Reduced order models for parameterized problems: Lecture One

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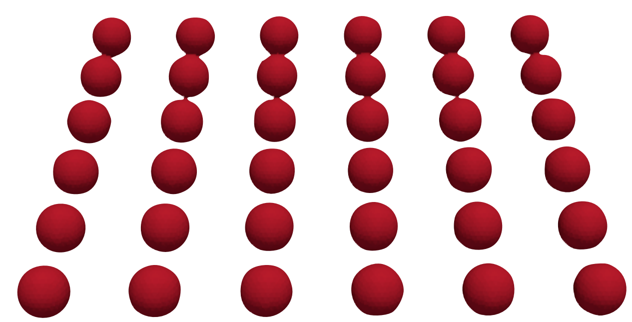
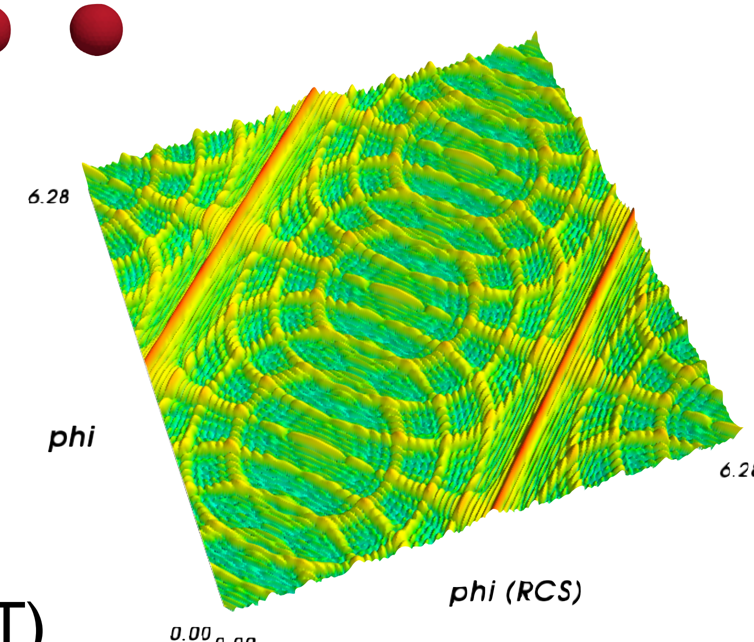




w/ assistance from B. Stamm (Aachen, D) and G. Rozza (SISSA, IT)

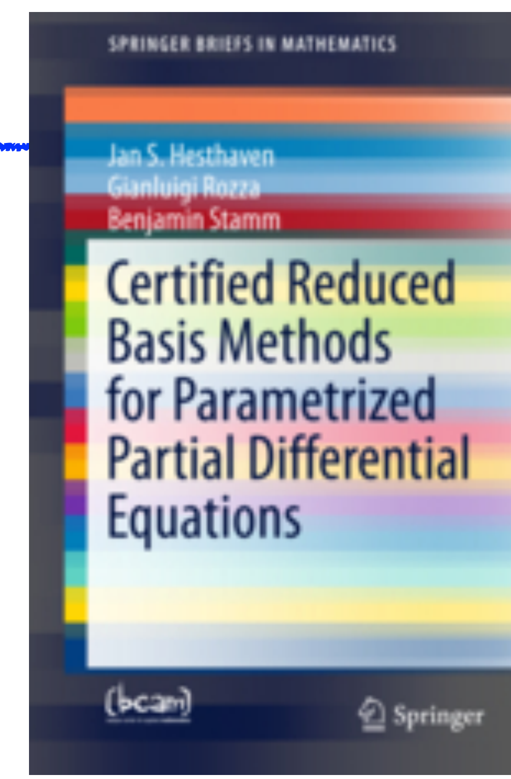
Overview of the lectures

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

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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 ?

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Understand Reduced models

WHAT do we mean by 'reduced models' ?

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DOES it work ?

WHAT's next ?

What we seek

What we need is an accurate way to evaluate the solution at new parameter values at reduced complexity.

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What we need is an accurate way to evaluate the solution at new parameter values at reduced complexity.

input: parameter value $\boldsymbol{\mu} \in \mathcal{D}$

PDE solver

$$\mathcal{L}_h(u_h(\boldsymbol{\mu}); \boldsymbol{\mu}) = 0$$

output: $s_h(\boldsymbol{\mu}) = l(u_h(\boldsymbol{\mu}); \boldsymbol{\mu})$

Reduced models ?

We do not consider reduced physics -

High-frequency vs low-frequency EM

$$\nabla \times \nabla \times \mathbf{E} + \omega^2 \mathbf{E} = \mathbf{f} \qquad \text{vs} \qquad -\nabla^2 \mathbf{E} = \mathbf{f}$$

Viscous vs inviscid fluid flows

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \mathbf{p} + \nu \nabla^2 \mathbf{u} \qquad \nabla \cdot \mathbf{u} = \mathbf{0}$$

vs

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \mathbf{p} \qquad \nabla \cdot \mathbf{u} = \mathbf{0}$$

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.. but reduced representations of the full problem

.. but WHY ?

Assume we are interested in

$$-\nabla^2 u(\mathbf{x},\mu) = \mathbf{f}(\mathbf{x},\mu) \qquad\qquad \mathbf{x} \in \boldsymbol{\Omega}$$

and wish to solve it accurately for many values of 'some' parameter μ

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We can use our favorite numerical method

$$\mathrm{A}_h \mathbf{u}_h(\mathbf{x},\mu) = \mathbf{f}_\mathbf{h}(\mathbf{x},\mu) \qquad \dim(\mathbf{u}_h) = \mathcal{N} \gg 1$$

For many parameter values, this is expensive - and slow !

.. but WHY (con't)

Assume we (somehow) know

$$\mathbf{u_h}(\mathbf{x},\mu) \simeq \mathbf{u_{RB}}(\mathbf{x},\mu) = \mathrm{V}\mathbf{a}(\mu) \qquad \mathrm{V}^T\mathrm{V} = \mathrm{I}$$

$$\dim(\mathbf{a}) = N \qquad \dim(V) = \mathcal{N} \times N$$

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Then we can recover a solution for a new parameter as little cost

$$(\mathrm{V}^T\mathrm{A}_h\mathrm{V})\mathrm{V}^T\mathbf{u}_h(\mu) = \mathrm{V}^T\mathbf{f}_h(\mu)$$

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.. if this behaves !

.. but WHY (con't)

So IF

- .. we know the orthonormal basis - V
- .. and it allows an accurate representation - $u_{RB}(\mu)$
- .. and we can evaluate RHS 'fast'- $\mathcal{O}(N)$

we can evaluate new solutions at cost - $\mathcal{O}(N)$

.. but WHY (con't)

So IF

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- .. and it allows an accurate representation - $u_{RB}(\mu)$
- .. and we can evaluate RHS 'fast'-

we can evaluate new solutions at cost -

So WHY ? - a promise to do more with less

When is that relevant ?

Examples in many application domains

- Optimization/inversion/control problems
- Simulation based data bases
- Uncertainty quantification
- Sub-scale models in multi-scale modeling
- In-situ/deployed modeling

When is that relevant ?

Examples in many application domains

- Optimization/inver

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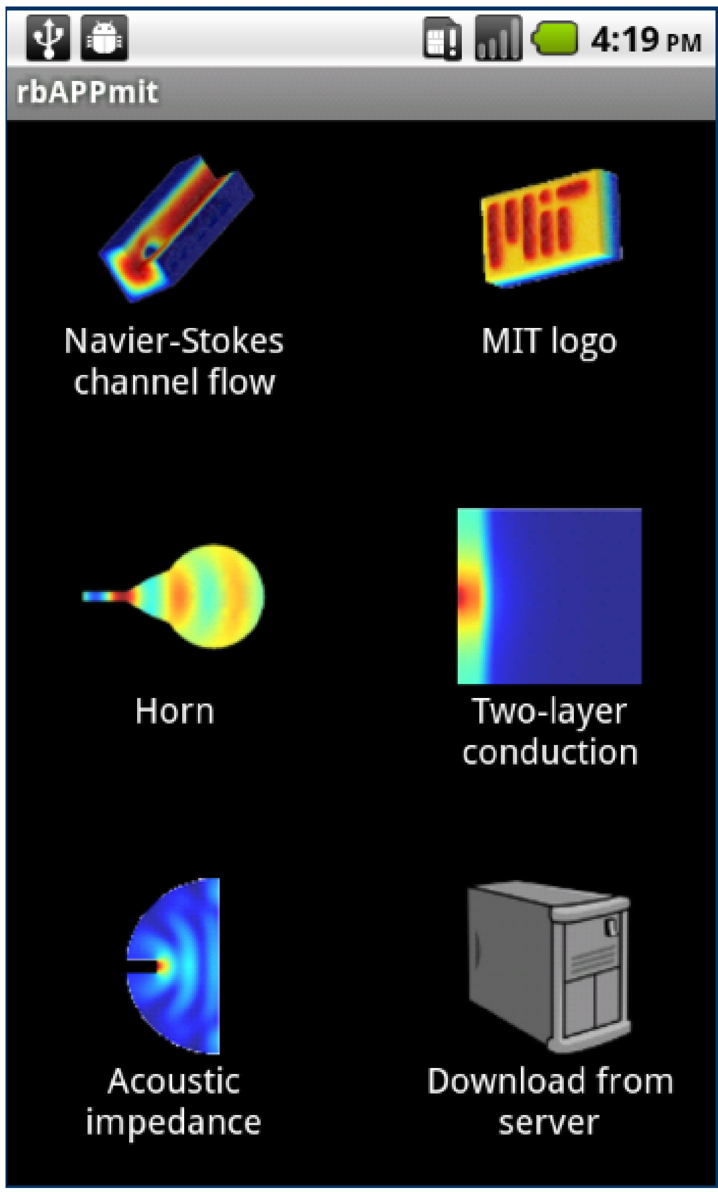


D. Knezevic et al, 2010

Before we continue

We consider projection based techniques, i.e.

$$\mathbf{u_h}(\mathbf{x},\mu) \simeq \mathbf{u_{RB}}(\mathbf{x},\mu) = \mathbf{V}\mathbf{a}(\mu)$$

There is a substantial literature for linear systems

$$\begin{cases} \boldsymbol{C}\dot{\boldsymbol{x}}(t) + \boldsymbol{G}\boldsymbol{x}(t) = \boldsymbol{B}\boldsymbol{u}(t), \\ \boldsymbol{y}(t) = \boldsymbol{L}^{\mathrm{T}}\boldsymbol{x}(t), \end{cases} \Leftrightarrow \begin{cases} \boldsymbol{C}_n\dot{\boldsymbol{z}}(t) + \boldsymbol{G}_n\boldsymbol{z}(t) = \boldsymbol{B}_n\boldsymbol{u}(t), \\ \tilde{\boldsymbol{y}}(t) = \boldsymbol{L}_n^{\mathrm{T}}\boldsymbol{z}(t), \end{cases}$$

Typically seeks to approximate the transfer function

$$\boldsymbol{H}(s) = \boldsymbol{L}^{\mathrm{T}}(\boldsymbol{G} + s\boldsymbol{C})^{-1}\boldsymbol{B}. \Leftrightarrow \boldsymbol{H}_n(s) = \boldsymbol{L}_n^{\mathrm{T}}(\boldsymbol{G}_n + s\boldsymbol{C}_n)^{-1}\boldsymbol{B}_n.$$

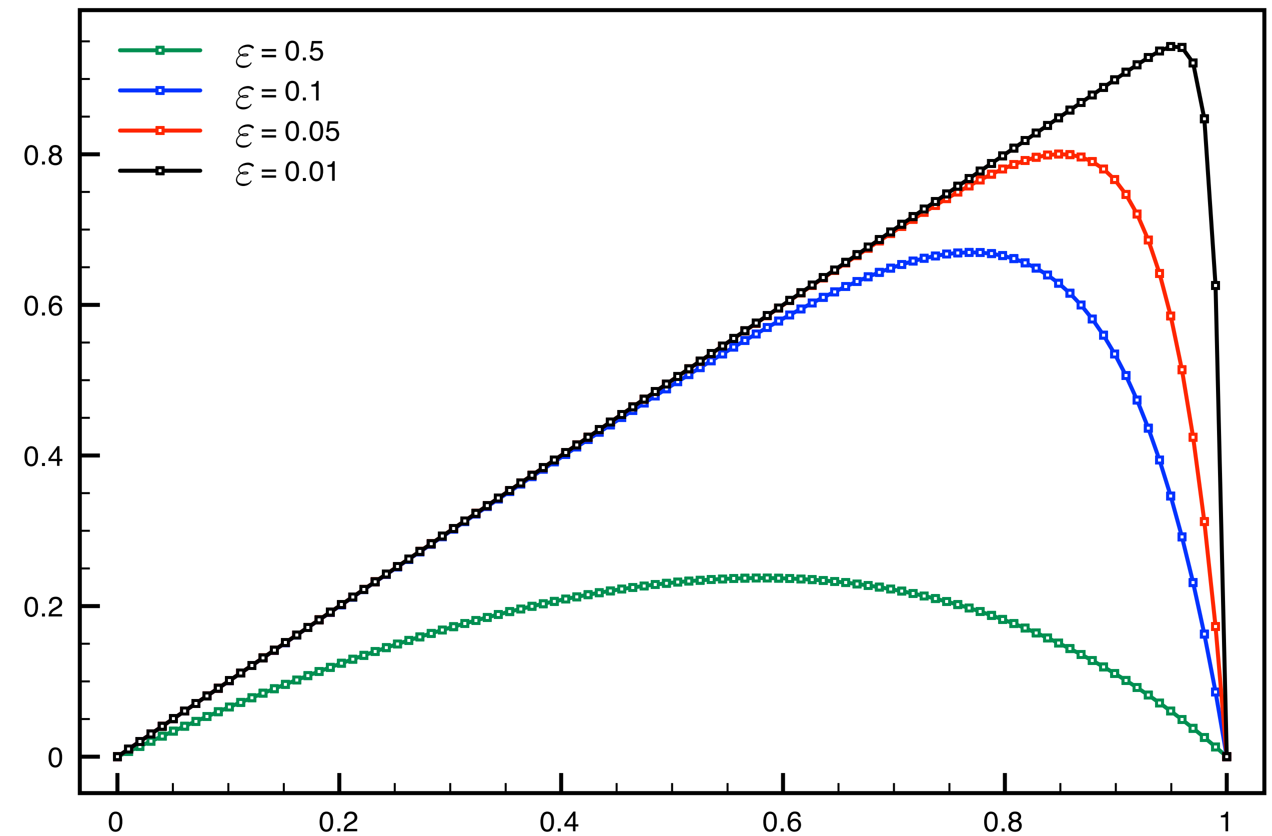
- Pade approximations
- Krylov subspace methods
- Balanced truncation

Non-linear problems ?

Parametrized problems - Ex 1

Convection-diffusion problem

$$\begin{aligned} \varepsilon u'' + u' &= 1, \qquad \text{in } (0,1), \\ u(0) = u(1) &= 0. \end{aligned}$$



Variational setting

$$\mathbb{V} = H_0^1(0,1),$$

$$a(u,v;\varepsilon) = \varepsilon \int_0^1 u'(x)v'(x)\,dx + \int_0^1 u'(x)v(x)\,dx,$$

$$f(v) = \int_0^1 v(x)\,dx.$$

Parametrized problems - Ex 1

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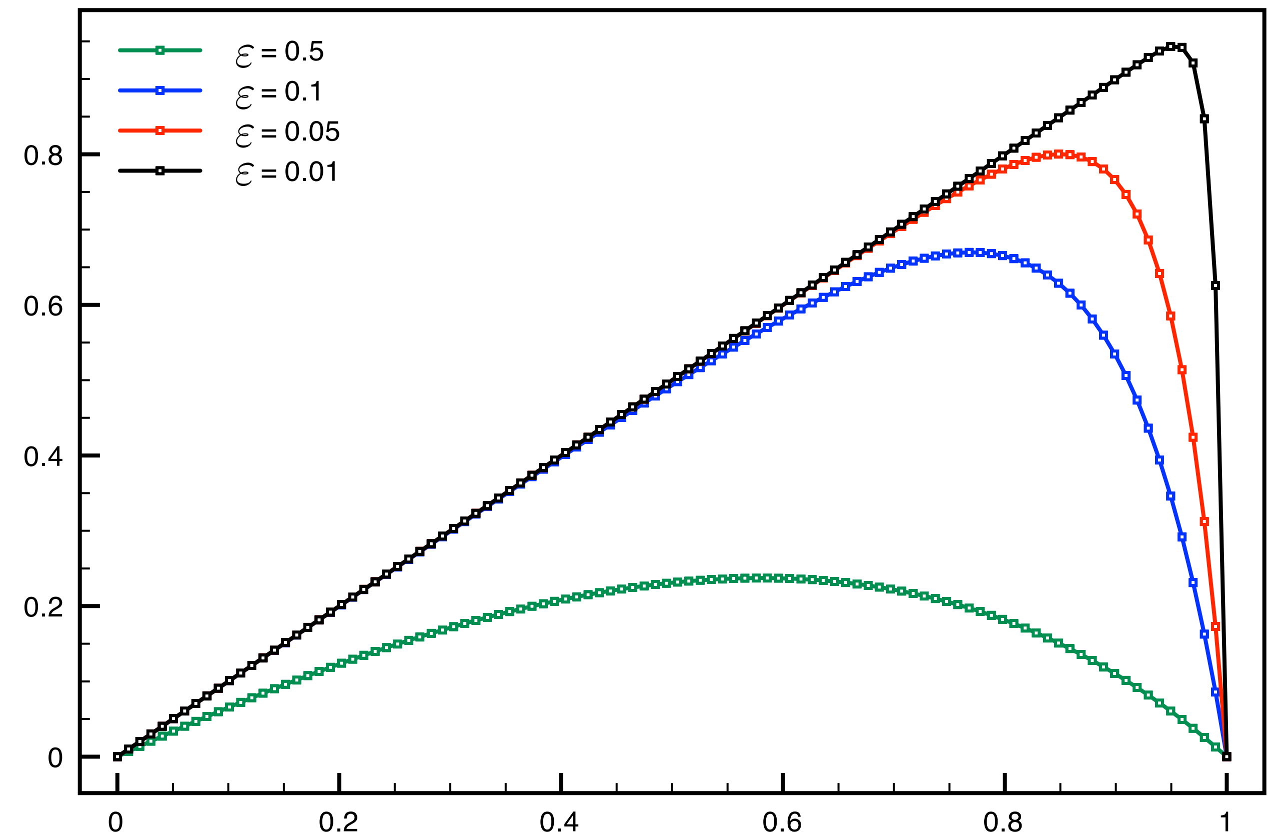

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$$f(v) = \int_0^1 v(x)\,dx.$$

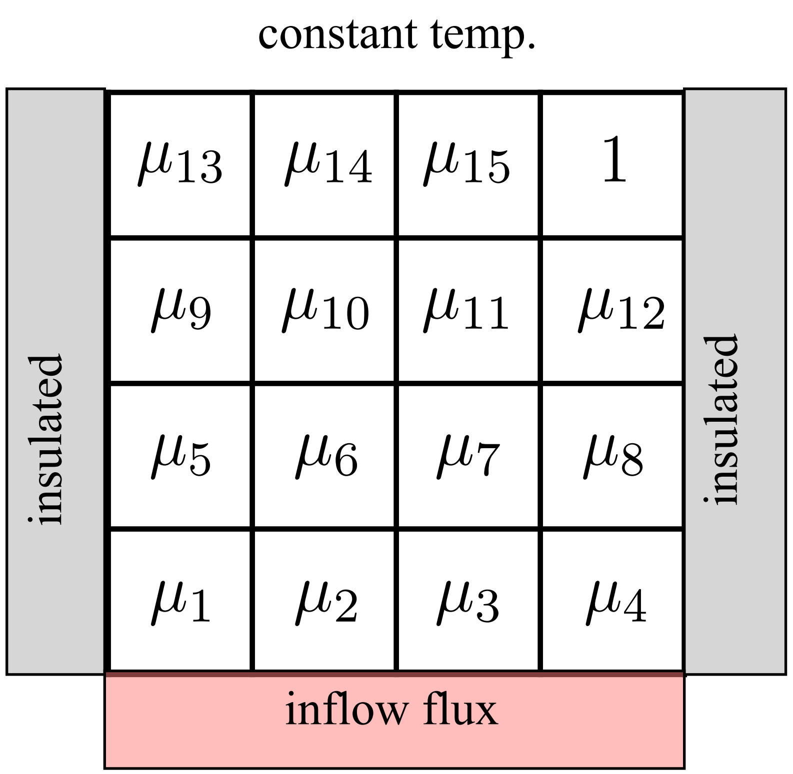
Parametrized problem: Given $\varepsilon \in [0.01, 0.5]$, find $u(\varepsilon) \in \mathbb{V}$ such that

$$a(u(\varepsilon), v; \varepsilon) = f(v), \qquad \forall v \in \mathbb{V}.$$

Then, compute $s(\varepsilon) = u(0.5; \varepsilon)$.

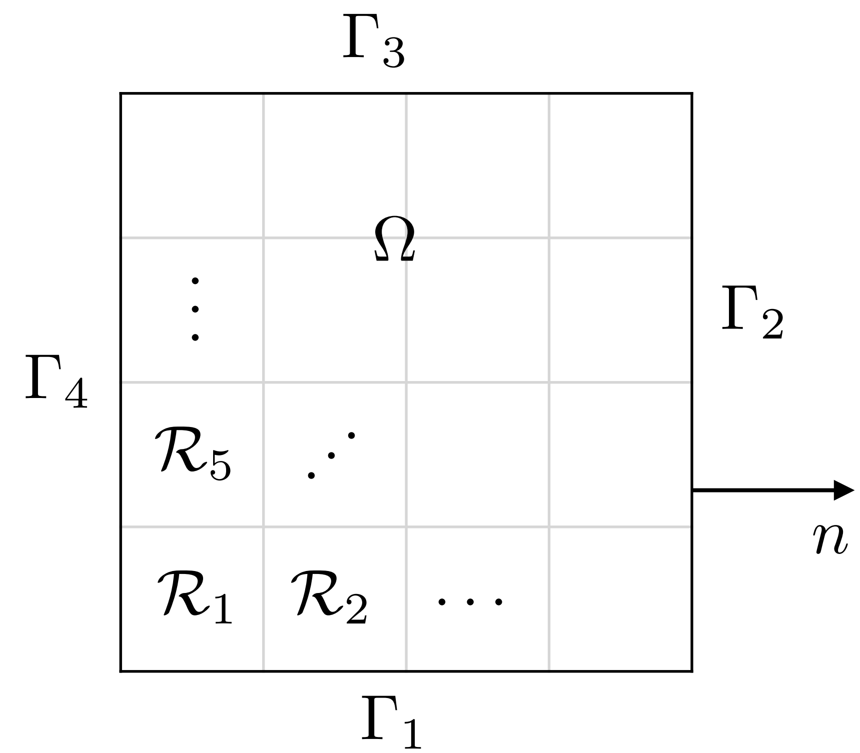
Parametrized problems - Ex 2

Physics:



$\mu_i \in \mathbb{R}$: conductivity of block $\mathcal{R}_i$

Mathematics:



$\mu : \Omega \to \mathbb{R}$ such that $\mu|_{\mathcal{R}_i} = \mu_i$

Find $u \in H^1(\Omega)$ such that:

$$\begin{aligned} \nabla \cdot \mu \nabla u &= 0, && \text{in } \Omega, \\ \nabla u \cdot n &= 1, && \text{on } \Gamma_1, \\ \nabla u \cdot n &= 0, && \text{on } \Gamma_2, \Gamma_4, \\ u &= 0, && \text{on } \Gamma_3. \end{aligned}$$

Output of interest is the average temperature over Γ_1:

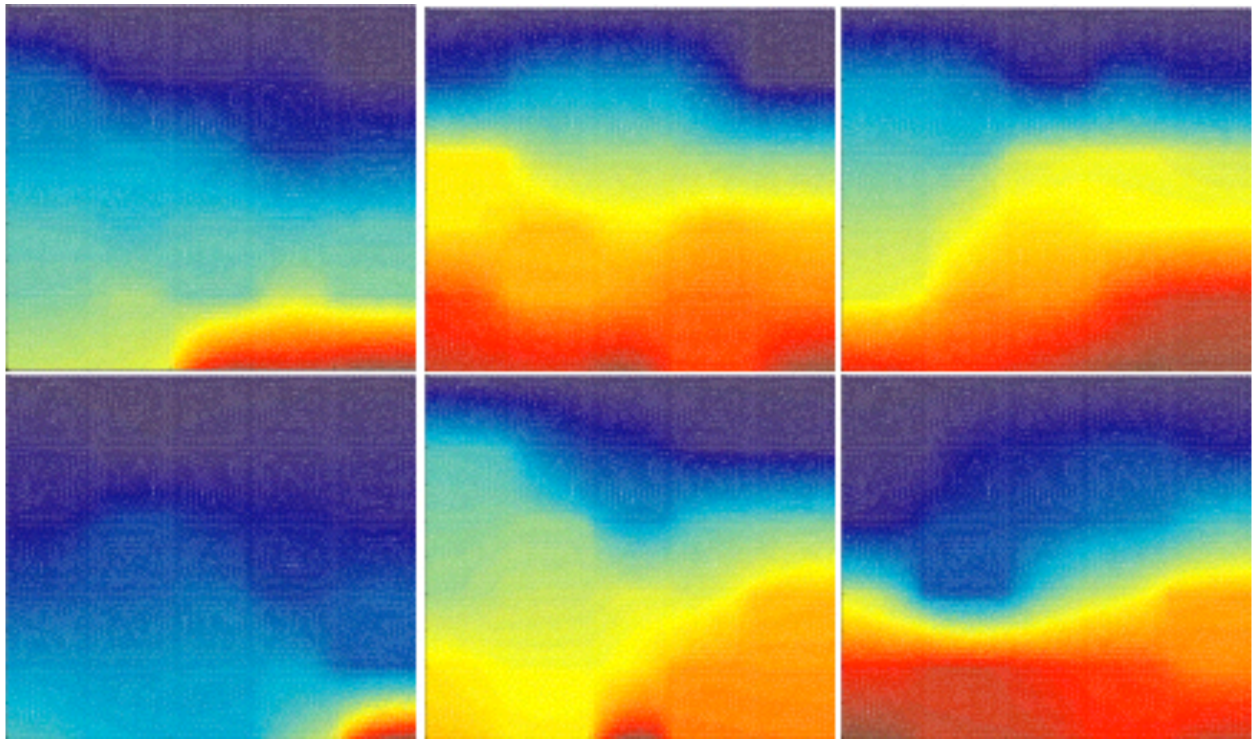
$$s(\mu) = \ell(u(\mu)) = \int_{\Gamma_1} u(\mu).$$

Parametrized problems - Ex 2

Parametrized problem setting:

Let $\mu = (\mu_1, \mu_2, \ldots, \mu_{15}) \in \mathbb{P} = [\mu_-, \mu_+]^{15}$. Then, for any $\mu \in \mathbb{P}$, compute $s(u(\mu))$.

Solutions $u(\mu)$ for different values of $\mu \in \mathbb{P}$:



Parametrized problems - Ex 2

Variational setting: Define

$$\mathbb{V} = \{v \in H^1(\Omega) \mid v|_{\Gamma_{top}} = 0\},$$

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

$$f(v) = \ell(v) = \int_{\Gamma_1} v.$$

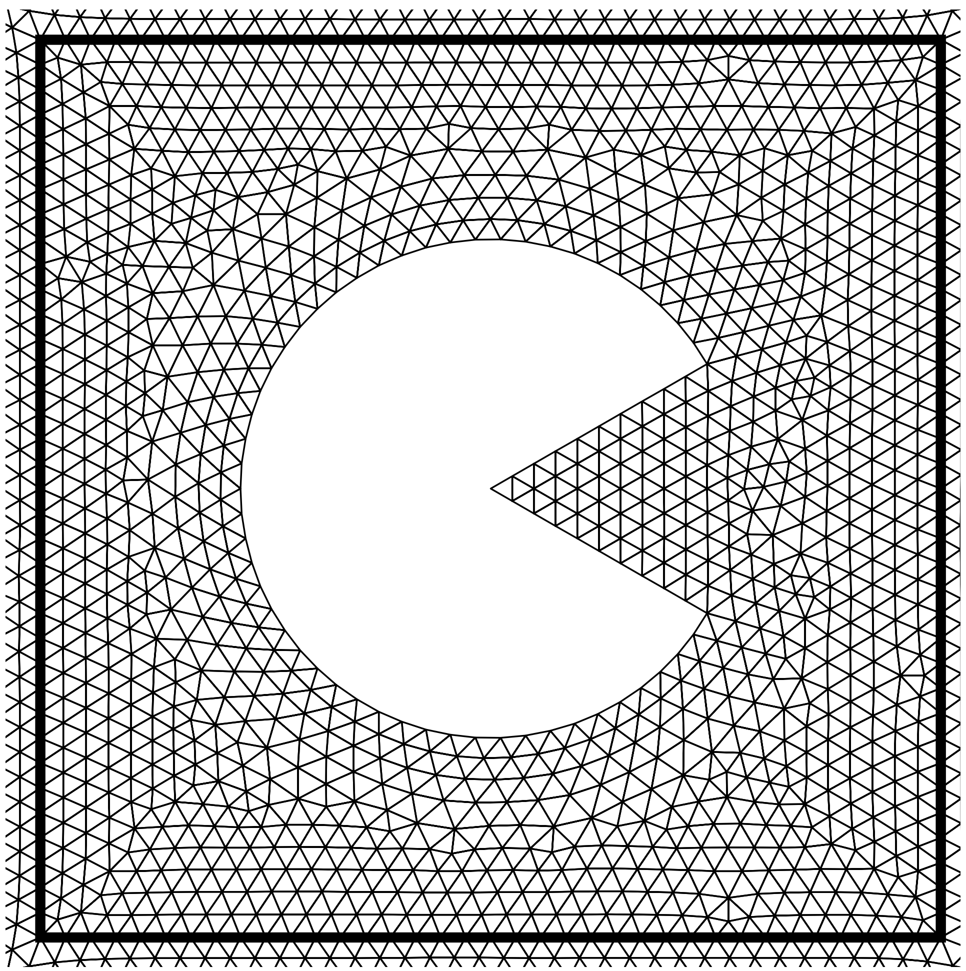
Parametrized problem setting:

For any $\mu \in \mathbb{P}$, find $u(\mu) \in \mathbb{V}$ s.t.

$$a(u(\mu), v; \mu) = f(v), \qquad \forall v \in \mathbb{V}.$$

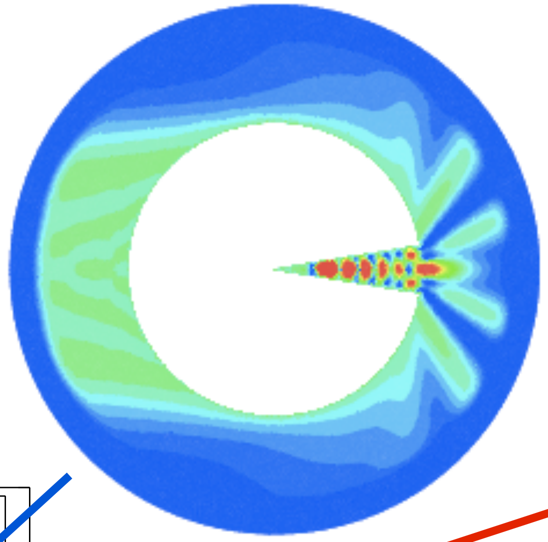
Then, compute $s(\mu) = \ell(u(\mu)) = \int_{\Gamma_1} u(\mu)$.

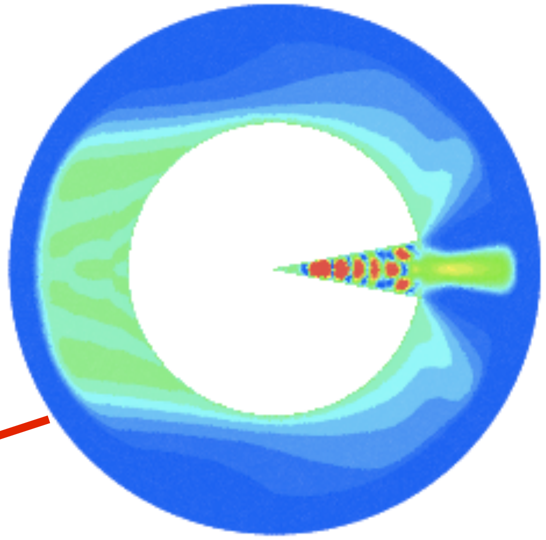
Parametrized problems - Ex 3

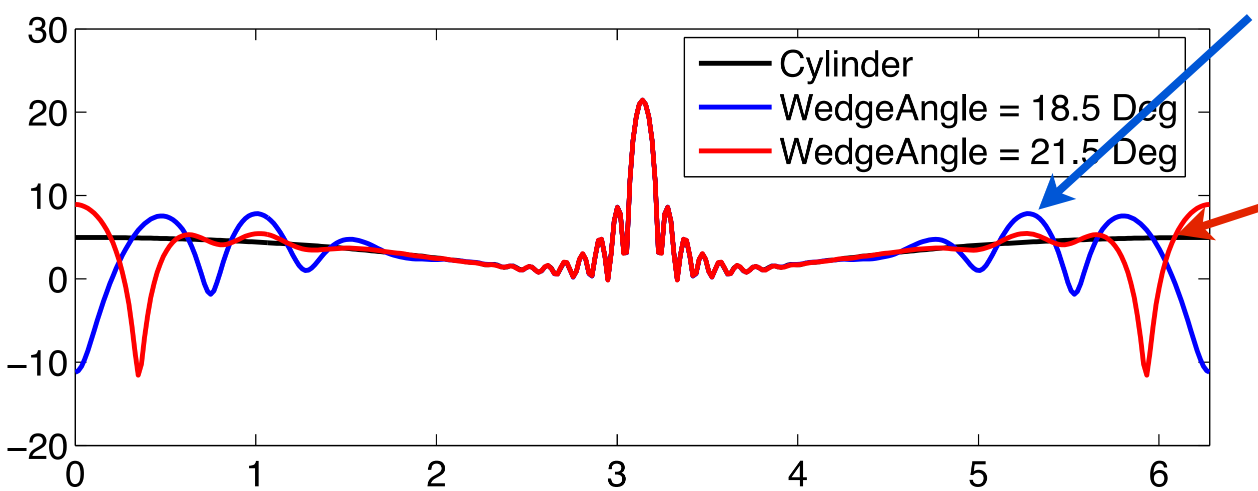


Scattering by 2D PEC Pacman

Backscatter depends very sensitively on cutout angle and frequency.







TM polarization

Difference in scattering is clear in fields

Parametrized problems - Ex 3

Assume that Ω is a homogenous media with magnetic permeability μ_0 and electrical permittivity ε_0.

Then, the electric field $E(\mu) = E^i(\mu) + E^s(\mu) \in H(\mathrm{curl}, \Omega)$ satisfies

$$\begin{aligned}
\mathrm{curl}\ \mathrm{curl}\ E(\mu) - k^2 E(\mu) &= 0 && \text{in } \Omega, && \text{Maxwell} \\
E(\mu) \times n &= 0 && \text{on } \Gamma, && \text{boundary condition} \\
\left| \mathrm{curl} E^s(x;\mu) \times \tfrac{x}{|x|} - ik E^s(x;\mu) \right| &= \mathcal{O}\left(\tfrac{1}{|x|}\right) && \text{as } |x| \to \infty. && \text{Silver-Müller radiation cond.}
\end{aligned}$$

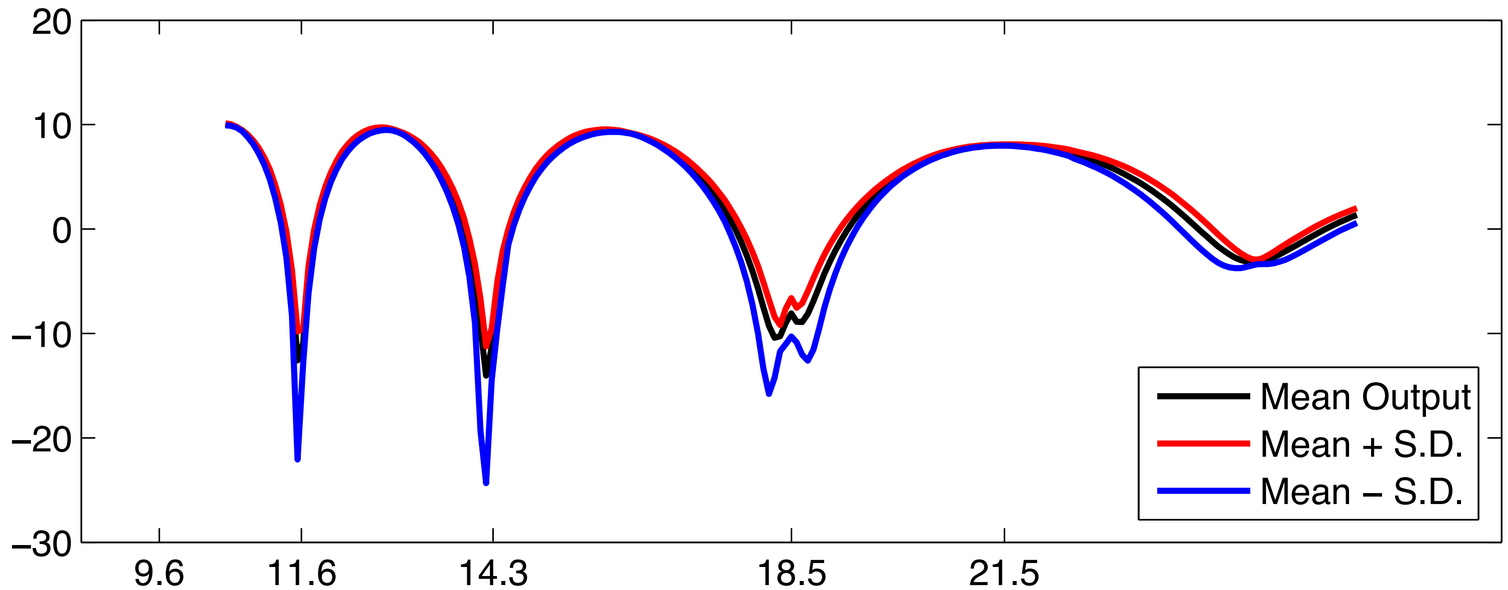
Boundary condition is equivalent to $\gamma_t E(\mu) = 0$ where γ_t denotes the tangential trace operator on surface Γ, $\gamma_t E(\mu) = n \times (E(\mu) \times n)$.

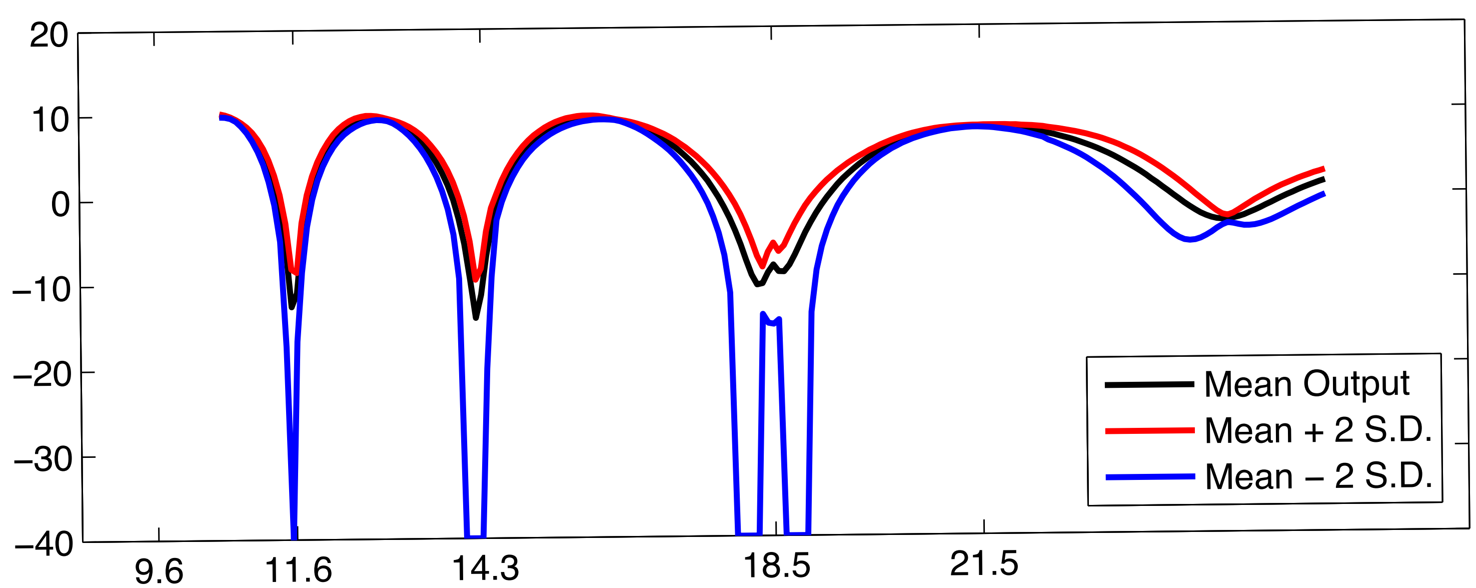
$k = \omega\sqrt{\mu_0 \varepsilon_0}$ is wave number and ω the angular frequency of the time-harmonic ansatz

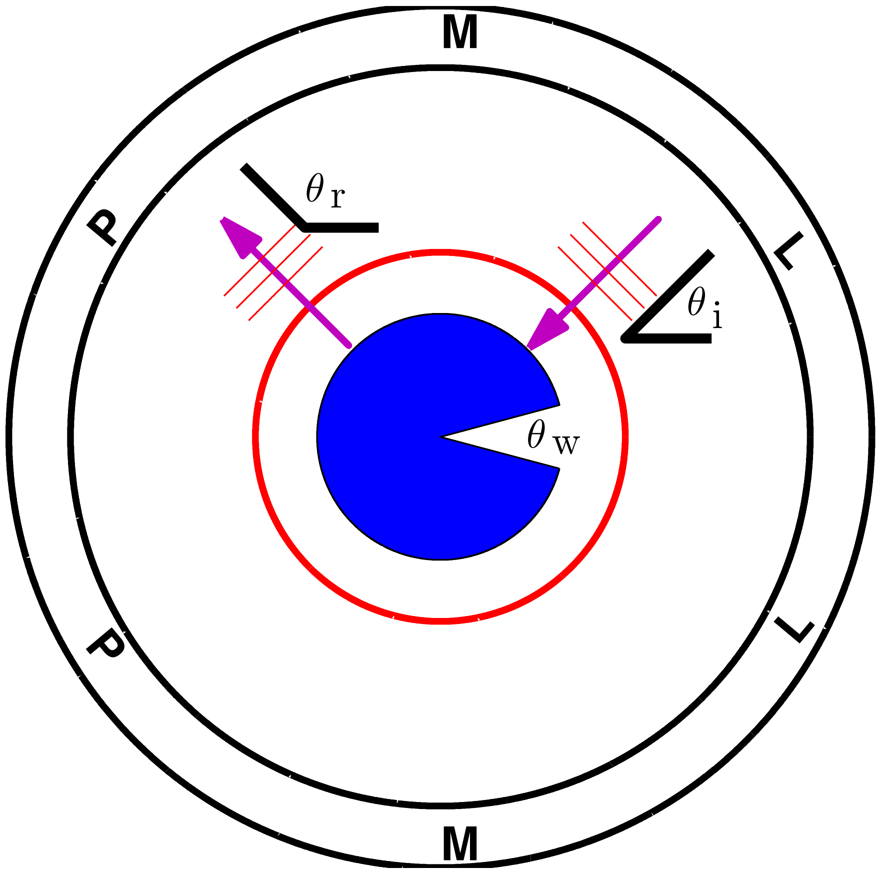
$$\hat{E}(x, t; \mu) = e^{-i\omega t} E(x; \mu).$$

Parametrized problems - Ex 3

Fast evaluation over parameter space allows for rapid uncertainty quantification





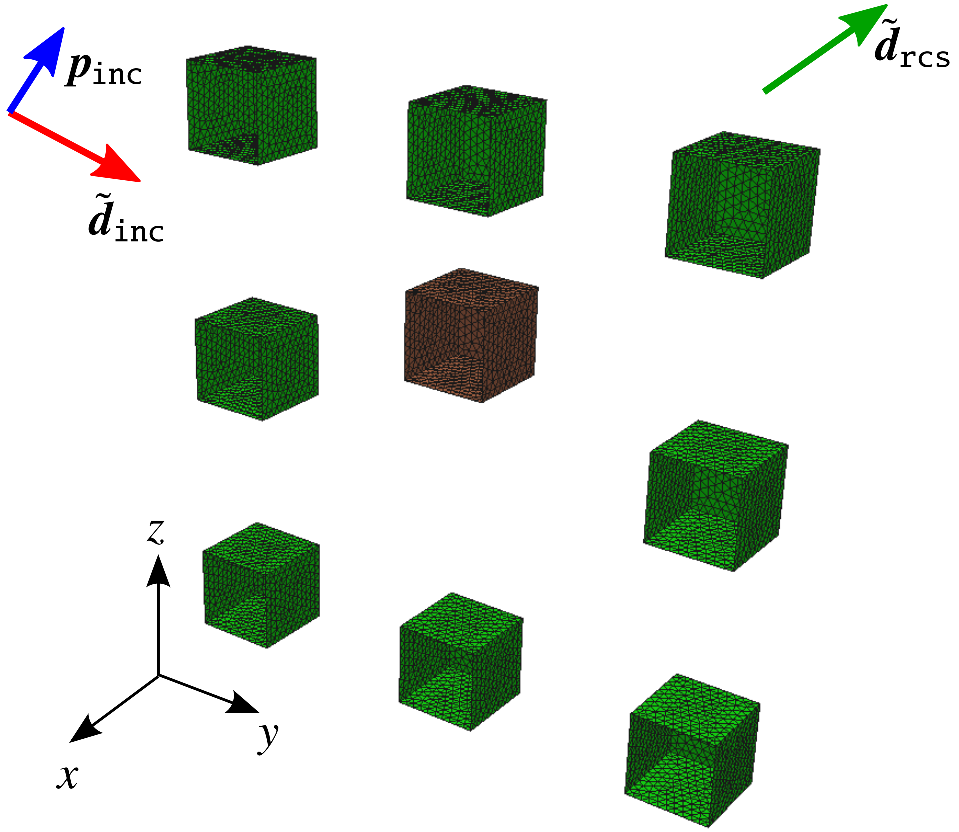


Uniformly distributed 5% randomness in gap angle

Parametrized problems

The parameters can describe

- Materials
- Sources
- Geometries
- Parameterized uncertainty
- Time
- etc



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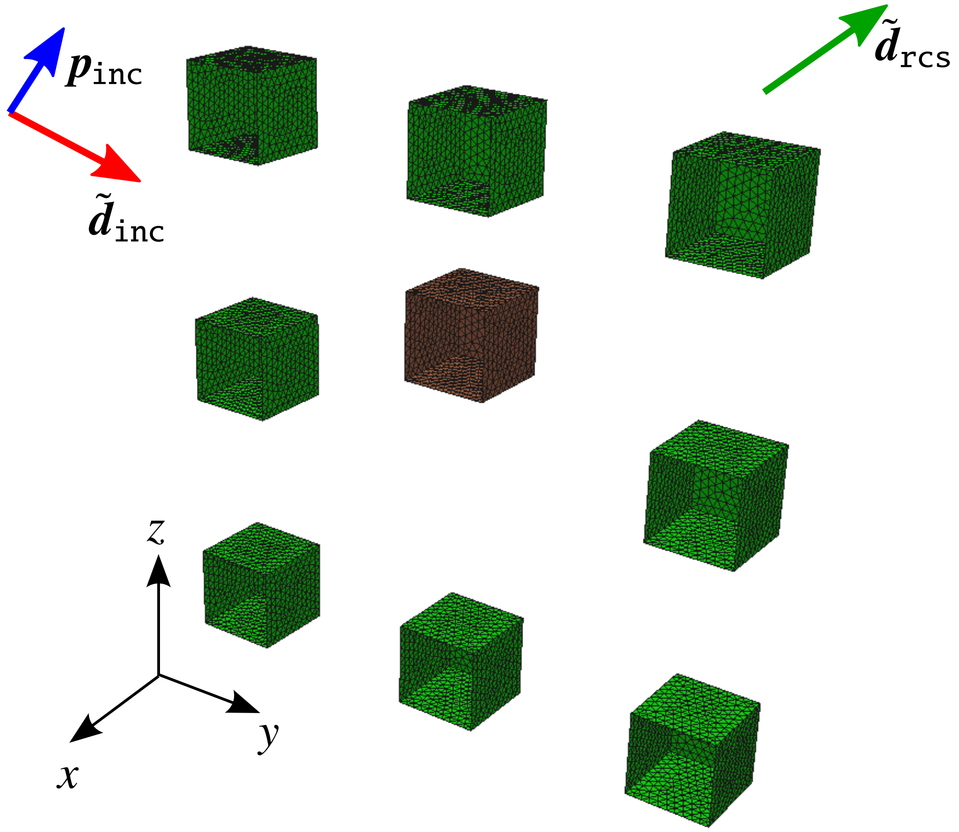


Does this always work, i.e., does a reduced model always exist ?

Probably not - we need to understand when and how to check

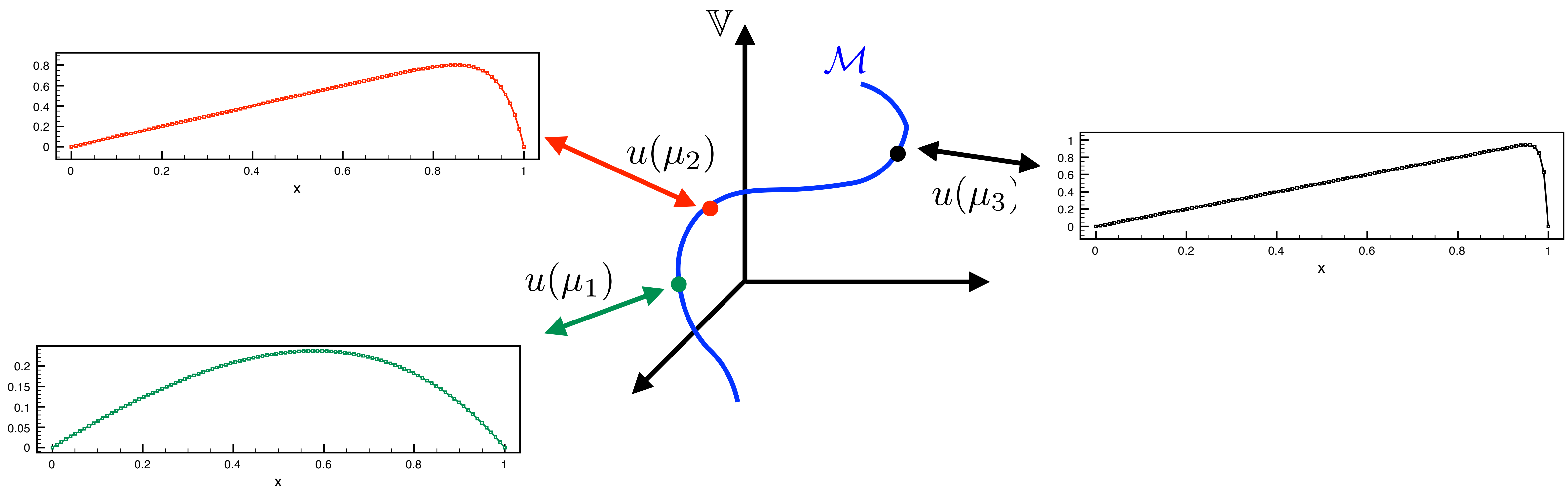
The solution manifold

Consider the "exact" and "discrete" solution manifolds

$$\mathcal{M} = \{u(\mu)\,;\,\forall \mu \in \mathbb{P}\} \subset \mathbb{V},$$

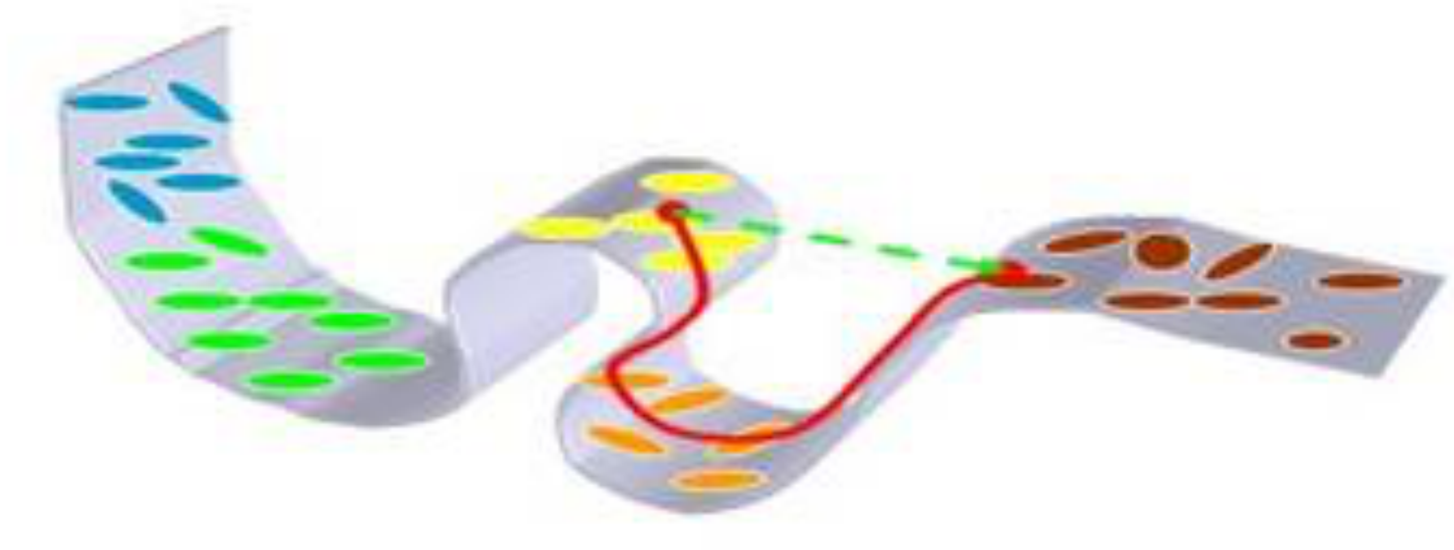
$$\mathcal{M}_\delta = \{u_\delta(\mu)\,;\,\forall \mu \in \mathbb{P}\} \subset \mathbb{V}_\delta,$$

where, for each $\mu \in \mathbb{P}$, $u(\mu)$ and $u_\delta(\mu)$ denote the solution of the underlying exact and discrete problems respectively.



The solution manifold

The key question is how well can the solution manifold $\mathcal{M}$ be approximated by $\mathcal{M}_\delta$ using an N-dimensional linear space ?



Clearly, if the solution space is (locally) smooth we have a good chance.

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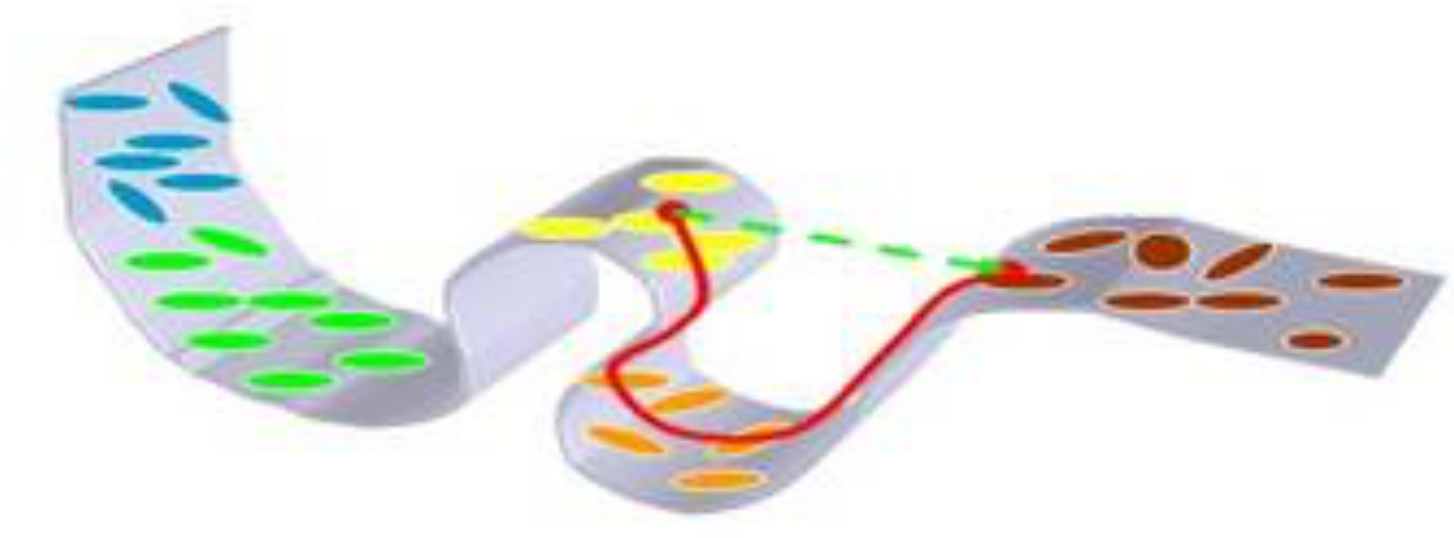

Clearly, if the solution space is (locally) smooth we have a good chance.

Highly sensitive/chaotic systems will be problematic as they have no structure

The solution manifold

For any N-dimensional space we define

$$E(\mathcal{M}, \mathbb{V}_{\texttt{rb}}) = \sup_{u(\mu)\in\mathcal{M}} \inf_{v_{\texttt{rb}}\in\mathbb{V}_{\texttt{rb}}} \|u(\mu) - v_{\texttt{rb}}\|_{\mathbb{V}}.$$

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The Kolmogorov N-width is defined as

$$d_N(\mathcal{M}) = \inf_{\mathbb{V}_{\mathtt{rb}}} E(\mathcal{M}, \mathbb{V}_{\mathtt{rb}}) = \inf_{\mathbb{V}_{\mathtt{rb}}} \sup_{u(\mu)\in\mathcal{M}} \inf_{v_{\mathtt{rb}}\in\mathbb{V}_{\mathtt{rb}}} \|u(\mu) - v_{\mathtt{rb}}\|_{\mathbb{V}},$$

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If this decays rapidly with N, we are in good shape

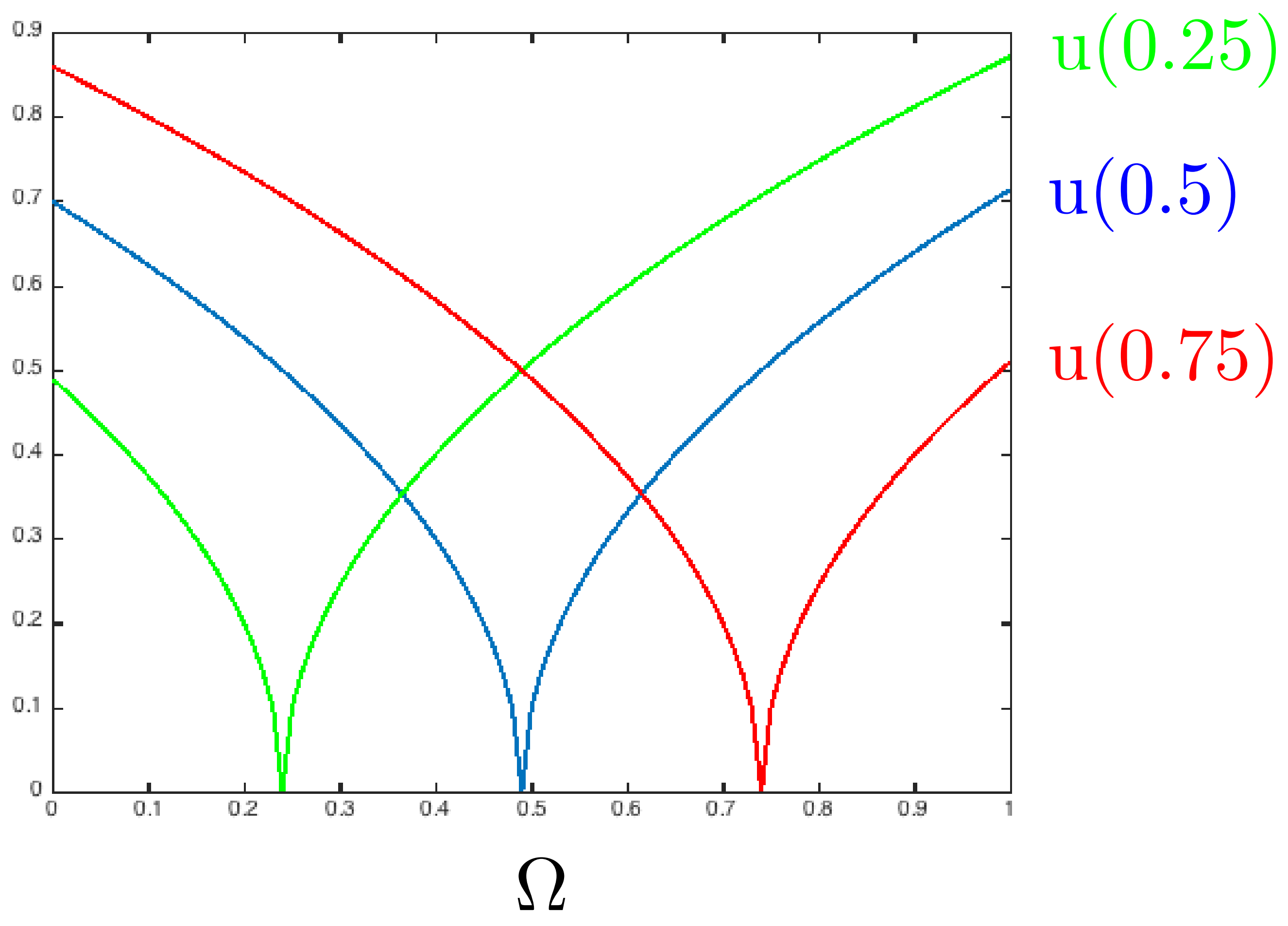
Identifying the optimal linear space by the Kolmogorov N-width is not practical — cost exponential in N

Solution manifold

The behavior of the Kolmogorov N-width is non-trivial

$$\mathcal{M} = \left\{ u(x,\mu) = |x-\mu|^{0.5} \;\middle|\; \mu, x \in (0,1) \right\}.$$

Singularity at varying location.



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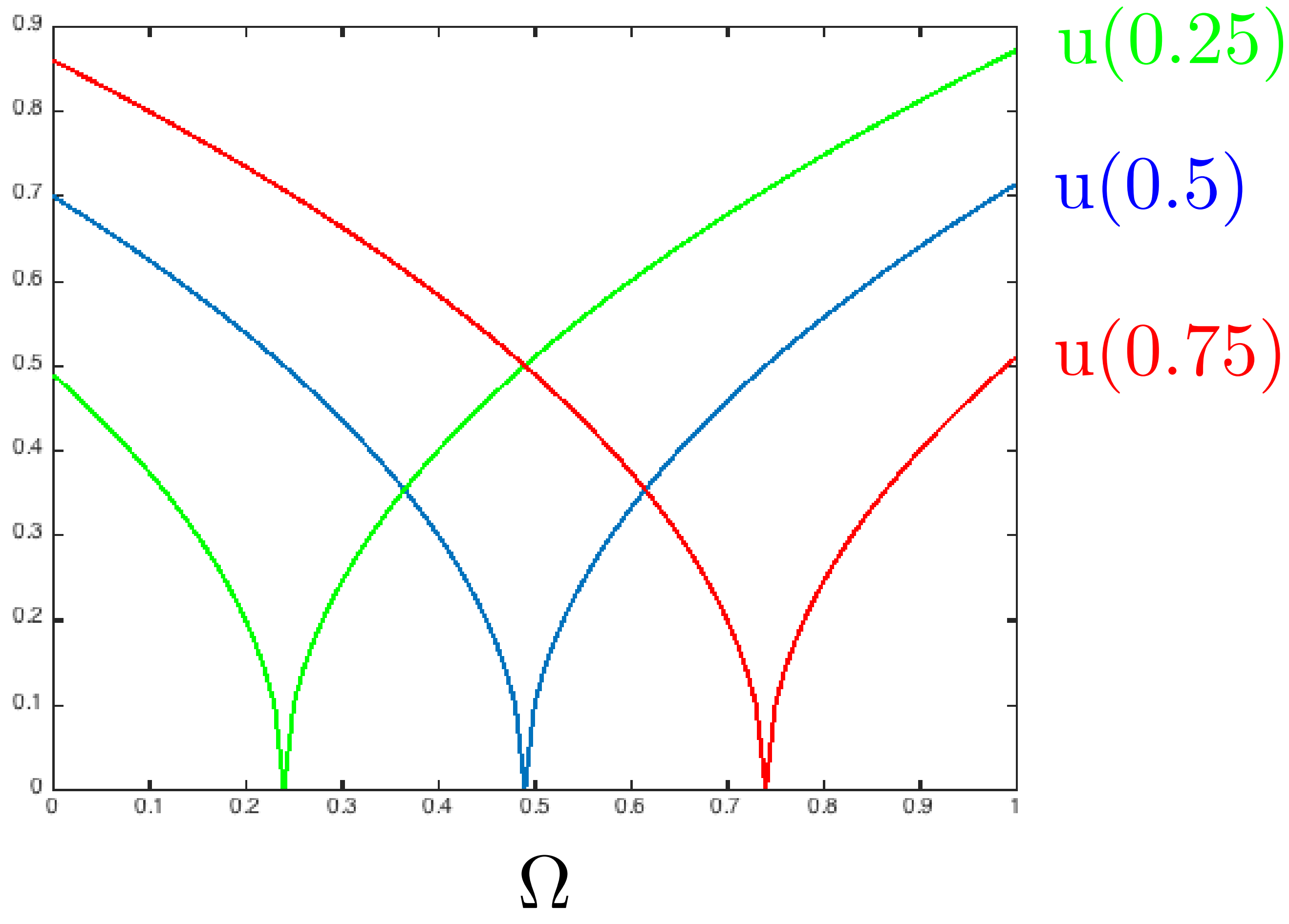
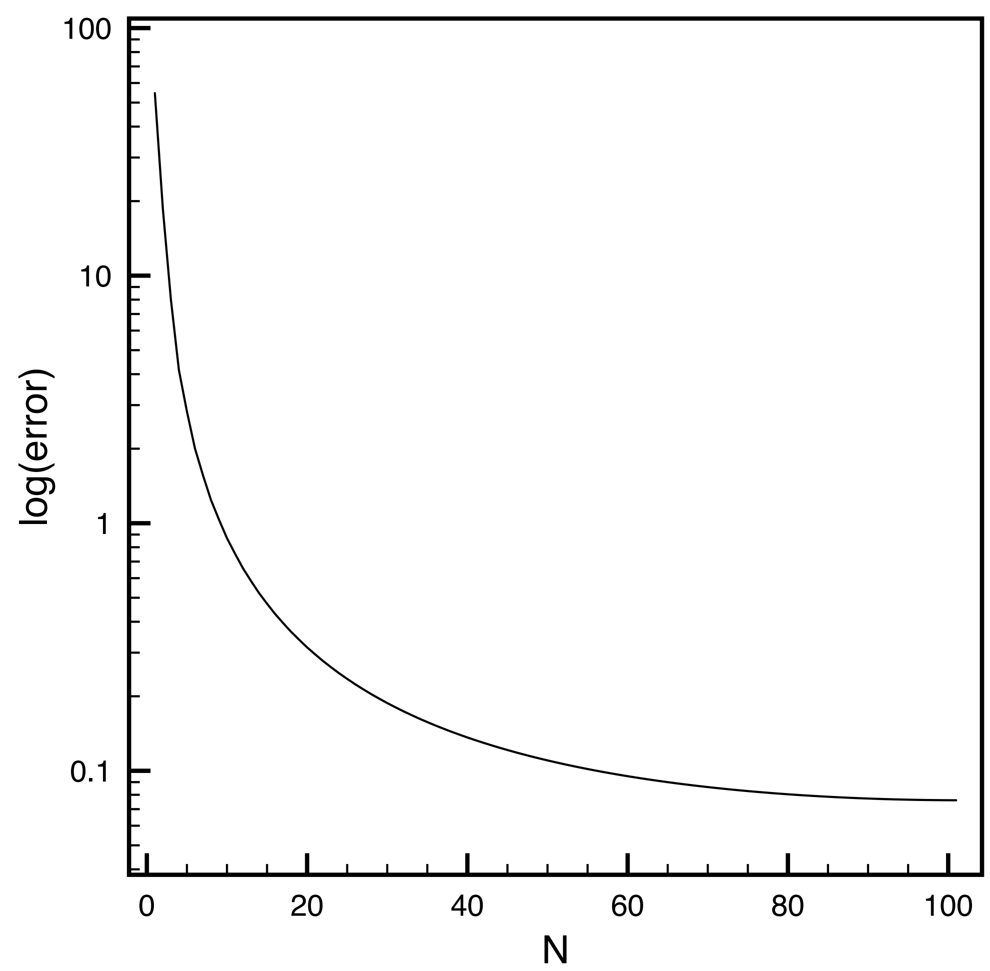


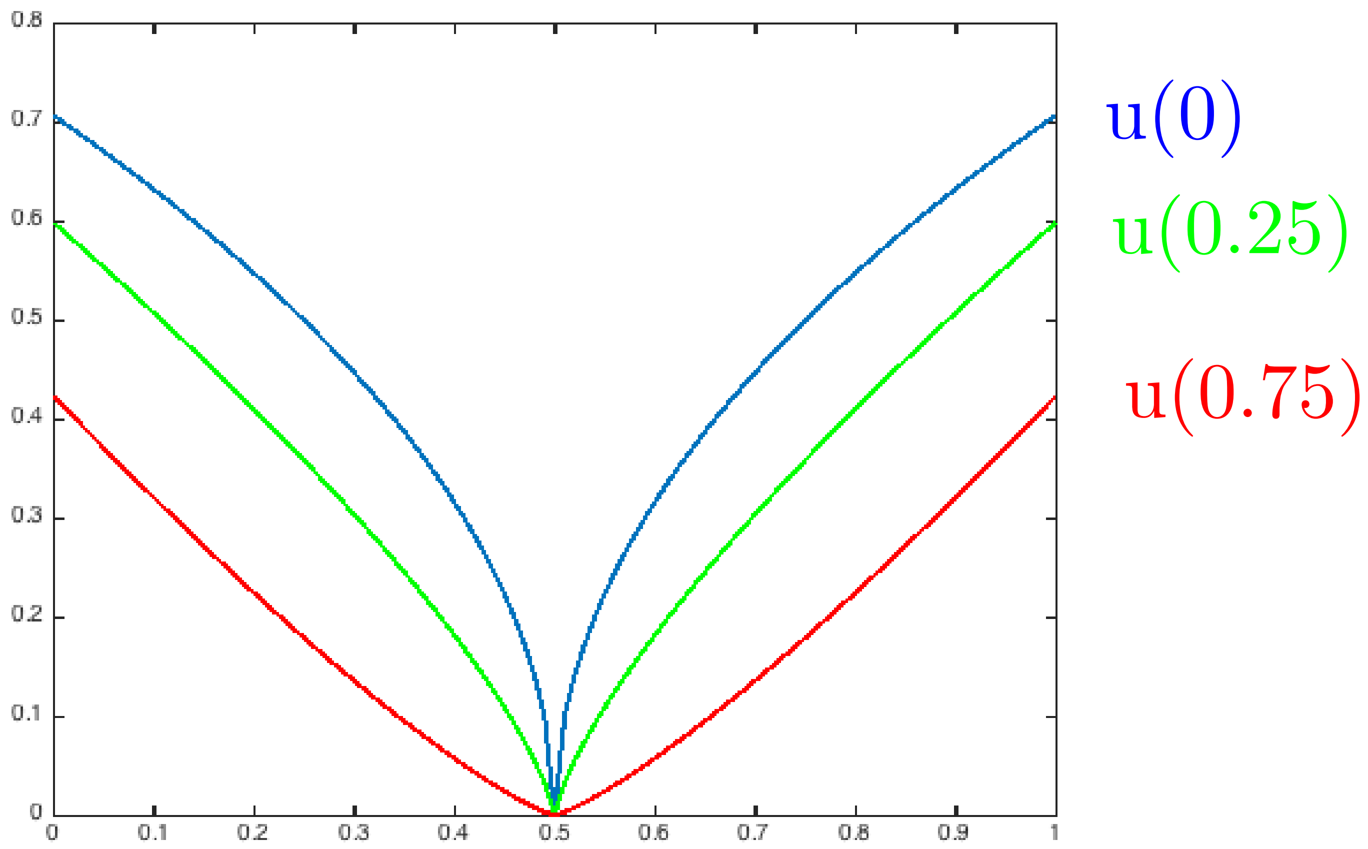
Error measure $d_N(\mathcal{M})$.



Solution manifold

$$\mathcal{M} = \left\{ u(x,\mu) = |x - 0.5|^{\mu+0.5} \;\middle|\; \mu, x \in (0,1) \right\}.$$

Singularity at fixed location
with varying width.



Solution manifold

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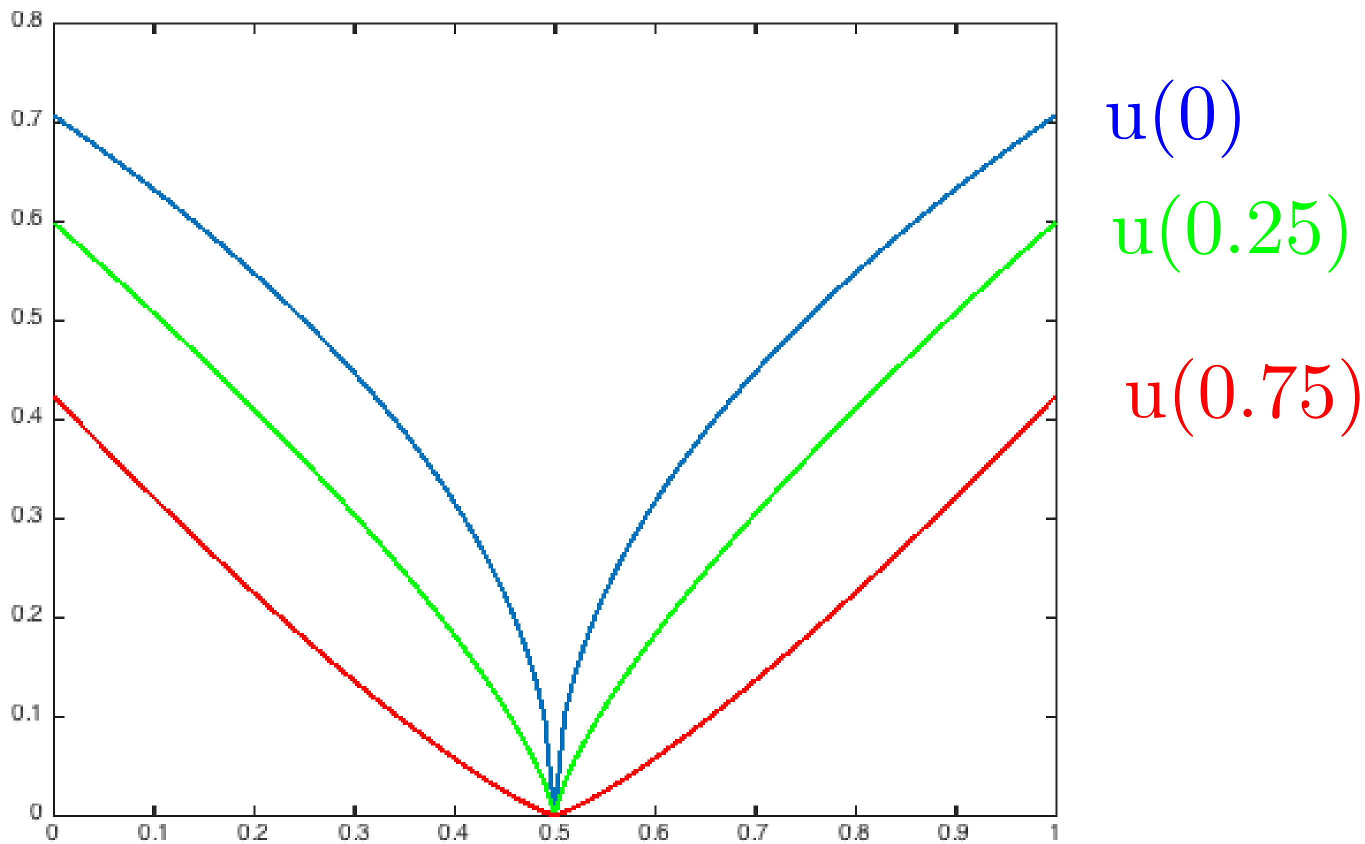

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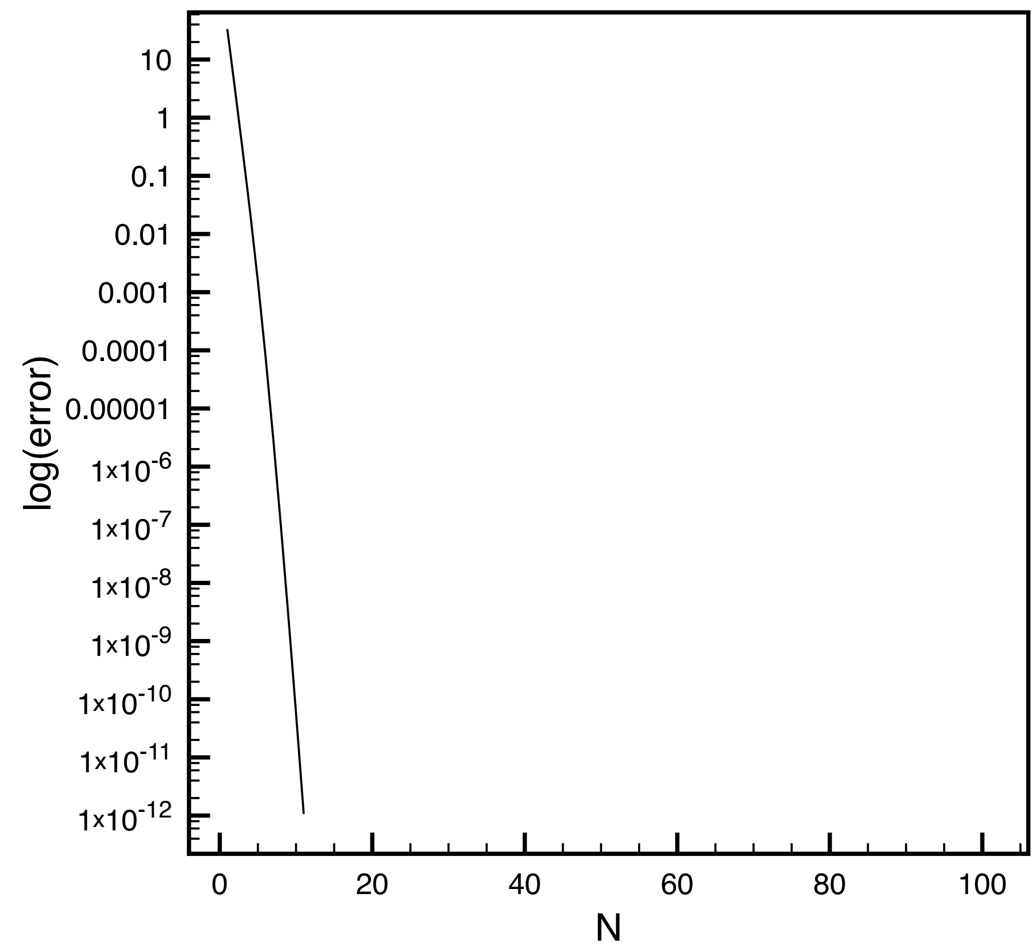
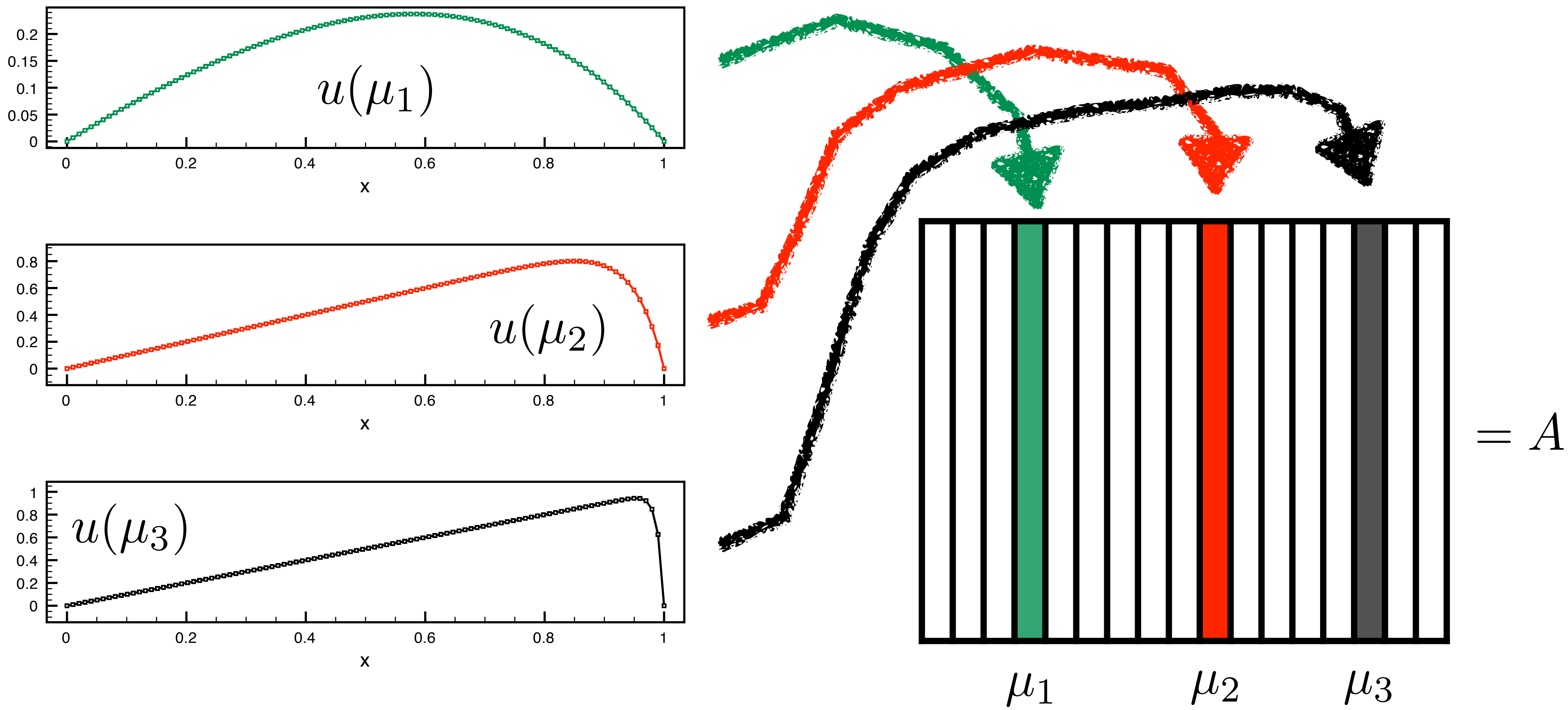


Morale: We need to check if a reduced space exists before going ahead

Solution manifold

We can get a good sense by a feasibility study

- Define a point-set $\mathbb{P}_h = \{\mu_1, \ldots, \mu_M\} \subset \mathbb{P}$.
- Compute for each μ_i the truth solution $u(\mu_i)$ using a simplified model.
- Store the degrees of freedom row-wise in a matrix A.

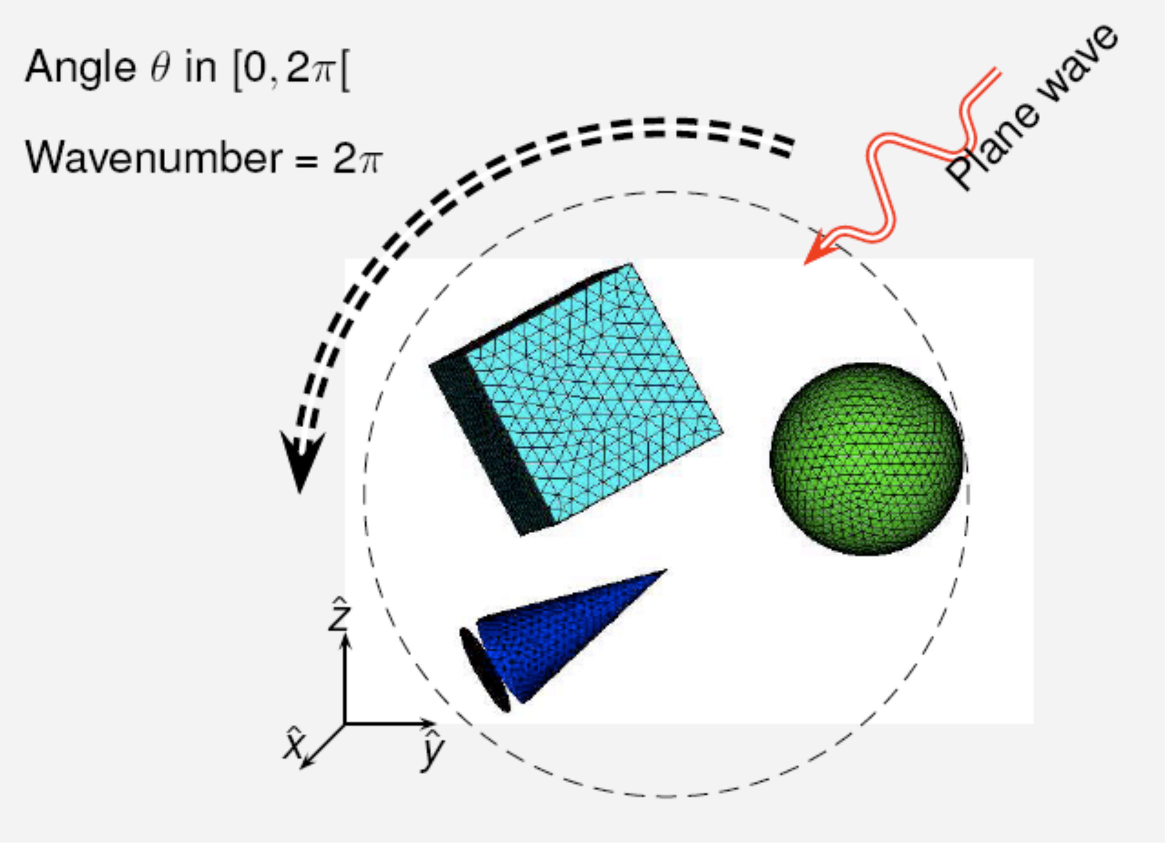


This samples the solution manifold

Solution manifold

3D EM scattering with the angle varying 0-360 deg. RCS is computed every 2 deg.

Computing the SVD of the 180 solutions shows that less than 60 samples would suffice -- and likely much less for applications

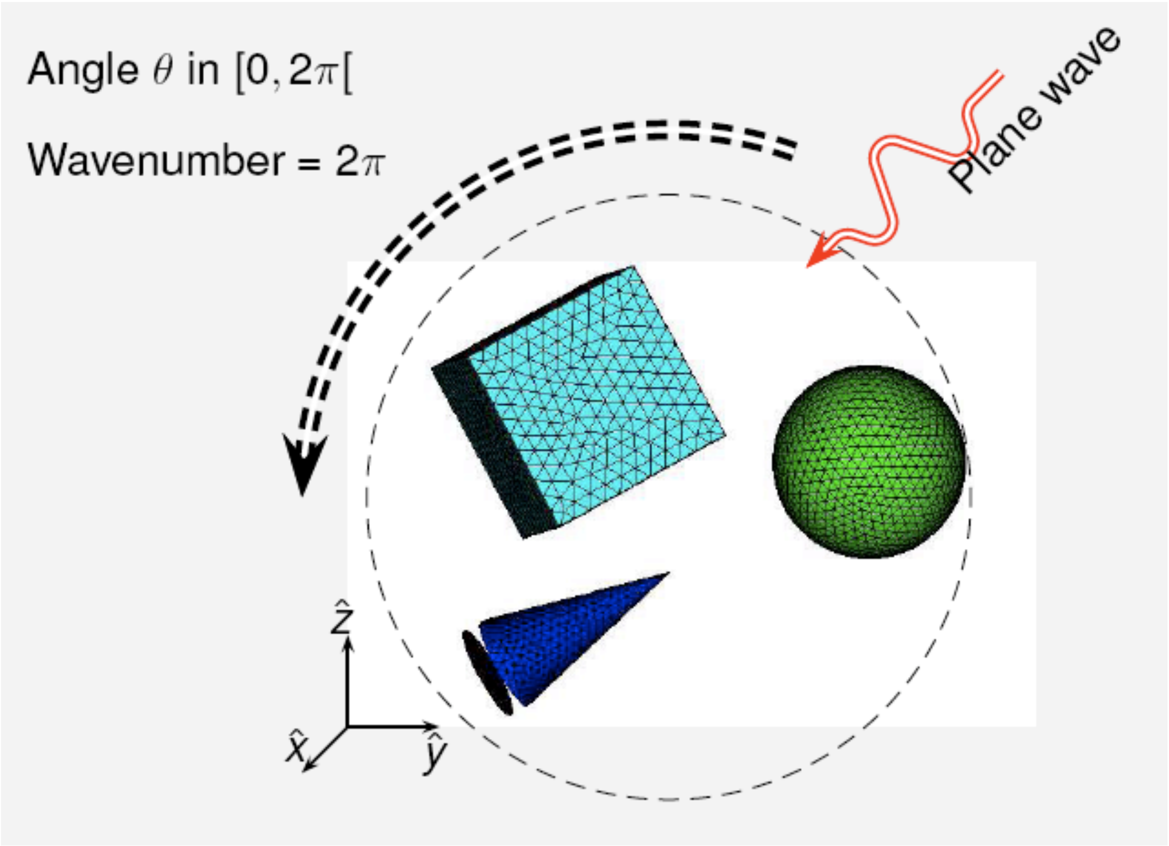


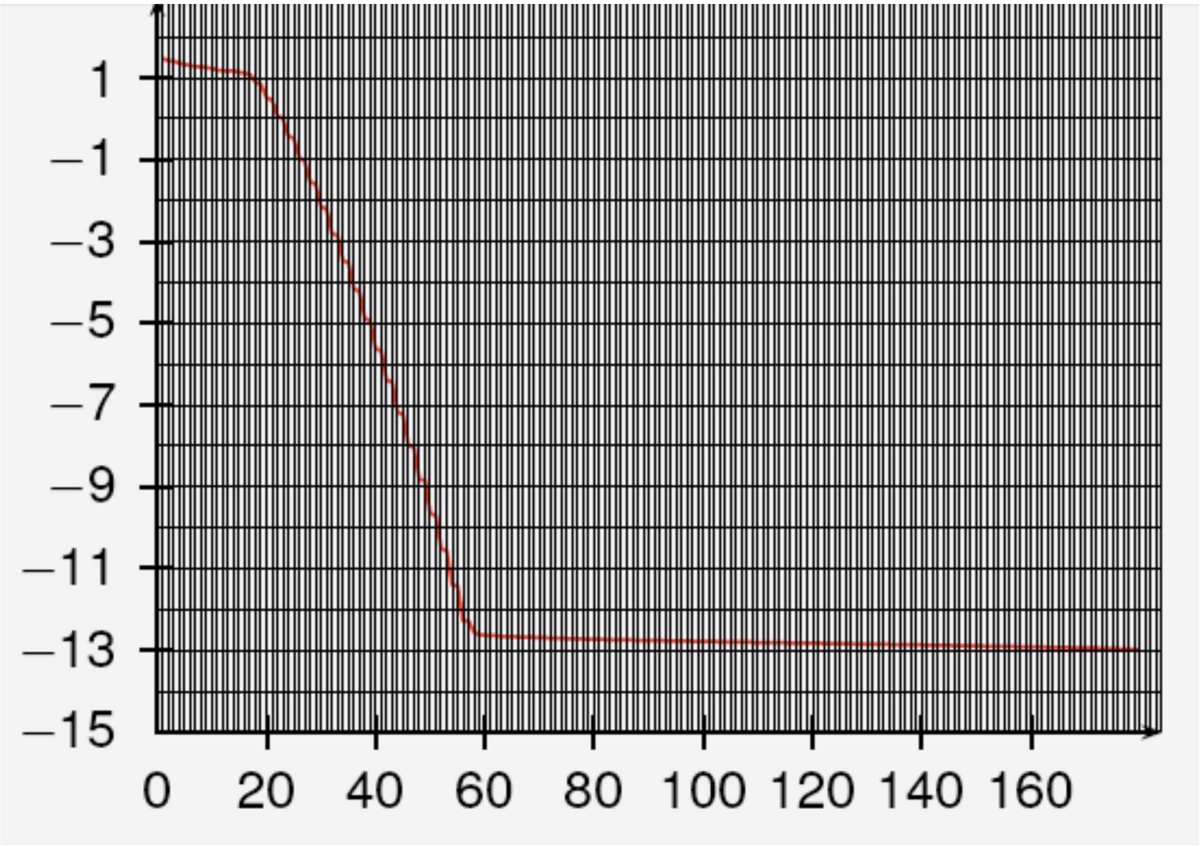
Computation by CERFACS

Solution manifold

3D EM scattering with the angle varying 0-360 deg. RCS is computed every 2 deg.

Computing the SVD of the 180 solutions shows that less than 60 samples would suffice -- and likely much less for applications



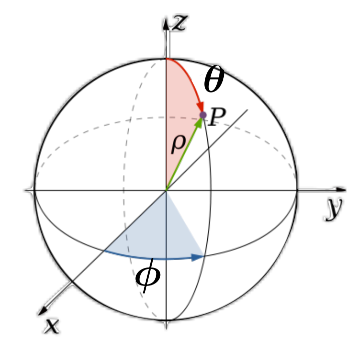


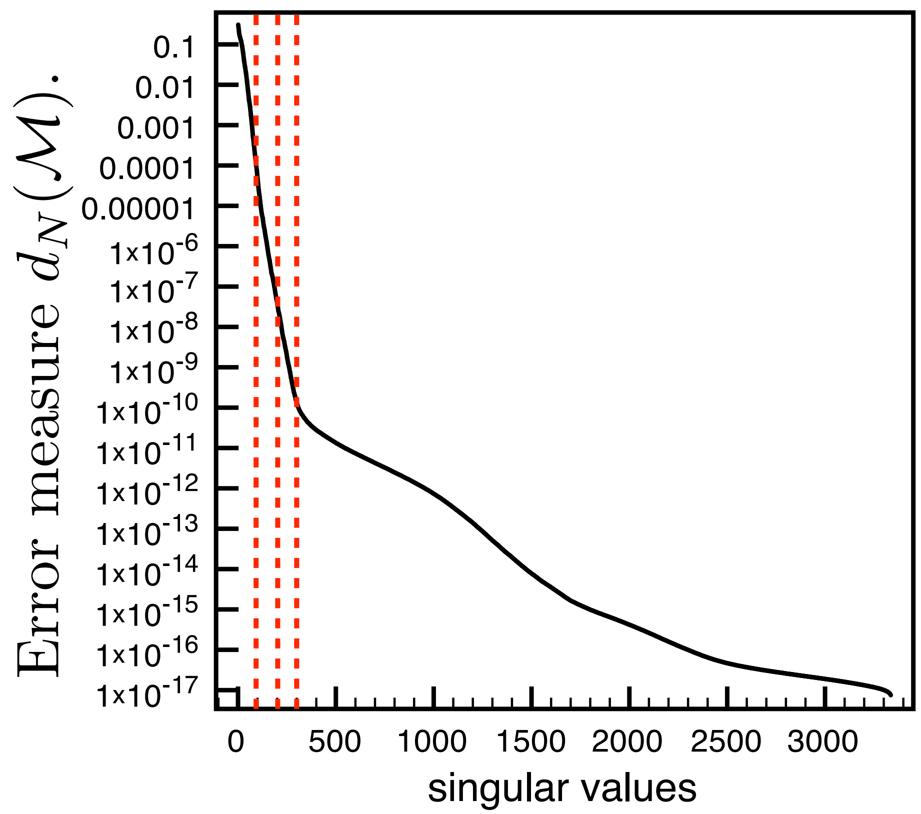
Computation by CERFACS

Solution manifold

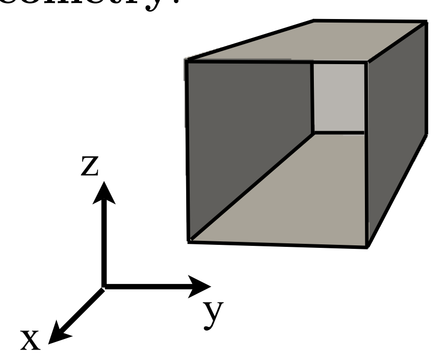
Computing the SVD of the solution matrix gives a measure of the decay of the Kolmogorov N-width

Example of the scattering problem: two dimensional parameterization with polar angle and frequency: $(k, \theta) \in [1, 25] \times [0, \pi]$, ϕ is fixed





Geometry:



With <100 basis functions you can reach a precision of 1e-3!

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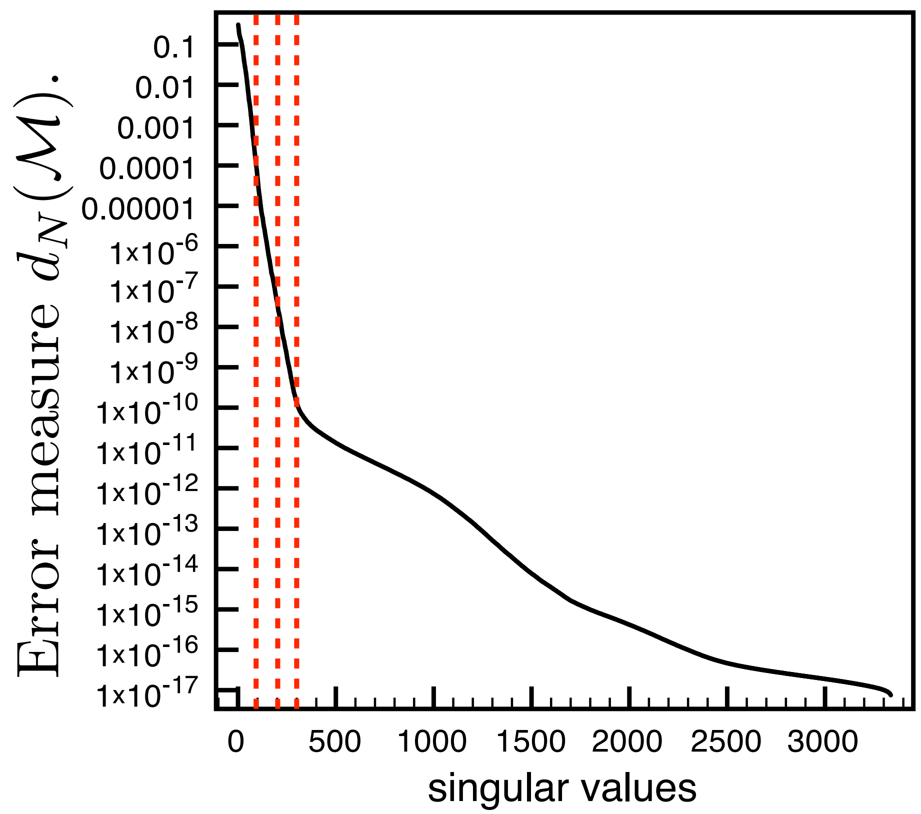

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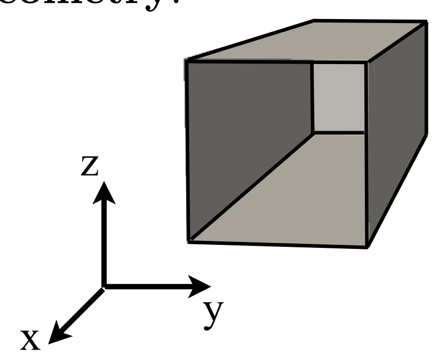

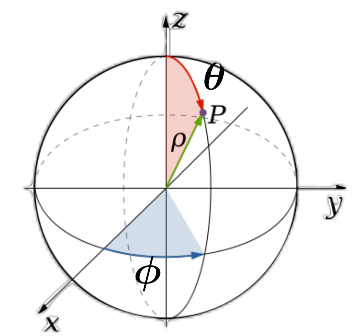

With <100 basis functions you can reach a precision of 1e-3!

Rigorous results are sparse for this - but there are some of the nature

$$d_N(\mathcal{M}) \leq Ce^{-cN}$$

Basic setting

We consider physical systems of the form

$$\mathcal{L}(\mathbf{x},\mu)u(\mathbf{x},\mu) = f(\mathbf{x},\mu) \qquad \mathbf{x} \in \Omega$$

$$u(\mathbf{x},\mu) = g(\mathbf{x},\mu) \qquad \mathbf{x} \in \partial\Omega$$

where the solutions are implicitly parameterized by

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where the solutions are implicitly parameterized by

$$\mu \in \mathcal{D} \in \mathcal{R}^N$$

- How do we find the basis.
- How do we ensure accuracy under parameter variation ?
- What about speed ?

Solutions and their behavior

Exact solution: For some parameter value $\mu \in \mathbb{P}$, find $u(\mu) \in \mathbb{V}$ such that

$$a(u(\mu), v; \mu) = f(v; \mu), \qquad \forall v \in \mathbb{V}.$$

Then, compute the value of the output functional $s(\mu) = \ell(u(\mu); \mu)$.

In practise, the exact PDE cannot be solved. A popular discretisation technique is the **Galerkin approach**: Replace the "continuous" space $\mathbb{V}$ by the finite dimensional subspace $\mathbb{V}_\delta$ such that

$$\lim_{\delta \to 0} \inf_{v_\delta \in \mathbb{V}_\delta} \|v - v_\delta\|_{\mathbb{V}} = 0, \qquad \forall v \in \mathbb{V}.$$

Galerkin solution: For some parameter $\mu \in \mathbb{P}$, find $u_\delta(\mu) \in \mathbb{V}_\delta$ such that

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

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$$\mathbf{A}_\delta^\mu \, \mathrm{u}_\delta^\mu = \mathrm{f}_\delta^\mu . \qquad s_\delta(\mu) = (\mathrm{u}_\delta^\mu)^T \, \mathrm{f}_\delta^\mu .$$

Convergence and stability

For coercive problems: Since $\mathbb{V}_\delta \subset \mathbb{V}$, there holds that the discrete coercivity constant

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

is uniformly bounded from below:

$$\boxed{0 < \alpha \leq \alpha_\delta(\mu),}$$

since

$$\boxed{0 < \alpha \leq \alpha(\mu) = \inf_{v \in \mathbb{V}} \frac{a(v, v; \mu)}{\|v\|_{\mathbb{V}}^2} \leq \inf_{v_\delta \in \mathbb{V}_\delta} \frac{a(v_\delta, v_\delta; \mu)}{\|v_\delta\|_{\mathbb{V}}^2}}$$

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Then

$$\|u(\mu) - u_\delta(\mu)\|_{\mathbb{V}} \;\leq\; \frac{\gamma(\mu)}{\alpha(\mu)} \|u(\mu) - v_\delta\|_{\mathbb{V}}, \quad \forall v_\delta \in \mathbb{V}_\delta$$

Let us construct our first model

Ultimative goal: a fast input-output computation: $\mu \mapsto s(\mu)$.

That is, for each $\mu \in \mathbb{P}$, evaluate $s(\mu) = \ell(u(\mu); \mu)$ where $u(\mu)$ is the solution of the parametrised weak problem: Find $u(\mu) \in \mathbb{V}$ s.t.

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In practise, the truth approximation is considered (instead of the exact solution): for $\mu \in \mathbb{P}$, evaluate $s_\delta(\mu) = \ell(u_\delta(\mu); \mu)$ where $u_\delta(\mu)$ is solution of: Find $u_\delta(\mu) \in \mathbb{V}_\delta$ s.t.

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Poor man's approach or **brute force approach**: For each new $\mu \in \mathbb{P}$, solve the above discrete problem to obtain $u_\delta(\mu)$ and compute the output $s_\delta(\mu)$.

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Too expensive

Basis by POD approach

$$\text{Seeking} \;\; u(x,t) \simeq u_\delta(x,t) \simeq V u_{rb}$$

Let $\mathbb{P}_h$ be a finite set of M points in $\mathbb{P}$ that are sampled "finely".

Introduce the error measure

$$\sqrt{\frac{1}{M} \sum_{\mu \in \mathbb{P}_h} \inf_{v_{\mathtt{rb}} \in \mathbb{V}_{\mathtt{rb}}} \|u(\mu) - v_{\mathtt{rb}}\|^2_{\mathbb{V}}}.$$

$\Rightarrow$ Average error of best approximation in $\mathbb{V}_{\mathtt{rb}}$ over $\mathbb{P}_h$.

The POD-space $\mathbb{V}_{\mathtt{POD}}$ is the N-dimensional sub-space of $\mathbb{V}_\delta$ that minimises the above error measure.

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Remark: The corresponding discrete Kolmogorov space would be the one that minimises the error measure

$$\boxed{\sup_{\mu \in \mathbb{P}_h} \inf_{v_{\mathtt{rb}} \in \mathbb{V}_{\mathtt{rb}}} \| u(\mu) - v_{\mathtt{rb}} \|_{\mathbb{V}}.}$$

Thus, this is question of L^∞ vs. L^2 over the parameter space $\mathbb{P}_h$.

Basis by POD approach

Proper Orthogonal Projection (POD):

1. Compute the solution $u_\delta(\mu)$ for all $\mu \in \mathbb{P}_h$ and define the correlation matrix

$$\boxed{C_{ij} = (u(\mu_j), u(\mu_i))_{\mathbb{V}}, \qquad i,j = 1,\dots,M.}$$

2. Find the eigen-pairs (λ_n, v_n) solution to $Cv_n = \lambda_n v_n$ for the N largest eigenvalues.
3. Define basis functions as

$$\boxed{\varphi_n = \sum_{i=1}^{M} (v_n)_i \, u(\mu_i).}$$

$\Rightarrow$ Basis functions are linear combinations of snapshots.

4. Set $\mathbb{V}_{\texttt{POD}} = \mathrm{span}\{\varphi_1, \dots, \varphi_N\}$.

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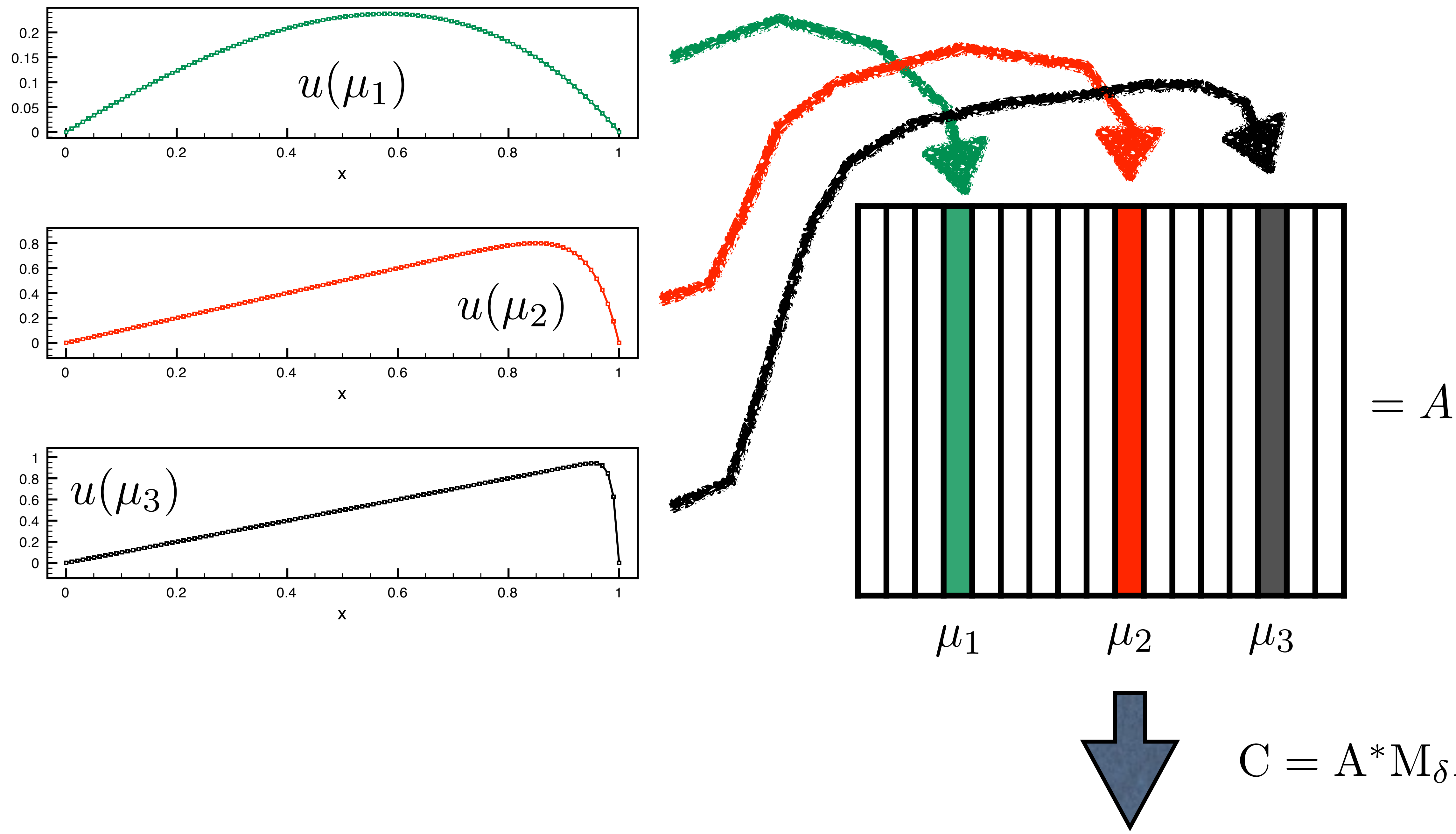
Result:

$$\boxed{\frac{1}{M} \sum_{i=1}^{L} \inf_{v \in \mathbb{V}_{\texttt{POD}}} \| u(\mu_i) - v \|_{\mathbb{V}}^2 = \sum_{n=N+1}^{M} \lambda_n.}$$

In practise: replace $u(\mu_i)$ by a truth approximation $u_\delta(\mu_i)$.

Basis by POD approach



$$\mathrm{C} = \mathrm{A}^* \mathrm{M}_\delta \mathrm{A}$$

Find eigen-decomposition of C

Basis by POD approach

The reduced model is now obtained as

$$A_h u_\delta = f_h \qquad \Rightarrow$$

$$(V^T A_h V) V^T u_\delta = V^T f_h \qquad V^T V = I$$

or

$$A_{rb} u_{rb} = f_{rb}$$

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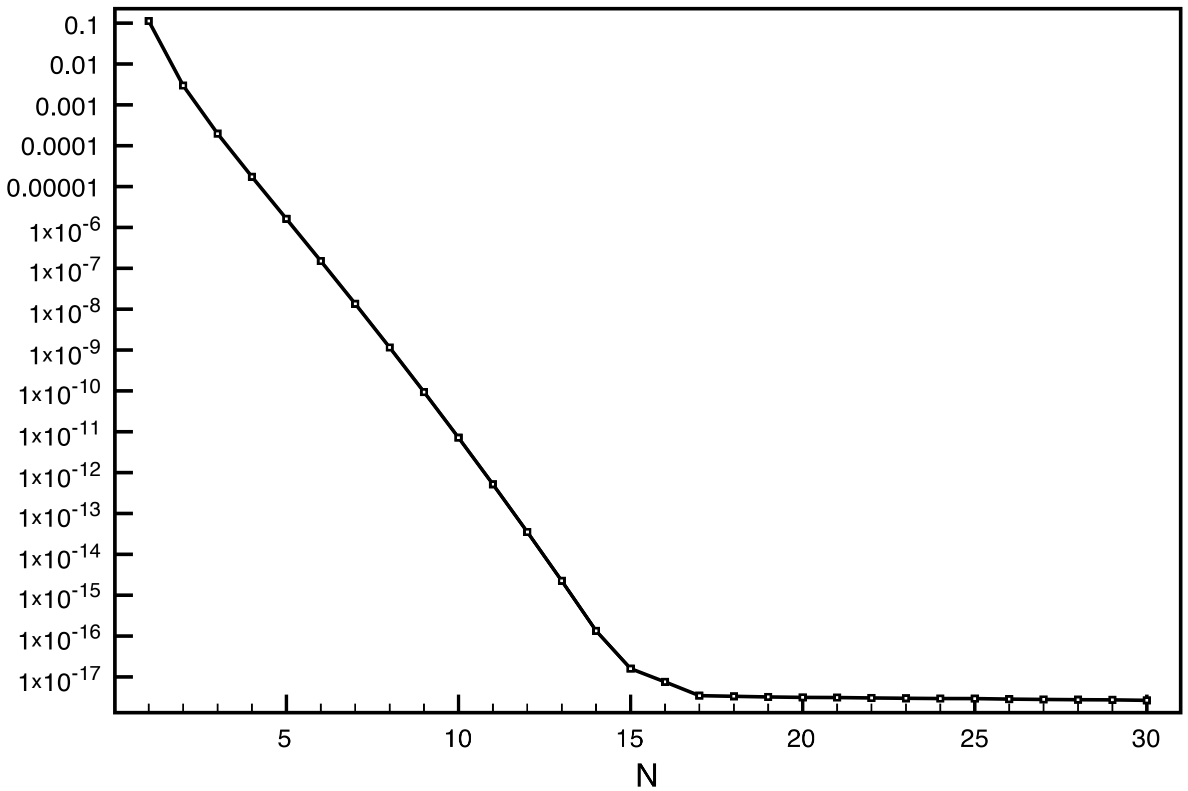
Since $N \ll \mathcal{N}$ we have the potential for speed

POD example - Ex 1

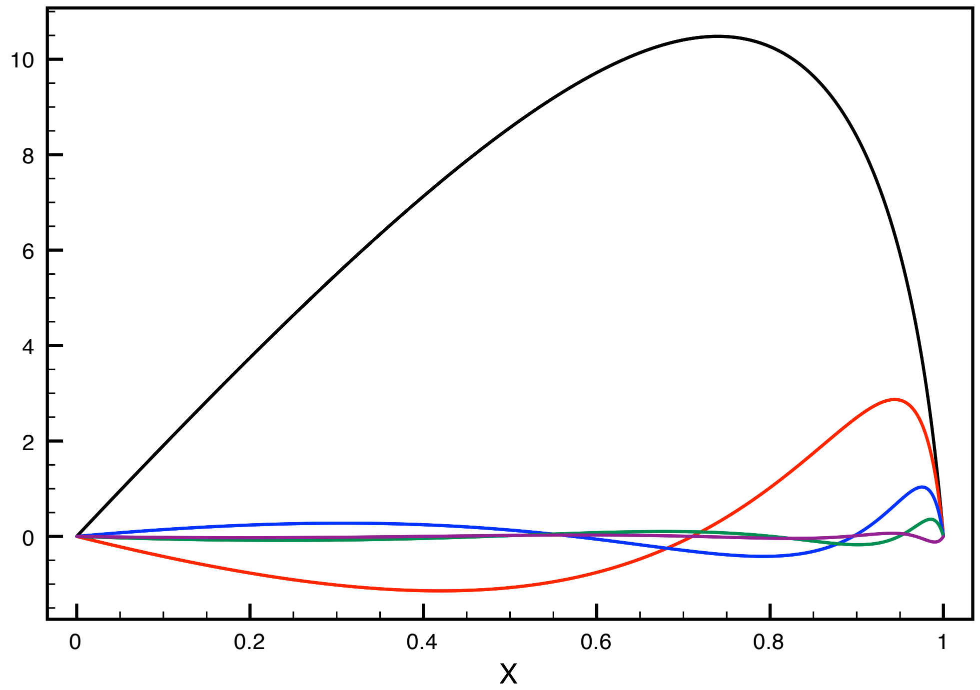
- Nodal values of exact solutions used instead of FE-approximations.
- $\mathbb{P}_h$: 491 equidistant points in $\mathbb{P} = [0.01, 0.5]$.

$$\begin{aligned} \varepsilon u'' + u' &= 1, \qquad \text{in } (0,1), \\ u(0) = u(1) &= 0. \end{aligned}$$

Eigenvalues:



5 first basis functions:



$\Rightarrow$ Precision of $\sim 10^{-6}$ with 5 basis functions.

POD methods

Method has several names -

- Karhunen-Loeve expansions
- Proper orthogonal expansions
- Empirical eigenfunctions

Properties -

- Simple and straightforward for linear systems
- Offline cost can be high
- Accuracy ? — did we sample carefully enough ?
- What about online cost for nonlinear problem

$$\nabla^2 u(x,\mu) = f(u,\mu) \quad \Rightarrow \quad A_{rb}(\mu) u_{rb}(x,\mu) = V^T f(V u_{rb},\mu)$$

Depends on $\mathcal{N}$

What's next

We need to develop methods that address these shortcomings

- Compute what we need - nothing more
- Control the error to certify results
- Ensure efficiency
- Deal with non-linear problems

This will be the main topics of Lecture 2

Questions ?