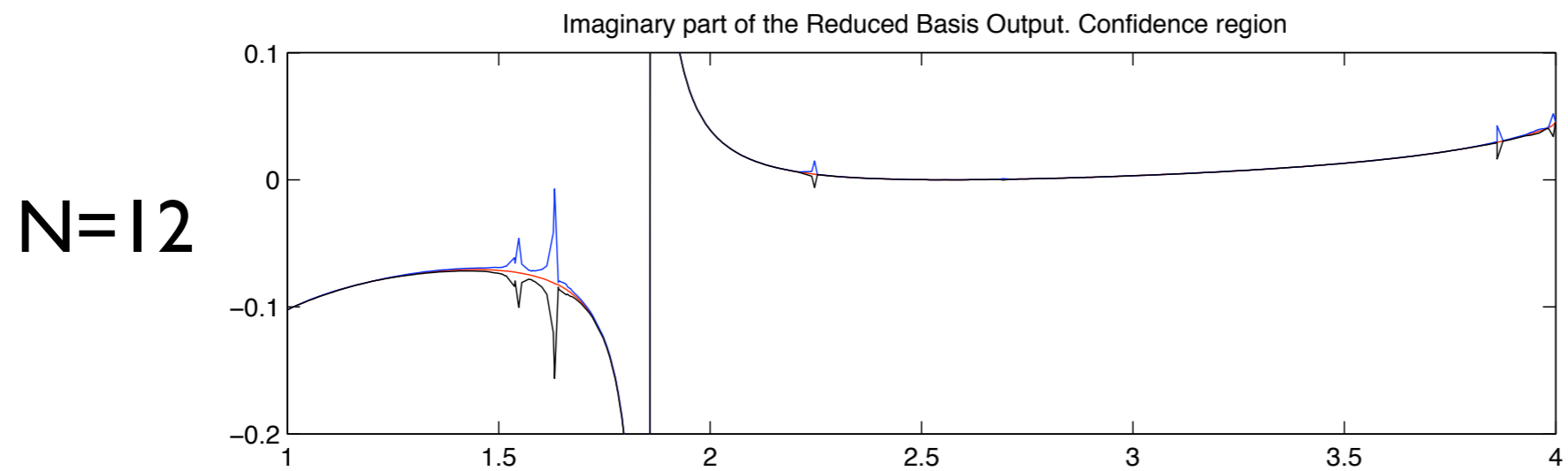
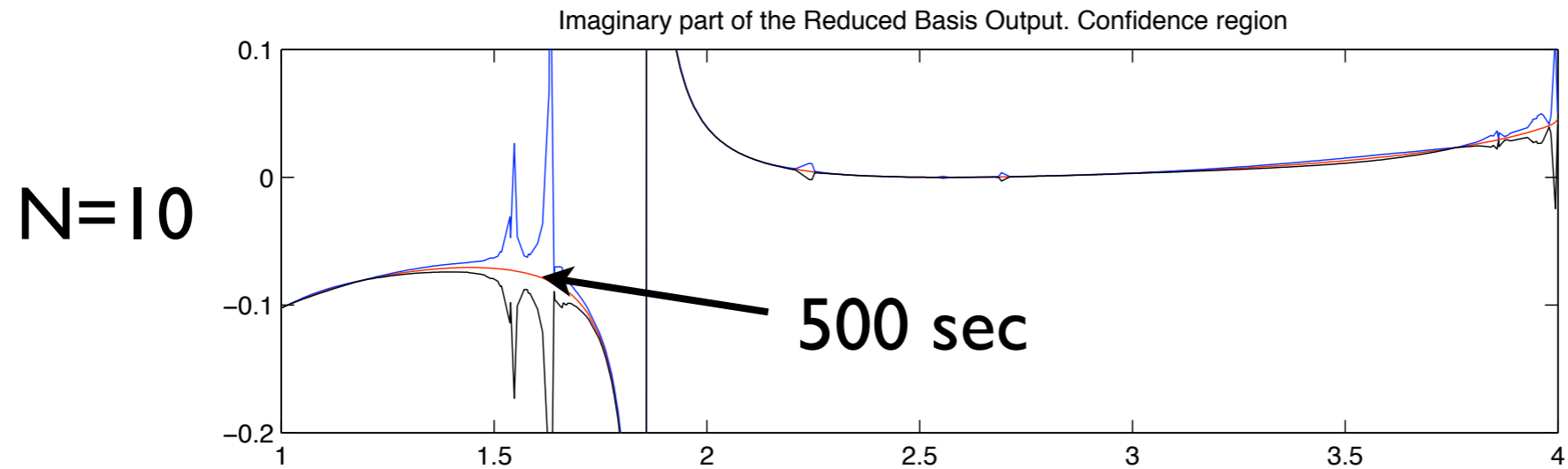
N=12



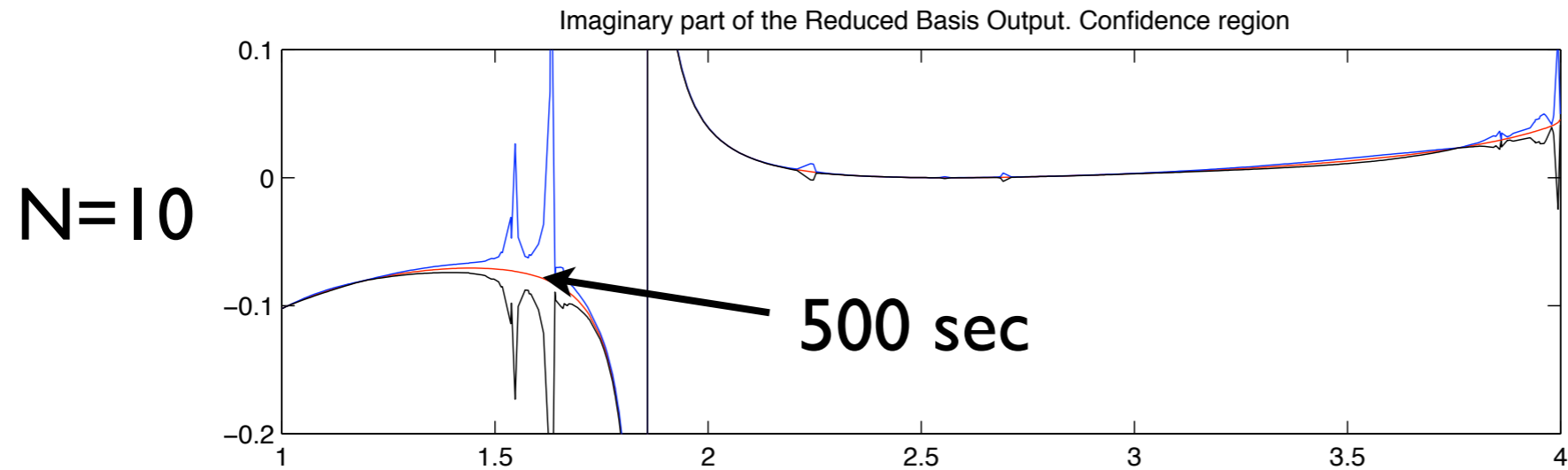
N=15



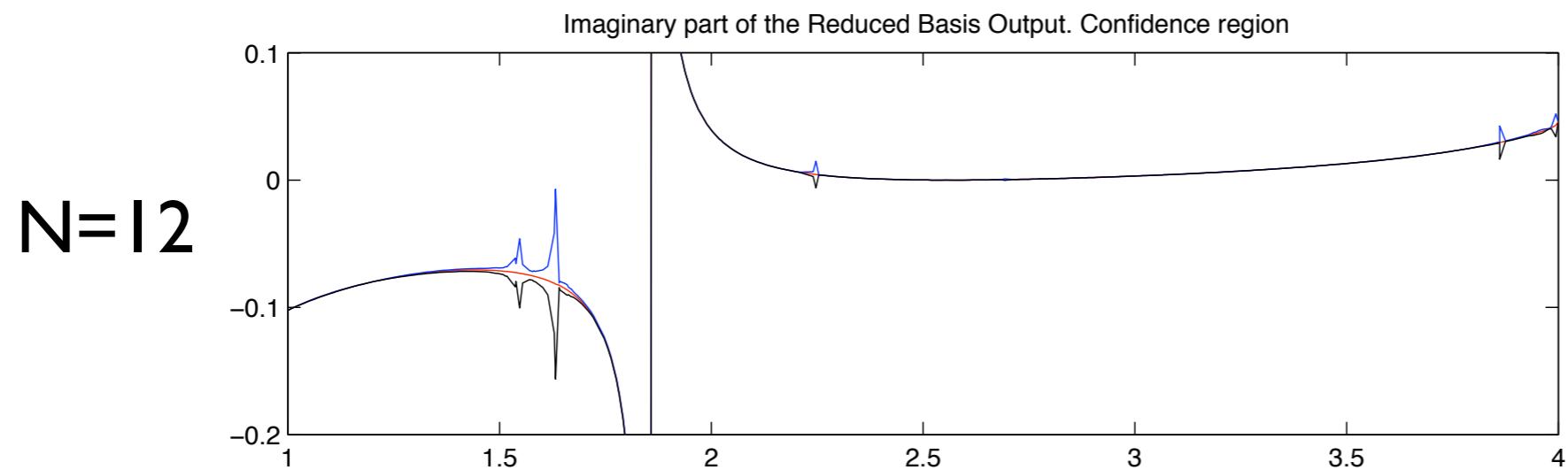
Lets see if it works



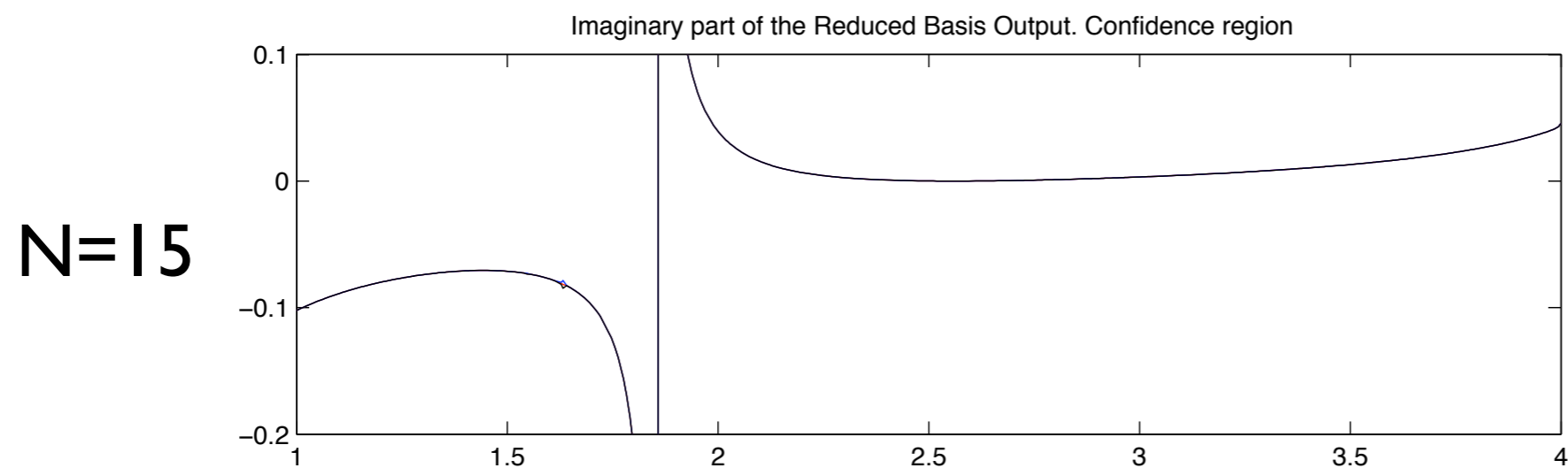
Lets see if it works



0.25 sec



0.28 sec

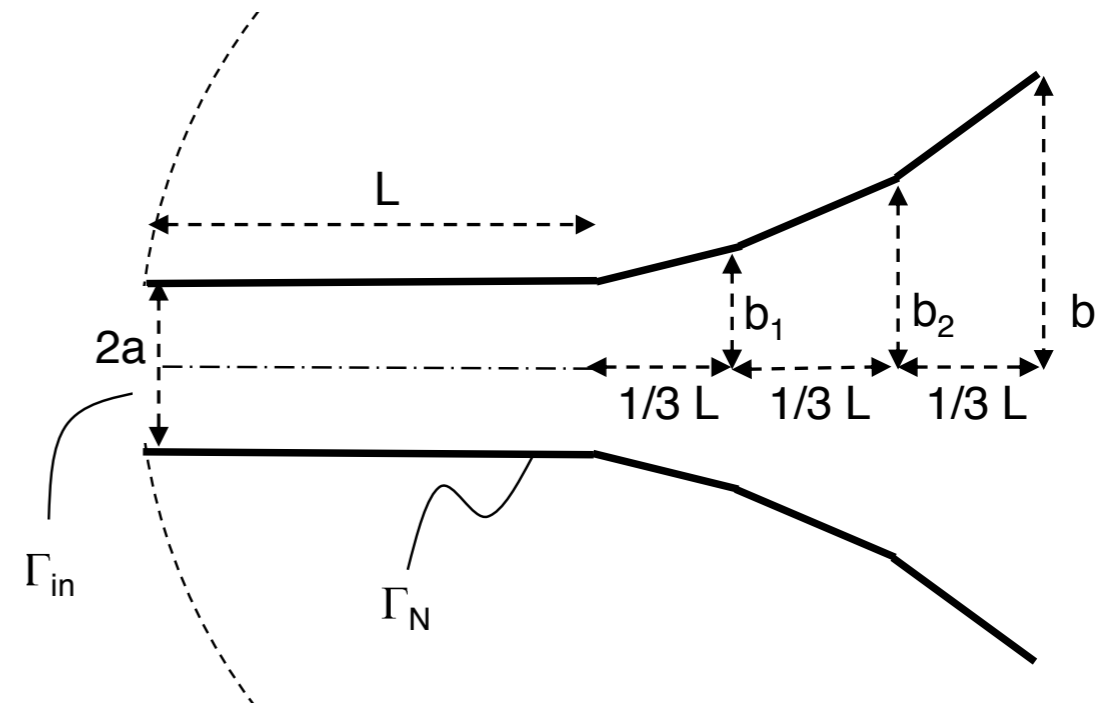


0.35 sec

An acoustic horn problem

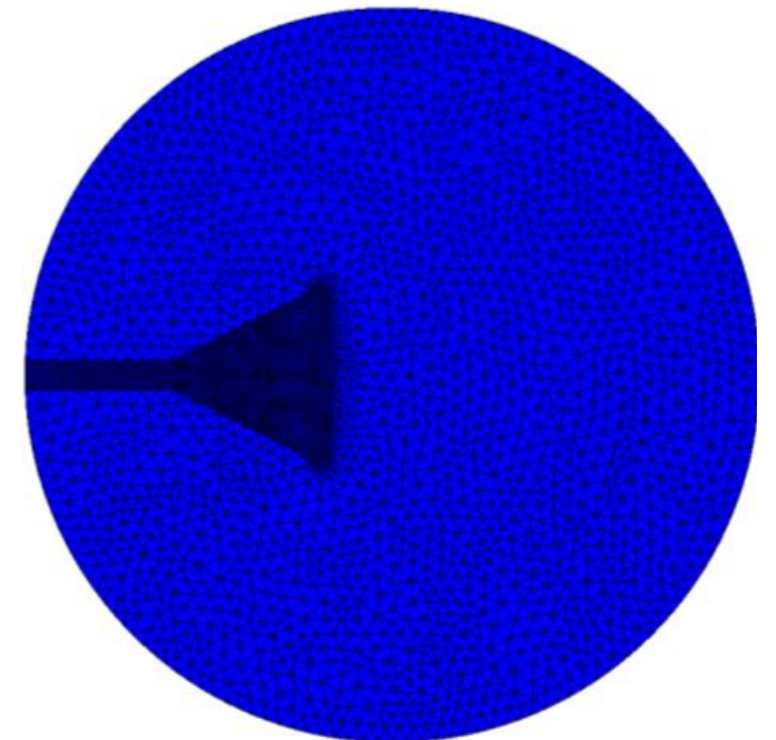
Geometry Parameters:

- 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



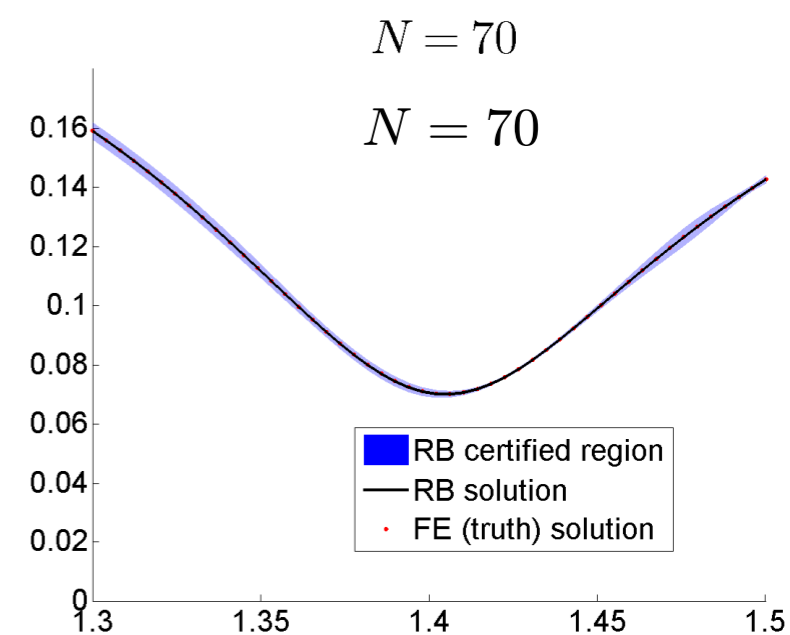
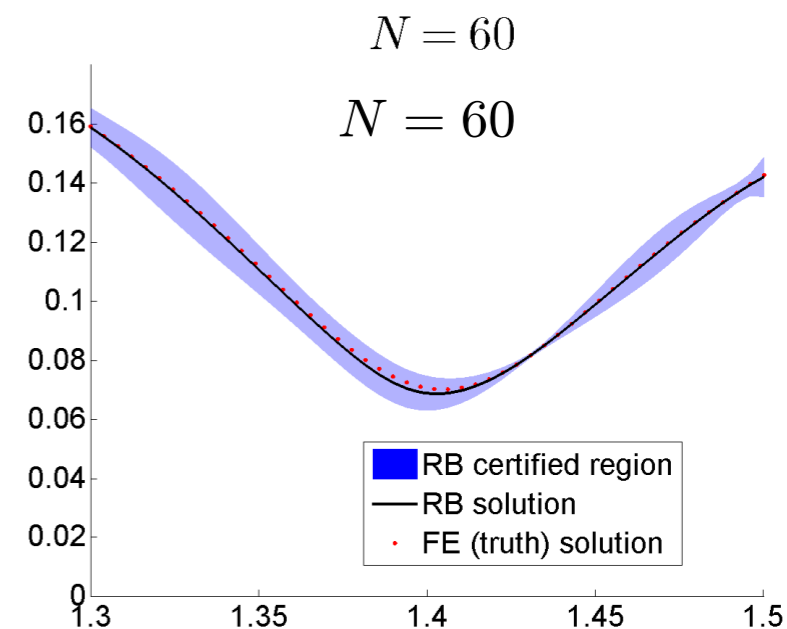
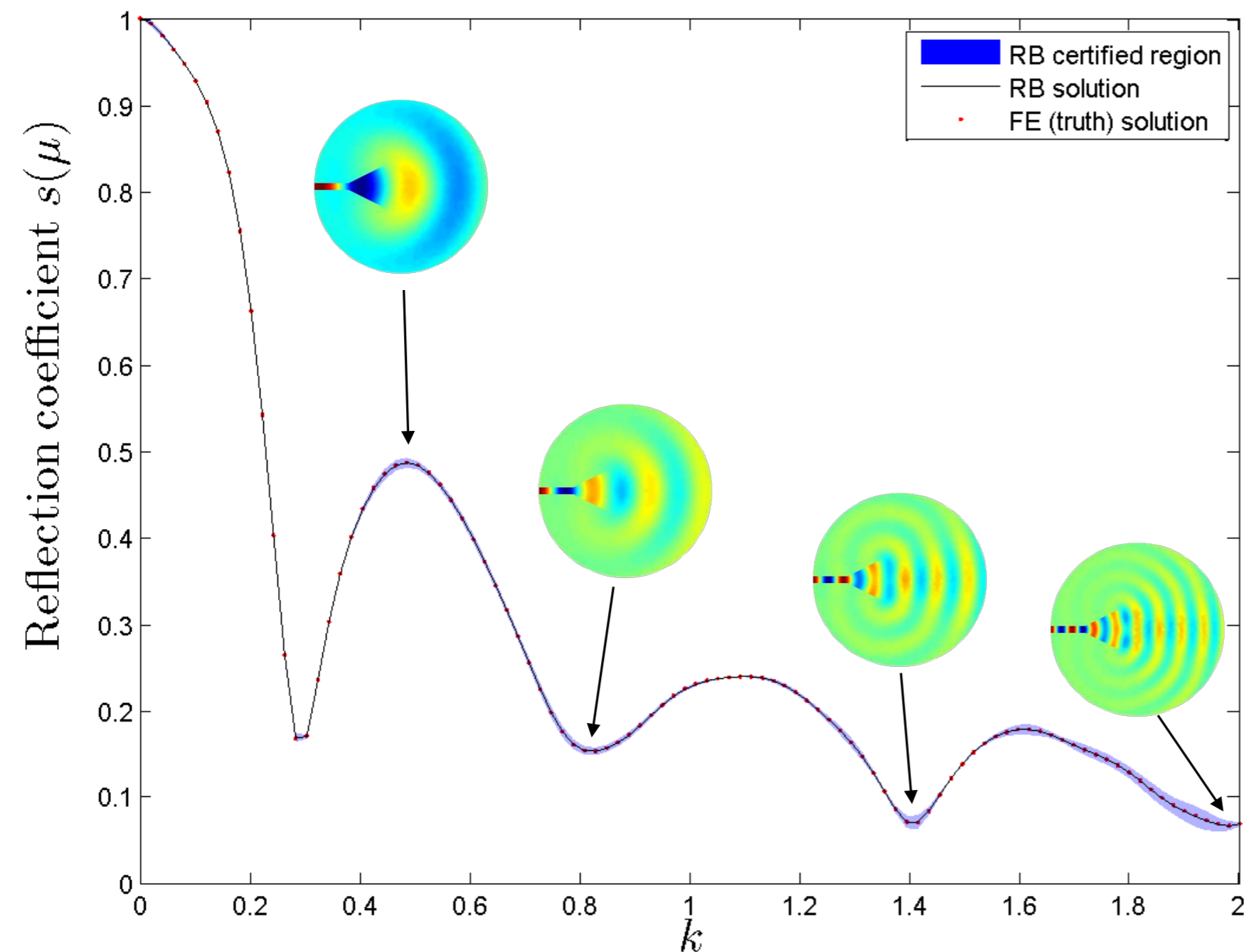
Governing Equation: Helmholtz equation

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

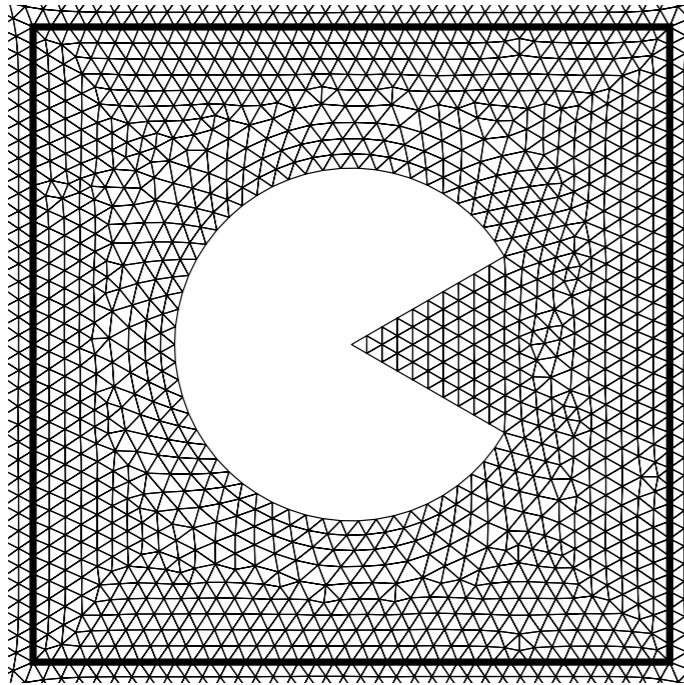


An acoustic horn problem

Wavenumber is parameter. $N=150$

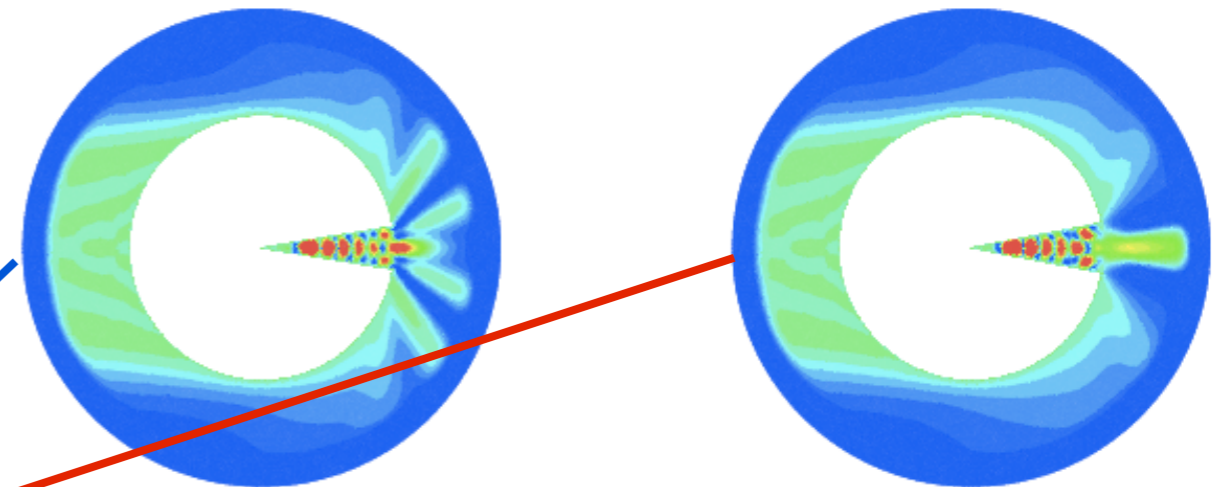
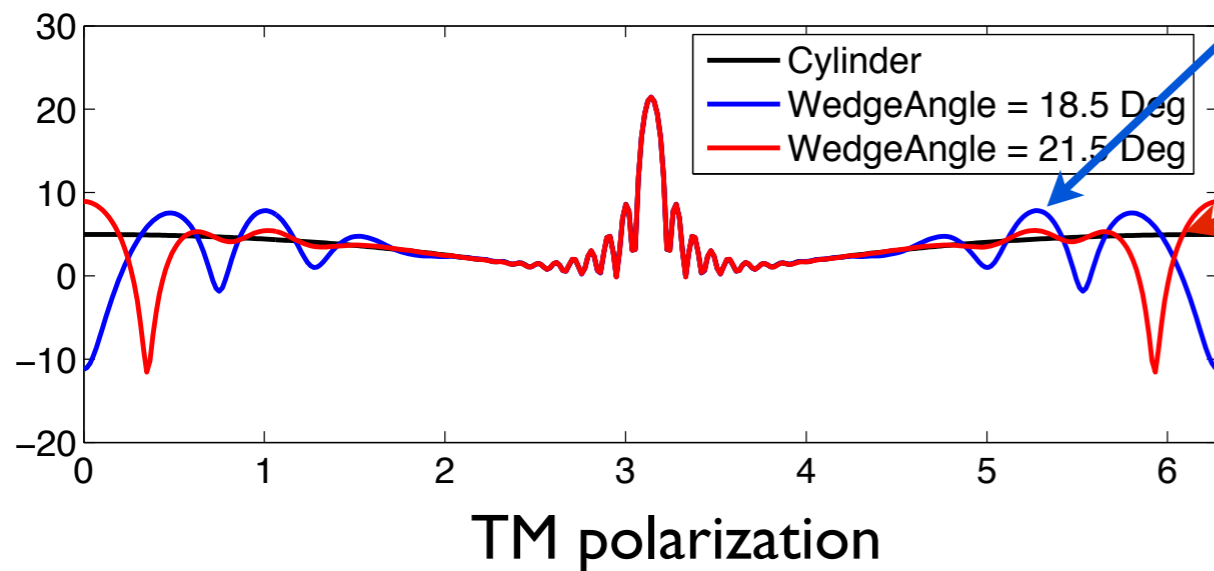


2D Pacman problem



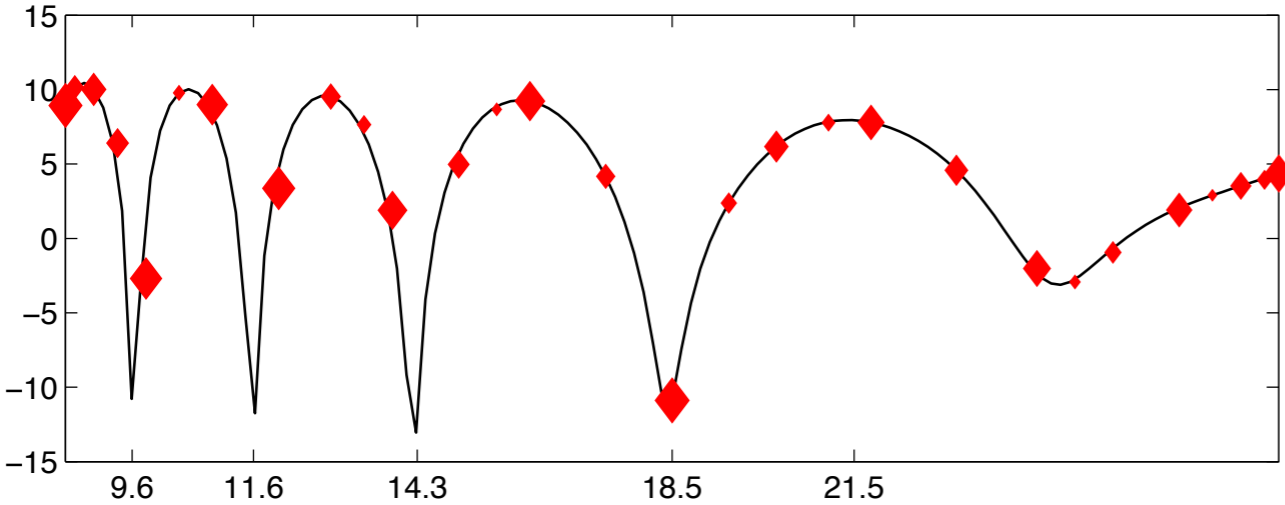
Scattering by 2D PEC Pacman

Backscatter depends very sensitively on cutout angle and frequency.

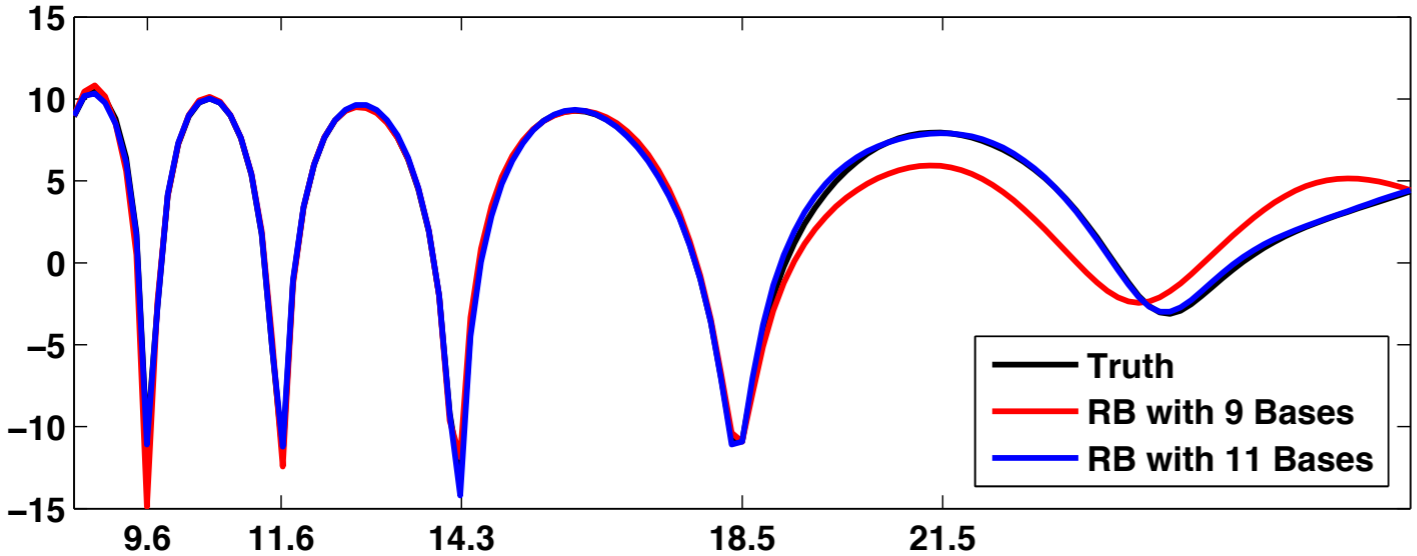
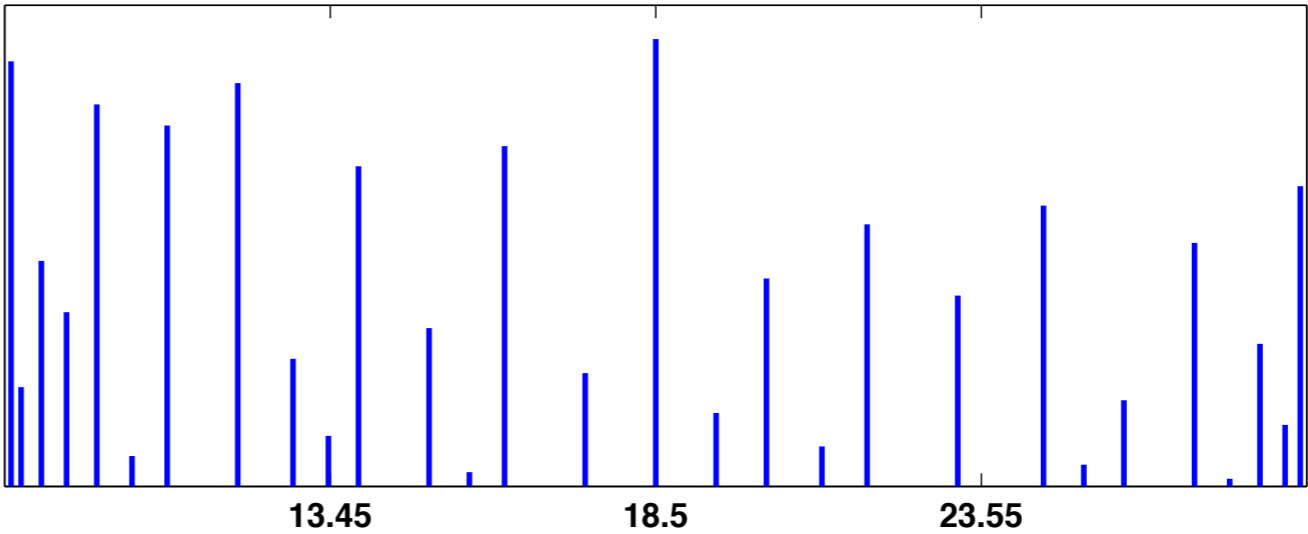


Difference in scattering is clear in fields

2D Pacman problem

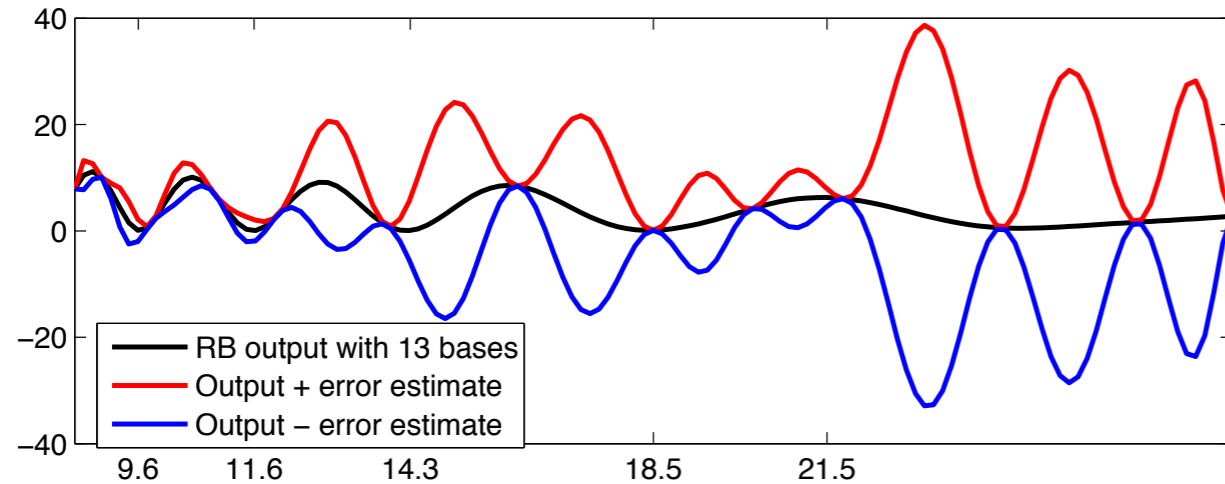


Greedy approach selects critical angles early in the selection process

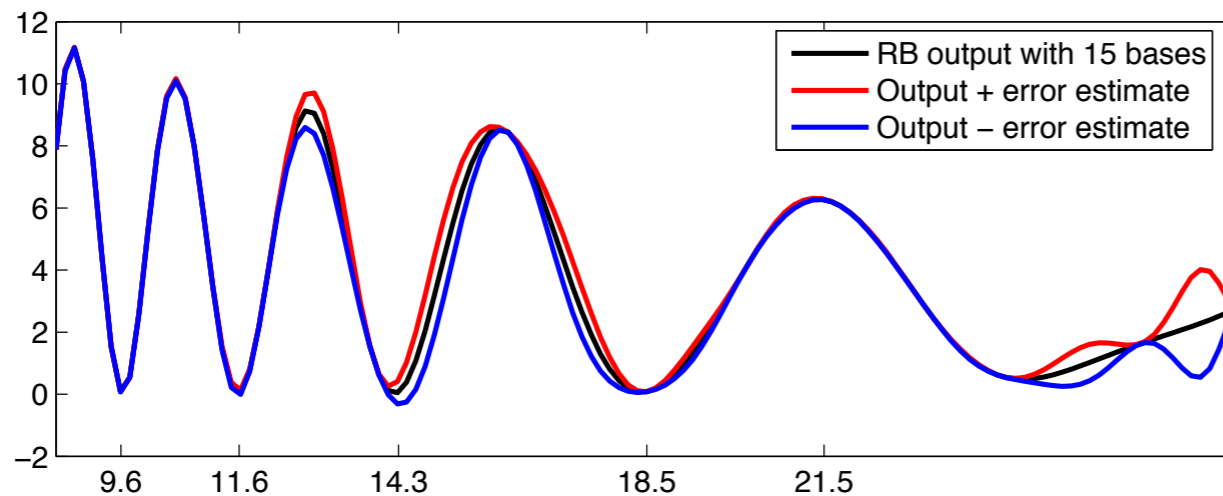


Convergence of output with $O(10)$ basis elements

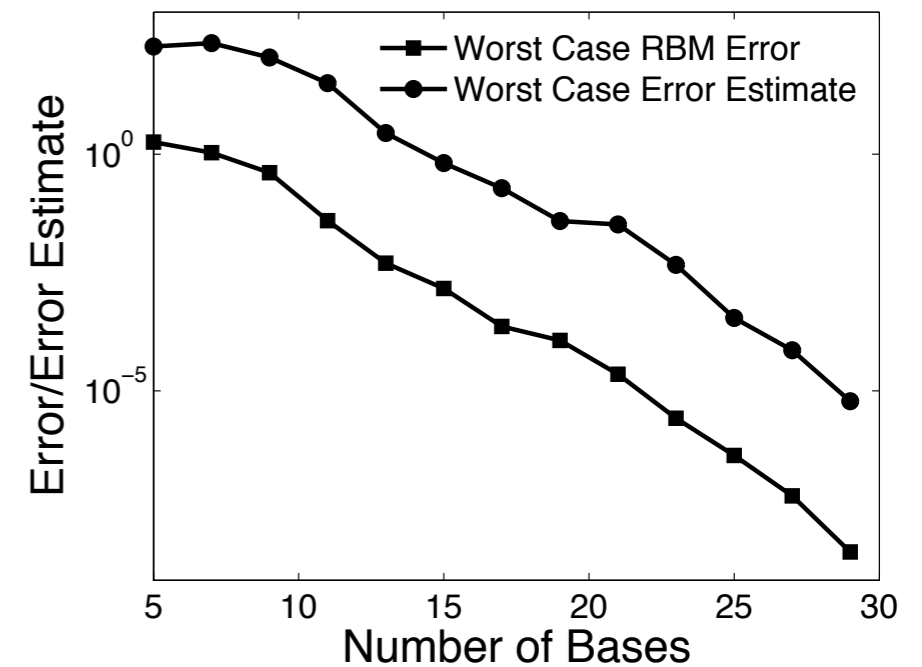
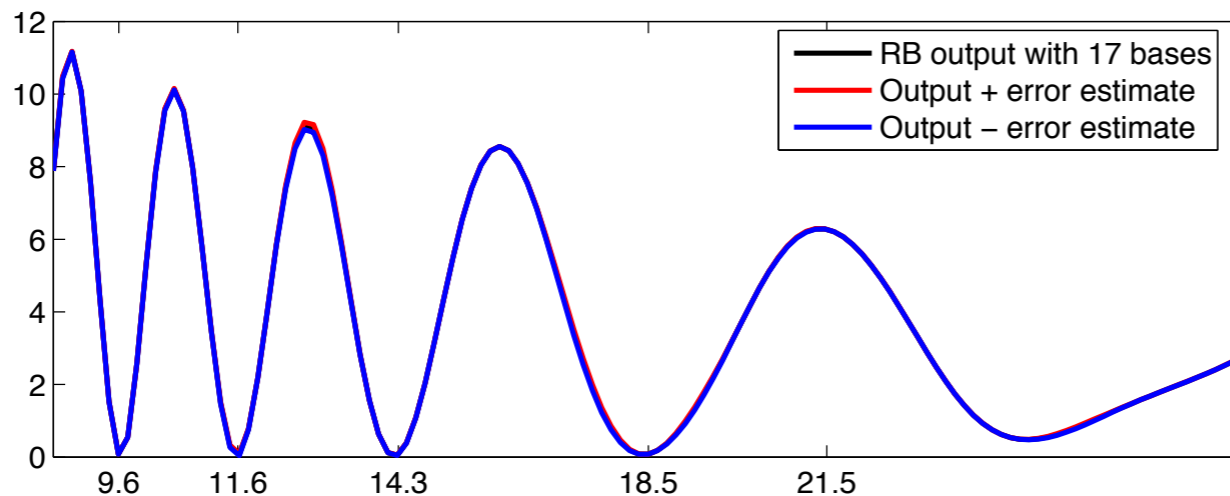
2D Pacman problem



Convergence of error bounds over full parameter range



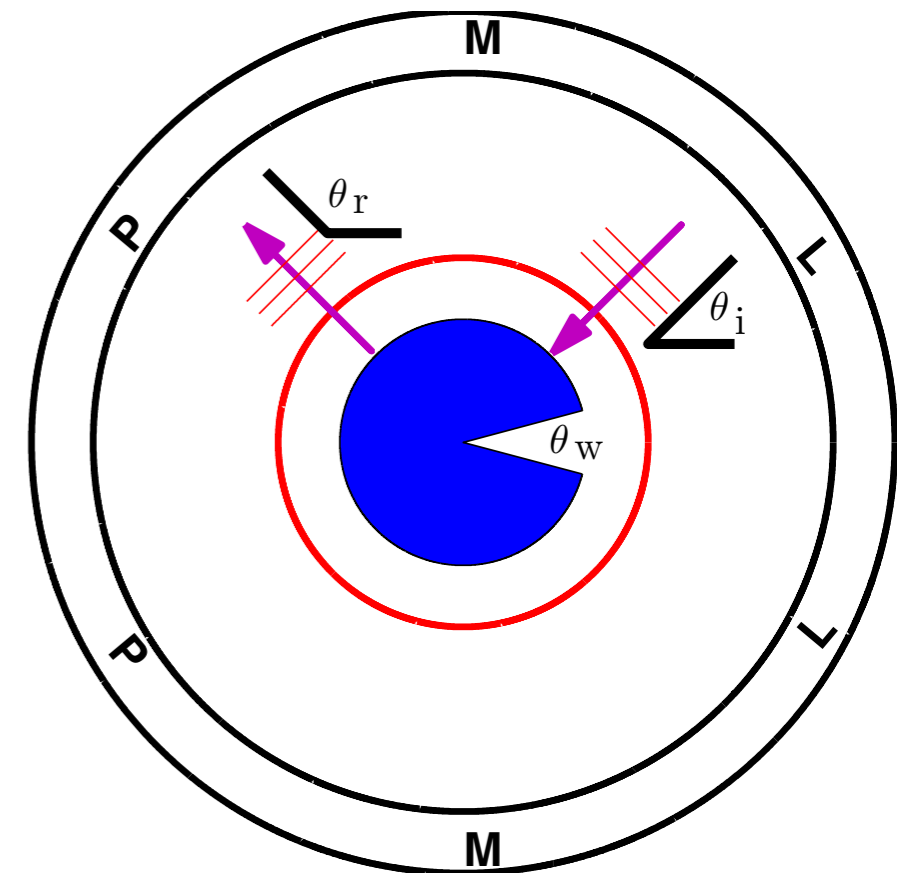
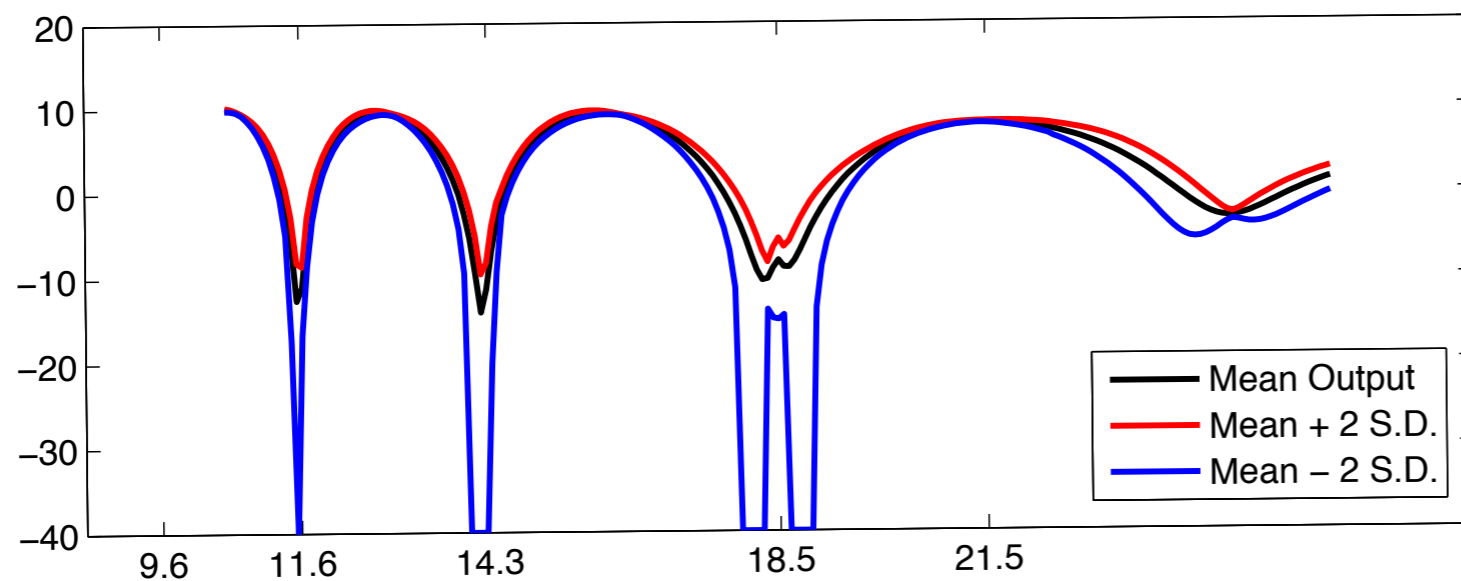
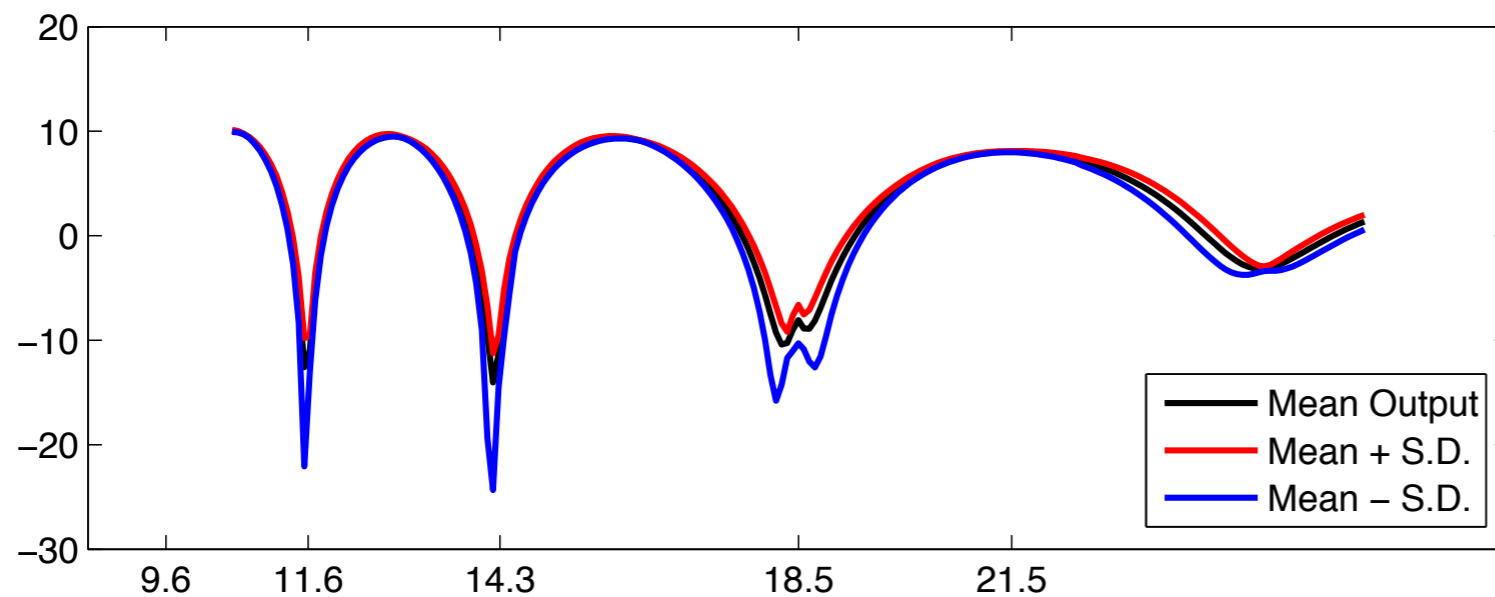
Exponential convergence of predicted error estimator and real error over large training set



Note: Linear scale, not db scale

2D Pacman prototype for UQ

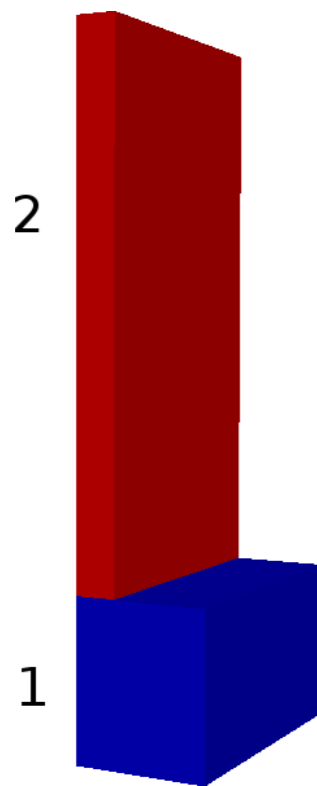
Fast evaluation over parameter space allows for rapid uncertainty quantification



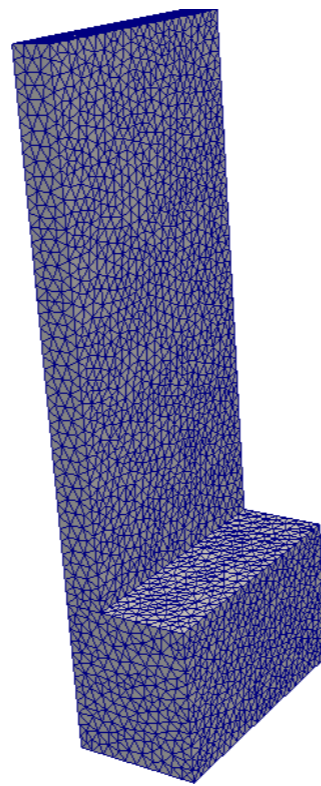
Uniformly distributed
5% randomness in
gap angle

One last example

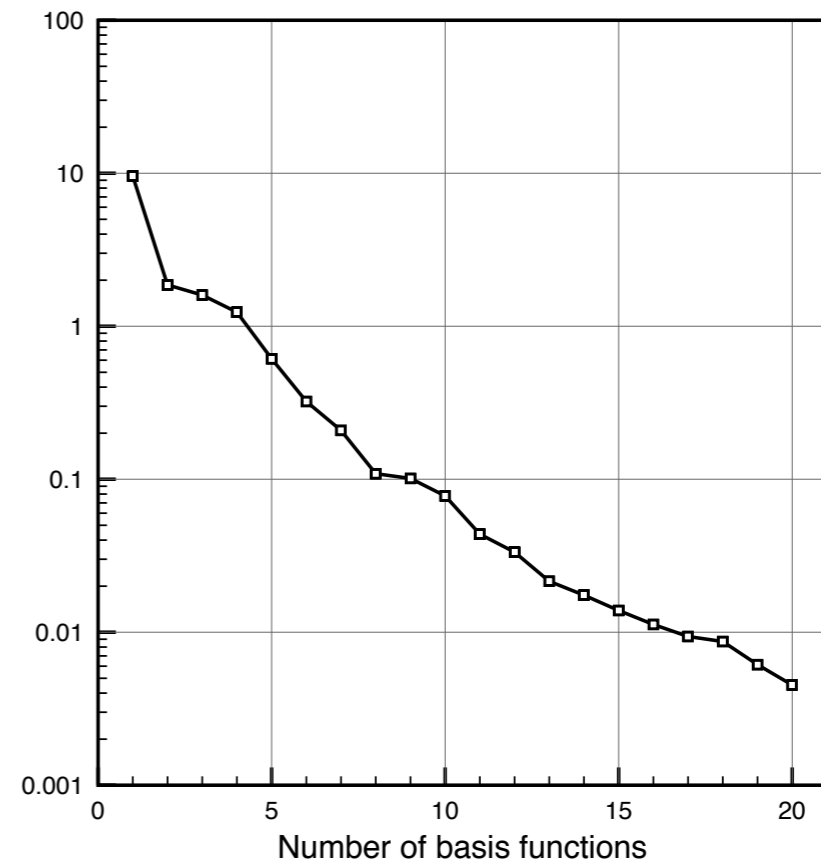
Thermal fin optimization



(a)



(b)



Three parameters

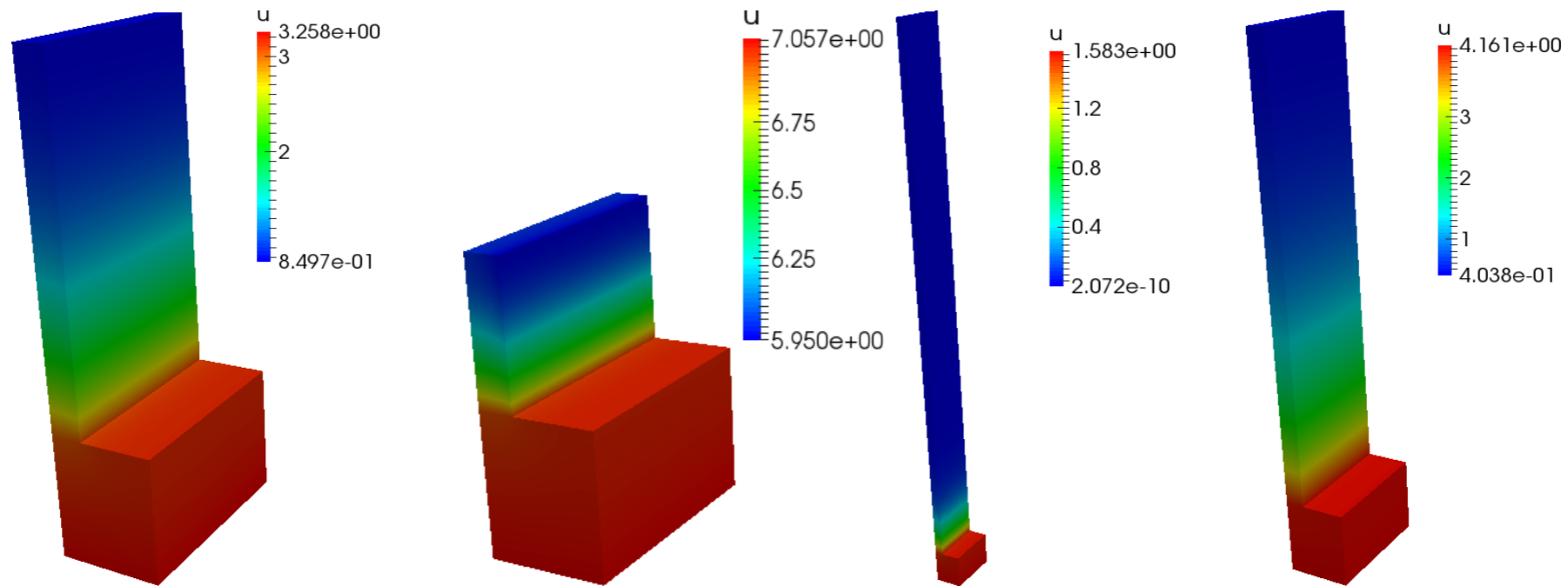
$$\mu_{[1]} \in [0.1, 1.0], \quad \mu_{[2]} \in [0.5, 10.0], \quad \mu_{[3]} \in [1.0, 10.0].$$

$$a_o(w, v; \mu) = \mu_{[3]} \int_{\Omega_o^1} \nabla w \cdot \nabla v + \int_{\Omega_o^2(\mu)} \nabla w \cdot \nabla v + \mu_{[1]} \int_{\Gamma_1} w v,$$

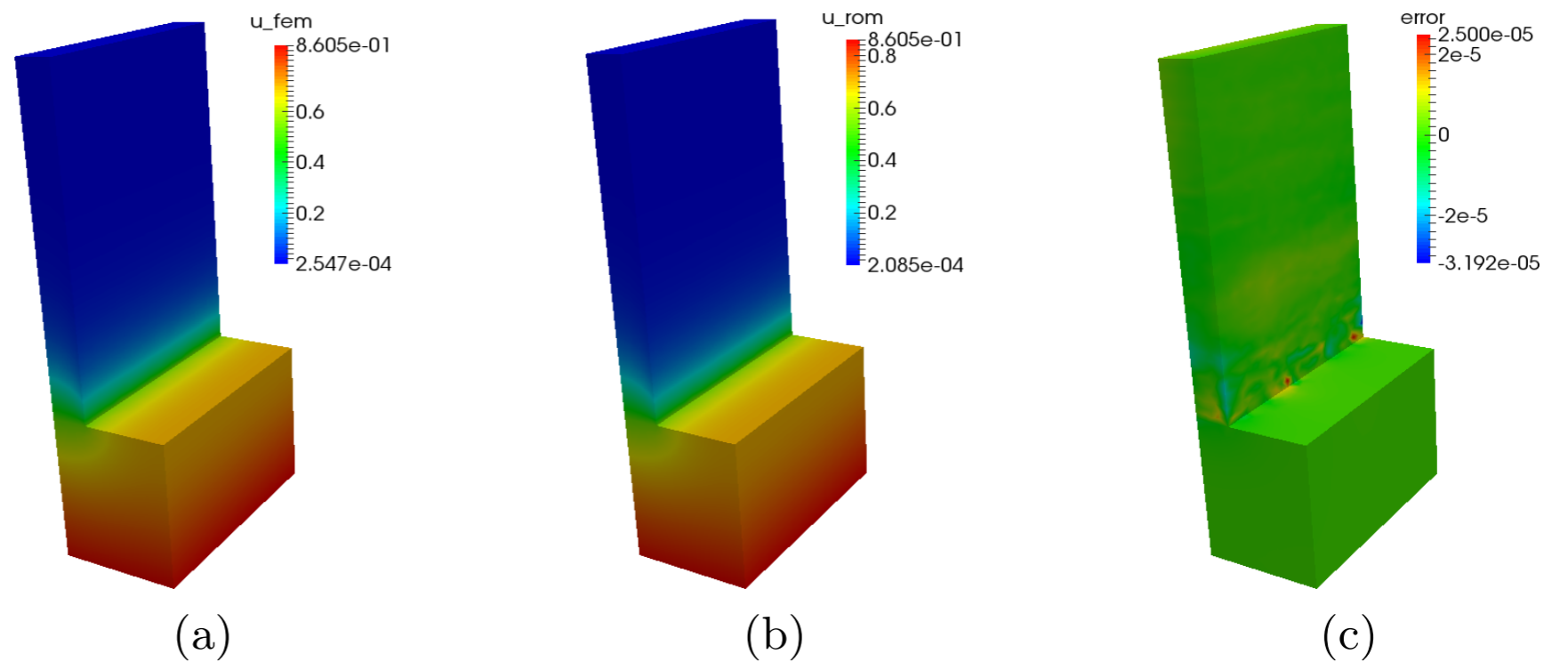
$$f_o(v) = \int_{\Gamma_{\text{bottom}}} v,$$

One last example

Basis functions



Verification



Where are we now ?

So far we have established

- ▶ Method works and efficient though greedy
- ▶ Performance depends on N
- ▶ Error is certified

Still to consider the 'non's'

- ▶ Non-affine problems
- ▶ Non-compliant problems
- ▶ Non-intrusive problems
- ▶ Non-stationary problems
- ▶ Non-standard problems

Lecture 3

Questions ?