Some Approaches to Complexity Reduction: Application to Computational Chemistry

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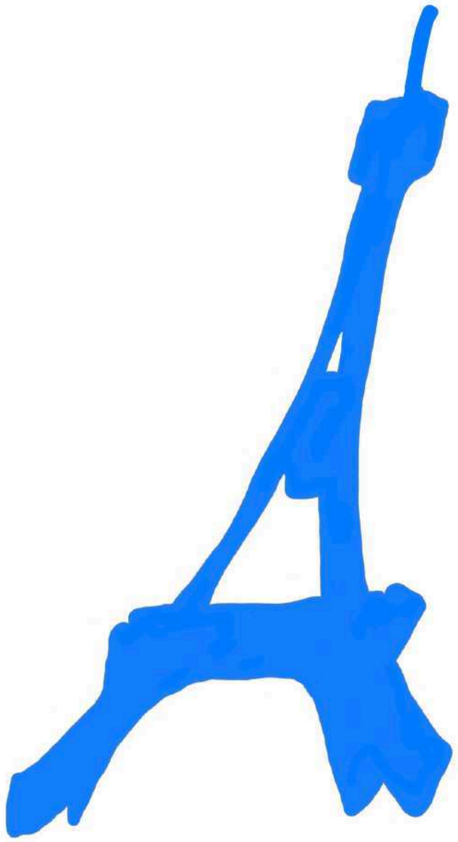
January 2020

ICODE workshop on numerical solution of HJB equations



Vague Statements

The quantities we are interested in, are functions, depending on space (and time), that are associated to the phenomenon we are interested in.

Mathematically this means that there are some parameters and that we are thus interested in $u(x, t; \mu)$

Here μ is a parameter well suited to the problem

A less vague statement

Where to look for $u(x,t;\mu)$?

$$\mathcal{S} = \{u(x,t;\mu),\ \text{when } \mu \text{ varies in } \mathcal{D}\}$$

REDUCTION OF COMPLEXITY

Looking for a needle in a Haystack
performance of SVEN SACHSALBER

REDUCTION OF COMPLEXITY

or looking for a needle in a needle cushion

REDUCTION OF COMPLEXITY

At the mathematical level, this translates into :

- looking for the approximation in some Banach space (e.g. L^2 or H^1) of regular enough functions : leading e.g. to finite element or spectral approximations
- or looking for the approximation of functions in a (well behaved) manifold (denoted as $\mathcal{S}$) : reduction of complexity

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Allows to use the knowledge of S

the right tool being then the Kolmogorov width.

Kolmogorov n-width

Definition Let X be a normed linear space, $\mathcal{S}$ be a subset of X and X_n be a generic n-dimensional subspace of $\mathcal{X}$. The deviation of $\mathcal{S}$ from X_n is

$$E(\mathcal{S}; X_n) = \sup_{u \in \mathcal{S}} \inf_{v_n \in X_n} \|u - v_n\|_X.$$

The *Kolmogorov n-width* of $\mathcal{S}$ in X is given by

$$d_n(\mathcal{S}, X) = \inf_{X_n} \sup_{u \in \mathcal{S}} \inf_{v_n \in X_n} \|u - v_n\|_X$$

The n-width of $\mathcal{S}$ thus measures the extent to which $\mathcal{S}$ may be approximated by a n-dimensional subspace of X.

Why should $\mathcal{S}$ have a small Kolmogorov width ?

Intuition

Verification

Mathematical Analysis

WHY SHOULD $\mathcal{S}$ HAVE A SMALL KOLMOGOROV WIDTH ?

MATHEMATICAL ANALYSIS

Until recently there was very few analysis on this matter[1] . . .

1 - Y. Maday, A.Patera, and G. Turinici. A priori convergence theory for reduced-basis approximations of single-parameter elliptic partial differential equations Journal of Scientific Computing 17, 437-446, 2002.

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Since, June 2014
Kolmogorov widths under holomorphic mappings by Albert Cohen and Ronald DeVore

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Why should $\mathcal{S}$ have a small Kolmogorov width ?

Simple fact : if L is a bounded linear operator mapping the Banach space X into the Banach space Y and $\mathcal{D}$ is a compact set in X, then the Kolmogorov widths of the image $L(\mathcal{D})$ do not exceed those of $\mathcal{D}$ multiplied by the norm of L.

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More involved statement : Cohen and DeVore have extended this result from linear maps to holomorphic mappings $\mathcal{L}$ from X to Y in the following sense:

when the n-widths of $\mathcal{D}$ are $O(n^{-r})$ for some $r > 1$, then those of $\mathcal{L}(\mathcal{D})$ are $O(n^{-s})$ for any $s < r - 1$,

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This can be the solution to some parameter dependent (elliptic) PDE, possibly nonlinear . . . : $\mu \in \mathcal{D}$ with small dimension $\Rightarrow \mathcal{S} = \{u(.,\mu), \mu \in \mathcal{D}\}$ has a small dimension !

but this can also be further applied to the situation e.g. : Assume $\mathcal{S}$ has a small Kolmogorov width, then : $\mathcal{S}^3 = \{u^3(.,\mu), \mu \in \mathcal{D}\}$ has also a small Kolmogorov width (and also $e^{\mathcal{S}} = \{e^{u(.,\mu)}, \mu \in \mathcal{D}\}$).

An example

The two group diffusion equation in matrix notation reads

$$\boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{\varphi} = \frac{1}{k_{eff}}\boldsymbol{F}(\boldsymbol{\mu})\boldsymbol{\varphi}$$

Where $\boldsymbol{\mu}$ is the parameters set, e.g. D, Σ, $\nu\Sigma_f$. $\boldsymbol{A}$ and $\boldsymbol{F}$ are 2×2 matrix and $\boldsymbol{\varphi}$ is a 2-element column vector:

$$\boldsymbol{A}(\boldsymbol{\mu}) = \begin{pmatrix} -\nabla\cdot D^1\nabla + (\Sigma_a^1 + \Sigma_s^{1\to 2}) & 0 \\ -\Sigma_s^{1\to 2} & -\nabla\cdot D^2\nabla + \Sigma_a^2 \end{pmatrix}$$

$$\boldsymbol{F}(\boldsymbol{\mu}) = \begin{pmatrix} \chi_1\nu\Sigma_f^1 & \chi_1\nu\Sigma_f^2 \\ \chi_2\nu\Sigma_f^1 & \chi_2\nu\Sigma_f^2 \end{pmatrix}$$

$$\boldsymbol{\varphi} = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$$

Where $D^i,\ i = 1,2$ is called the *diffusion coefficient* of each group; $\Sigma_a^i,\ i = 1,2$ is the absorption cross section of each group; $\varphi_i,\ i = 1,2$ is the neutron flux of each group; $\Sigma_s^{1\to 2}$ is called the removal cross section from group 1 to group 2; $\nu\Sigma_f^1,\ i = 1,2$ is the fission source term of each group; $\chi_i,\ i = 1,2$ is called the fission spectrum of each group; finally k_{eff} is the effective multiplication factor, also the *eigenvalue* of equation.

In 1D, this looks like

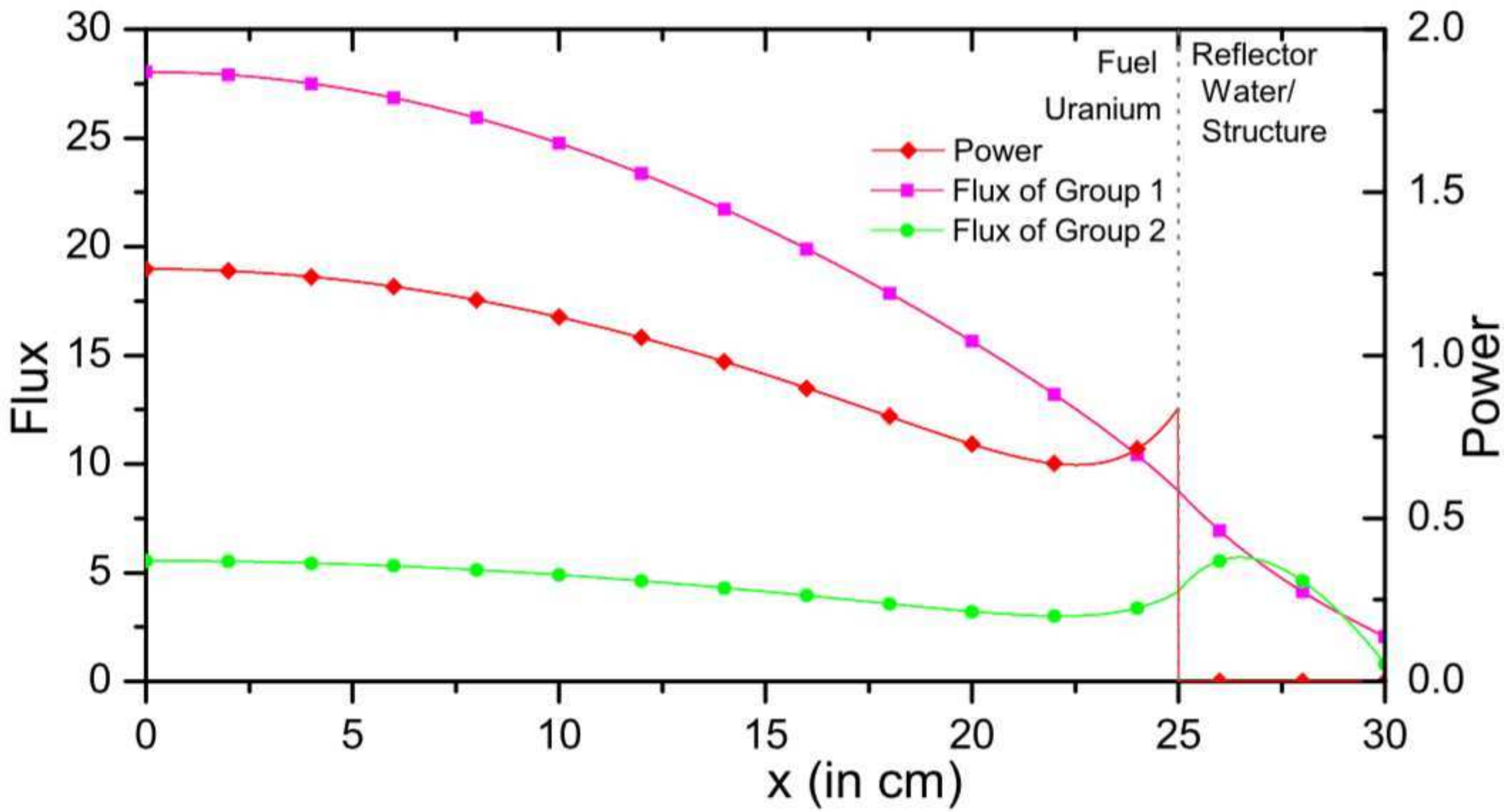
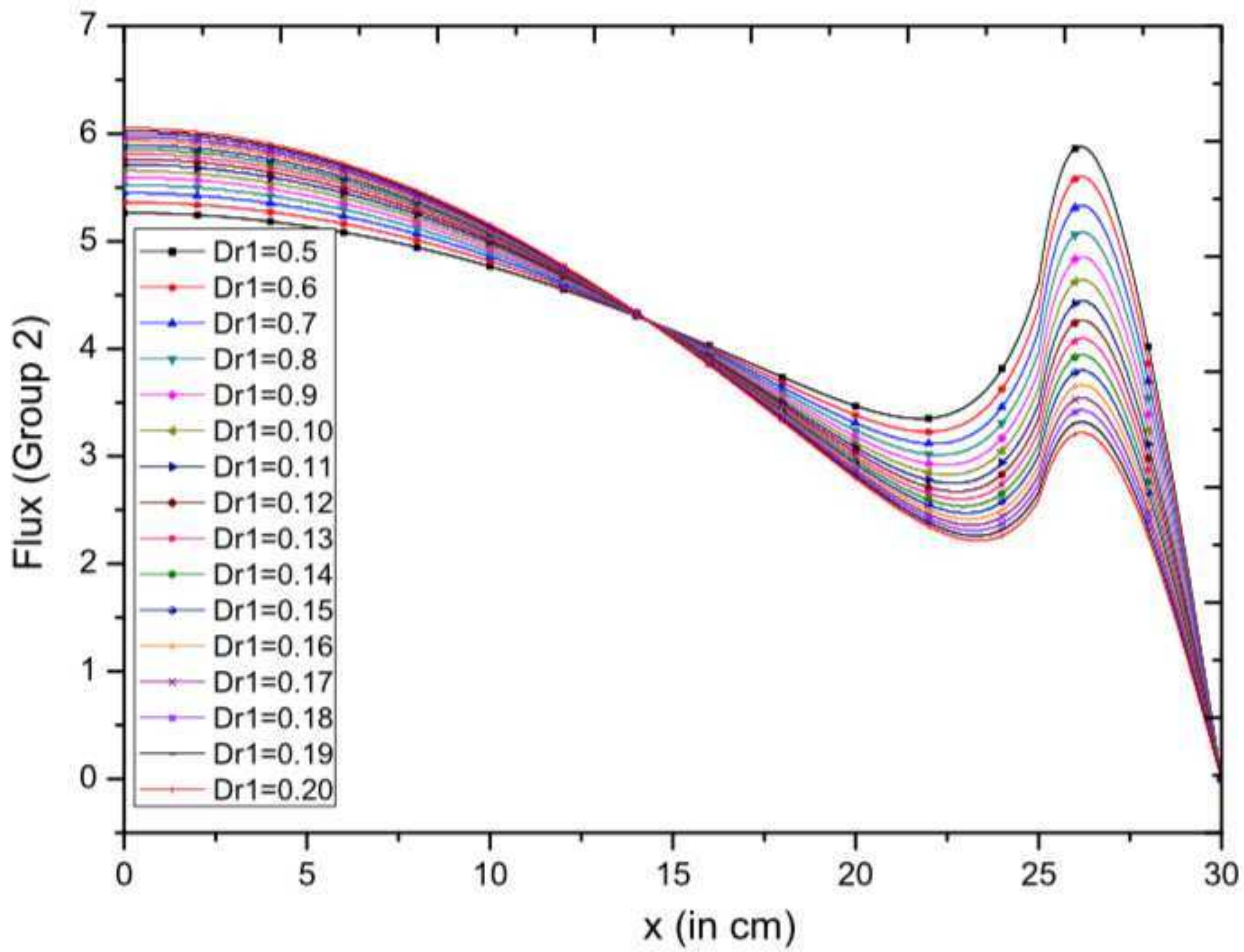


Figure 1: Flux and power distribution in the Core for the benchmark problem

In order you are convinced that the Kolmogorov dimension is small



Another example

Another example

less simple

$$u(\mu) = \text{Arg} \inf_{\int u^2 = 1} E(u, \mu)$$

where

$$E(u, \mu) = \frac{1}{2} \int_\Omega |\nabla u|^2 dxdy + \int_\Omega V(., \mu) u^2 dxdy + \int_\Omega \int_\Omega \frac{u^2(x) u^2(y)}{|x - y|} dxdy$$

With the potential

$$V(x, y, \mu) = \frac{\mu_2}{\sqrt{(x + \mu_1/2)^2 + y^2}} + \frac{\mu_2}{\sqrt{(x - \mu_1/2)^2 + y^2)}}$$

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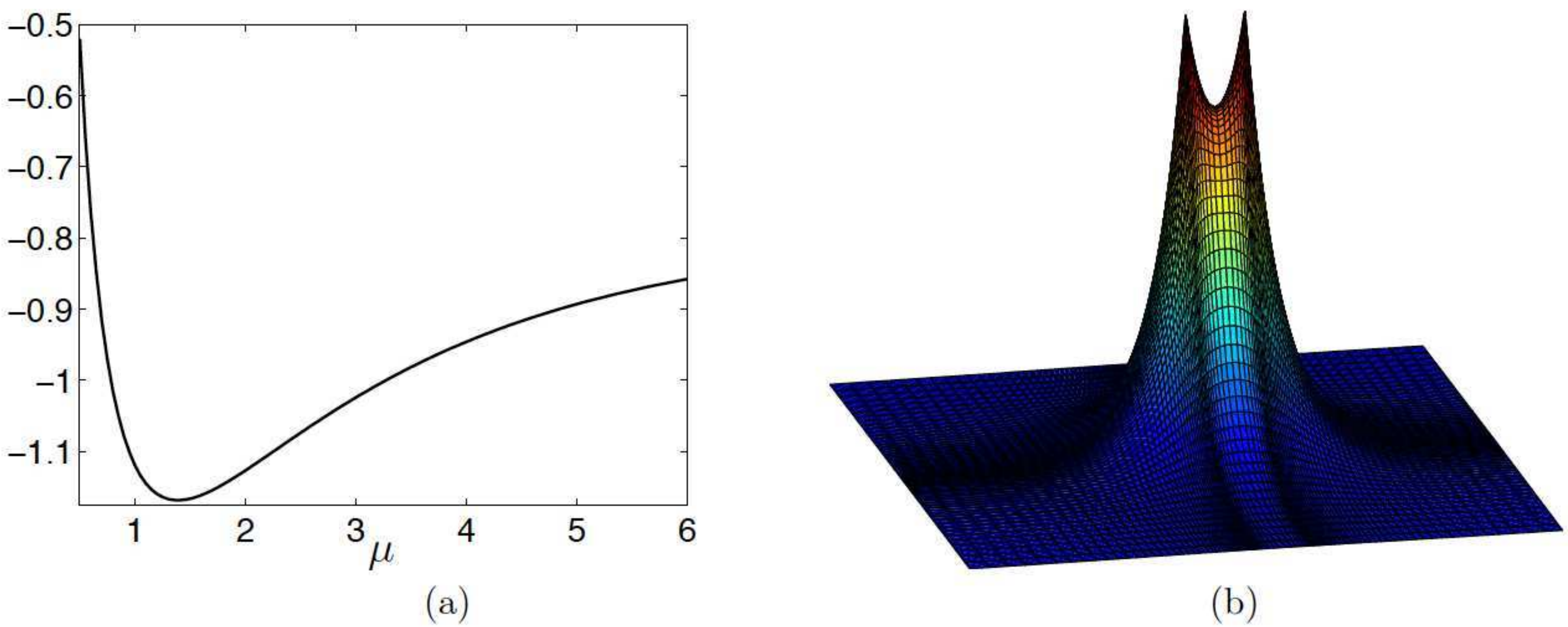

FIGURE (a) $\mathcal{E}_{H_2}$ as a function of μ, and (b) $u(\mu)$ at the equilibrium internuclear separation

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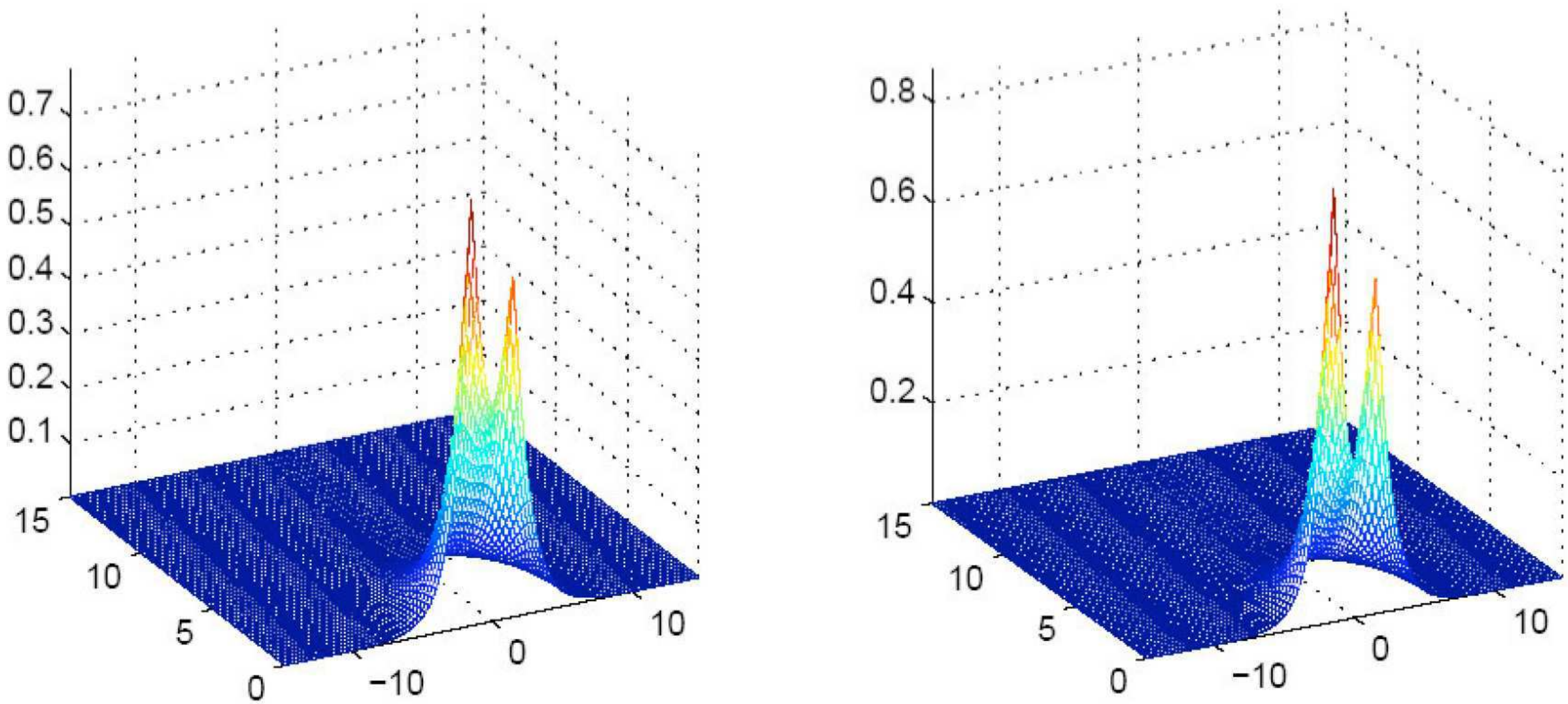

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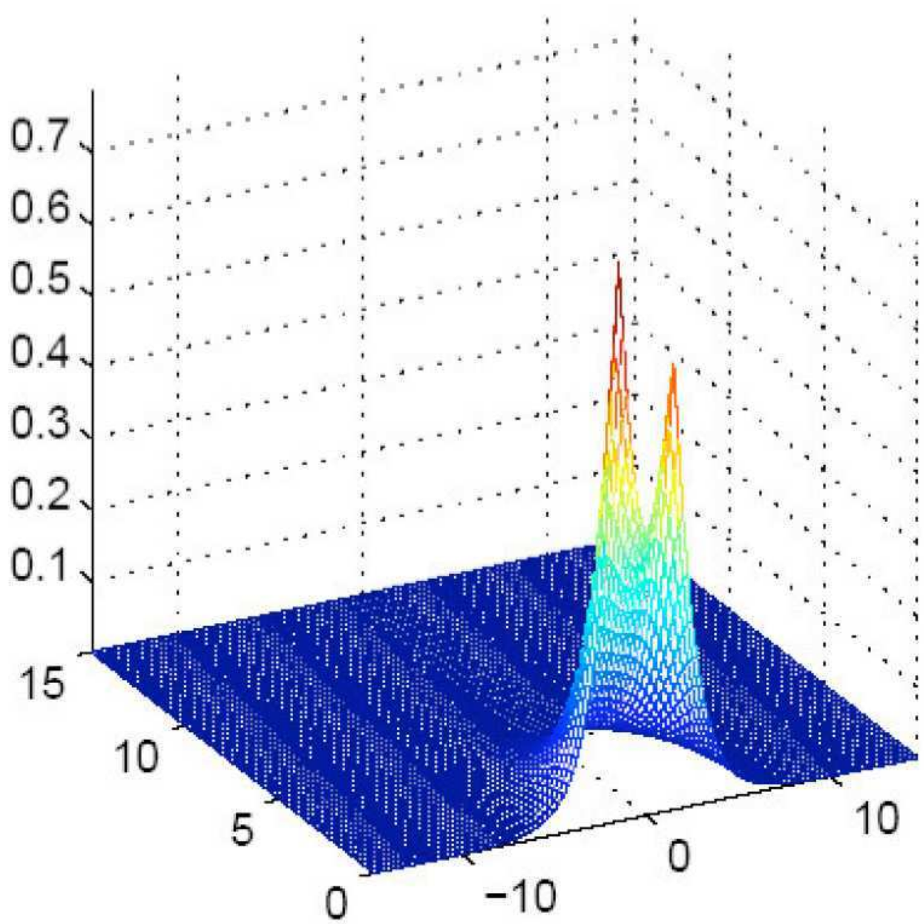

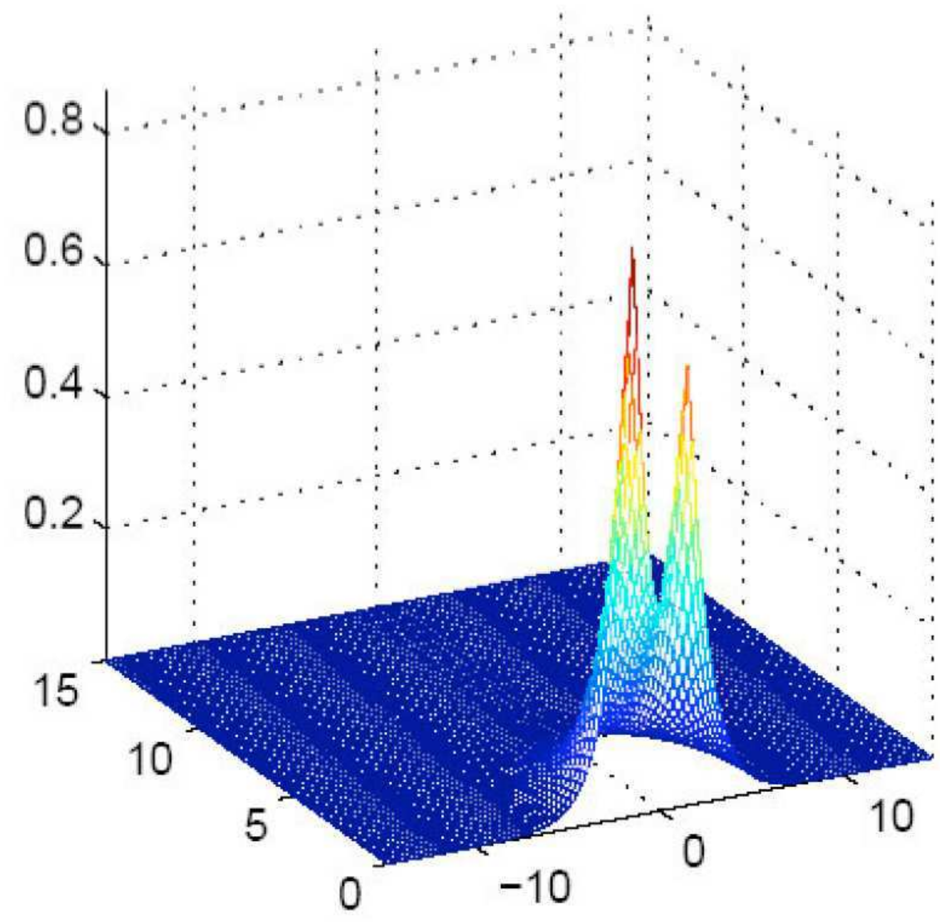

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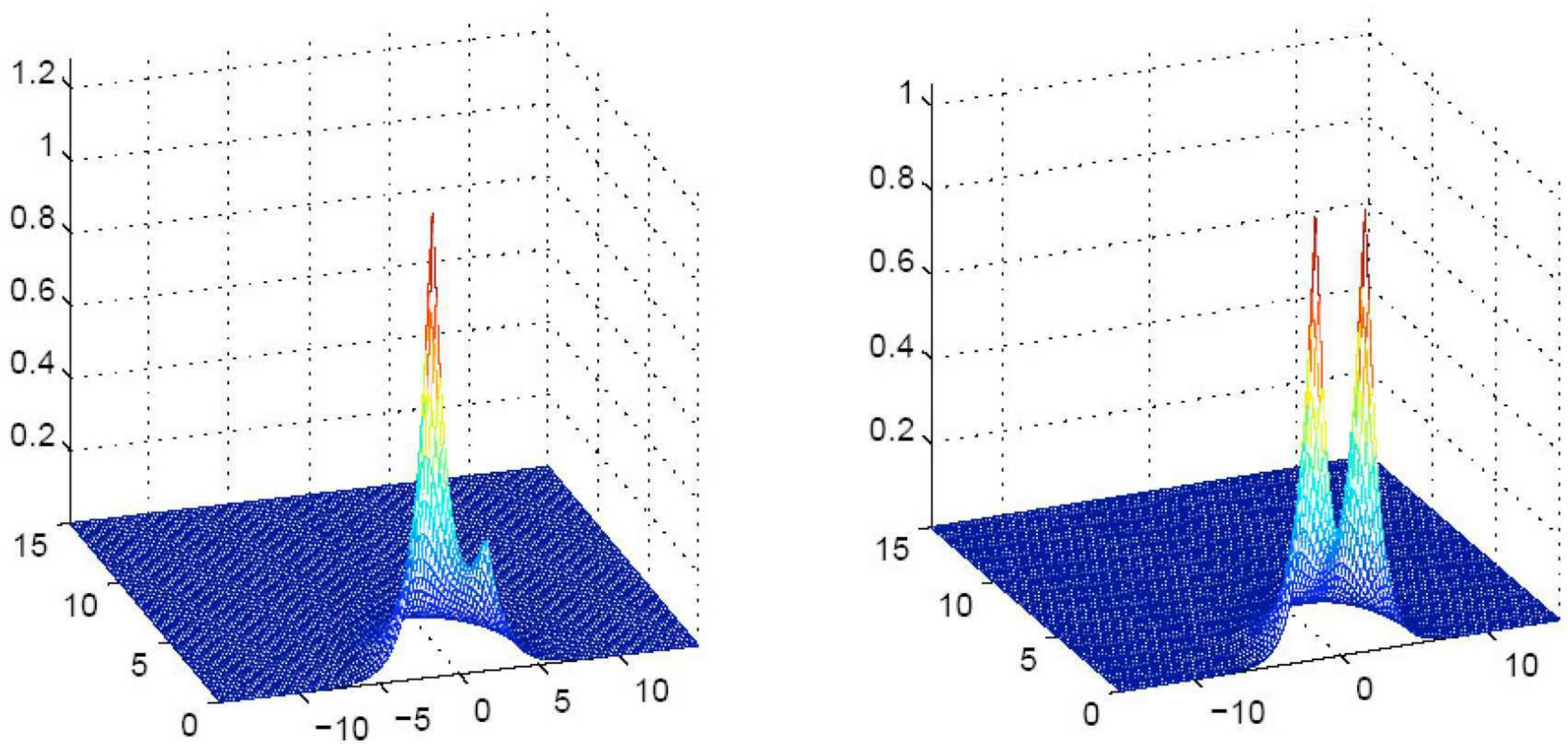

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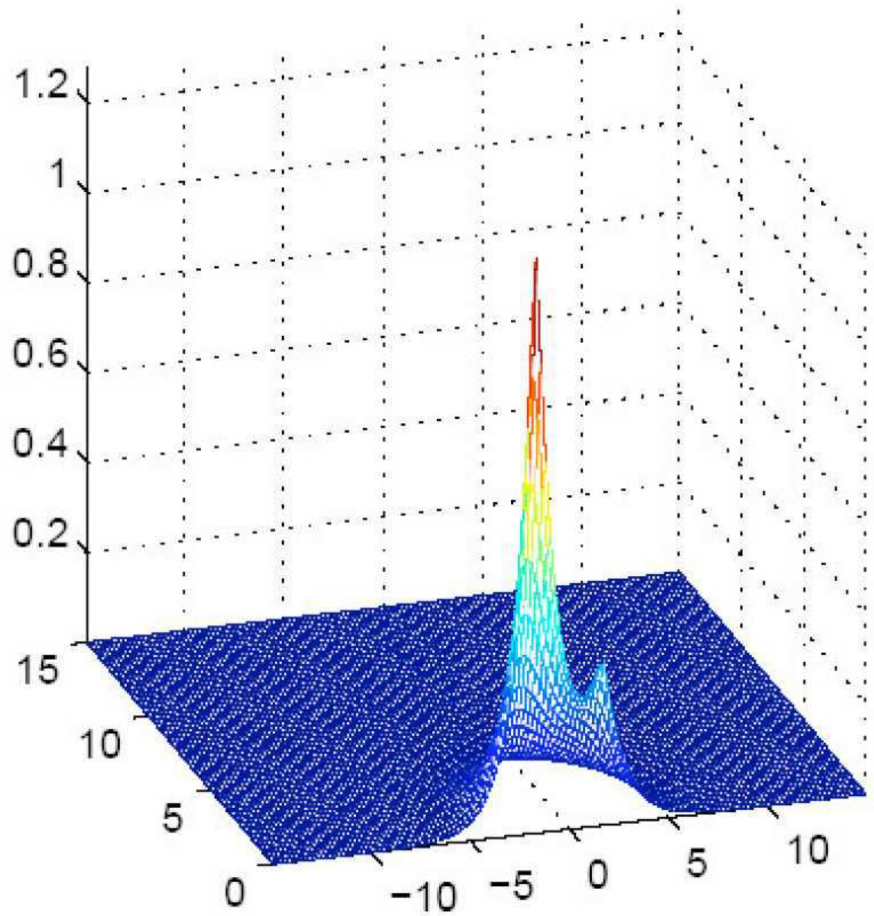

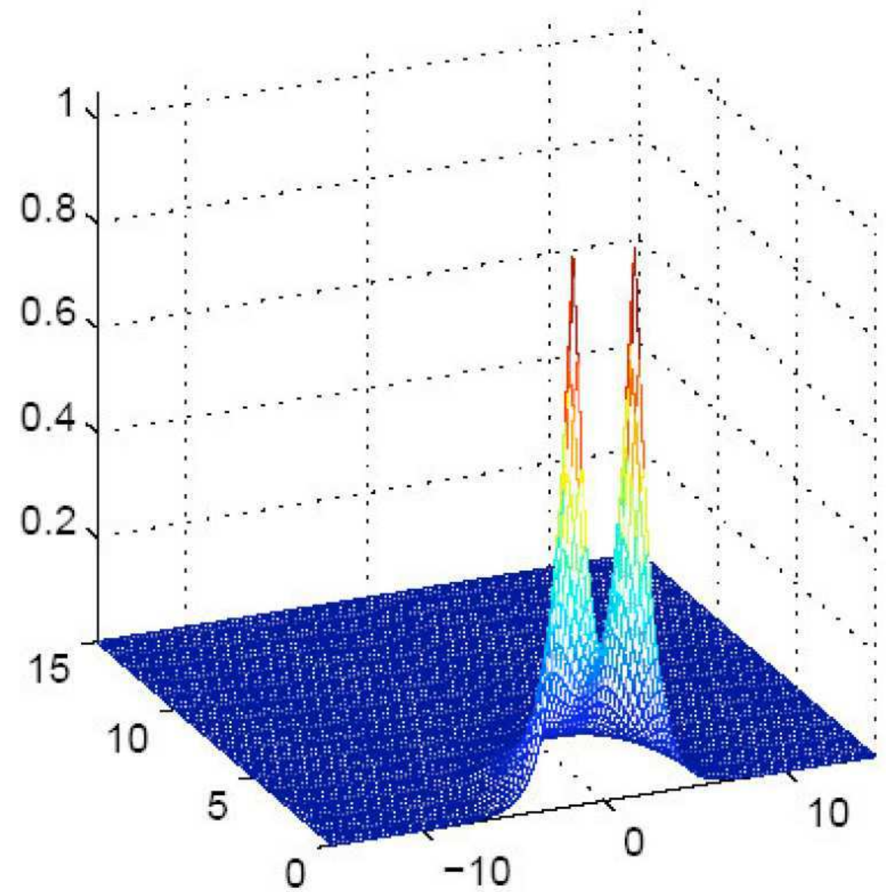

One should align the position of the nuclei ….

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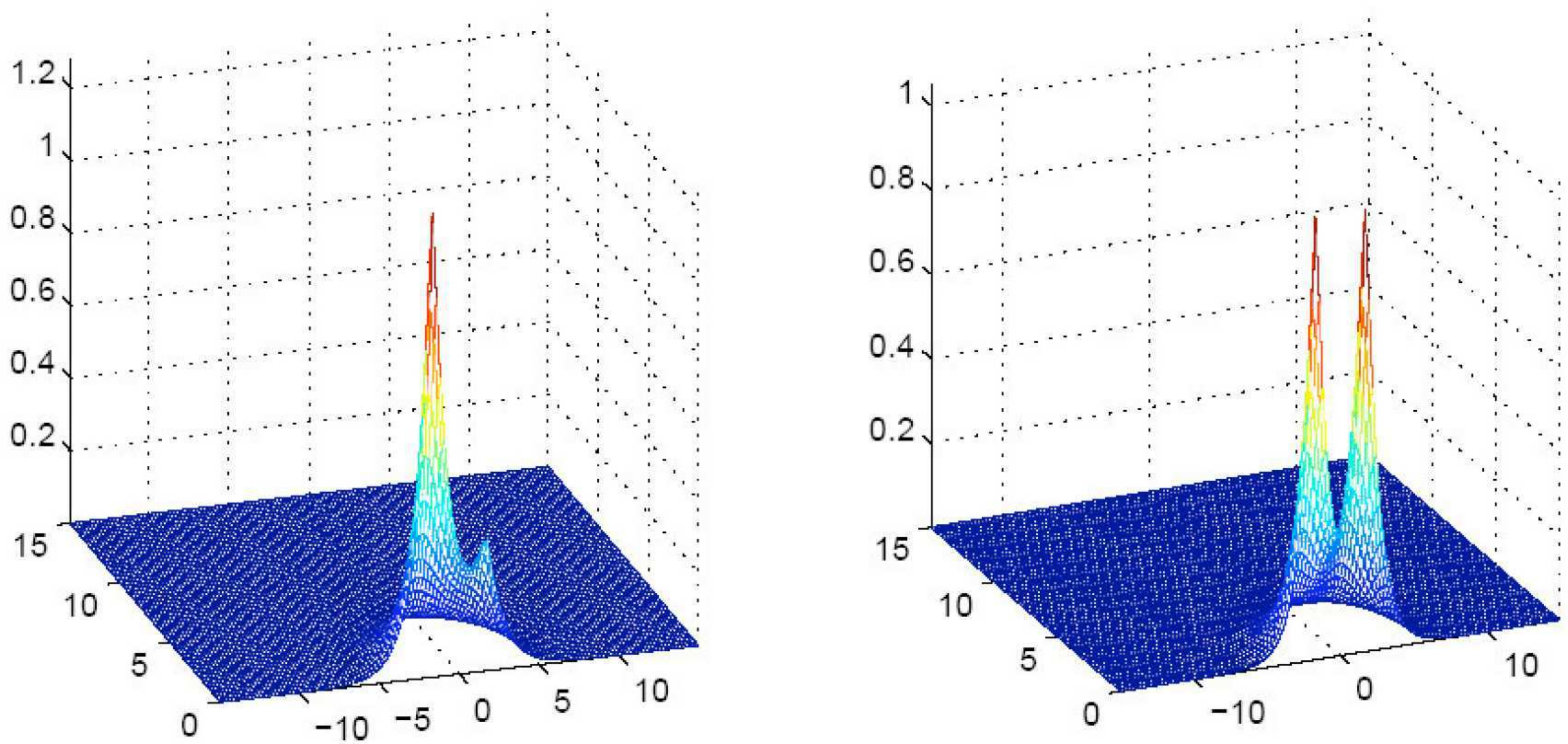

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another way is through greedy approach

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proven to be close to optimal

Framework

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Possibly inaccurate and suffering from bias

Let us assume that we have such a space Z_N

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and a model

Reduced basis method : approximation of a PDE

With such a Z_N…

Perform a Galerkin approximation

With domain decomposition : Reduced basis element method

Much to say : off-line, on-line

2 books : J. Hesthaven; G. Rozza; B. Stamm & A. Quarteroni, F. Negri, A. Manzoni

Reduced basis method : approximation of a PDE

With such a Z_N…

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Much to say : off-line, on-line

for on-line efficiency for non linear problems : a fundamental ingredient is …

EIM/GEIM

EIM/GEIM

Reconstruction from data .. only

EIM/GEIM

Reconstruction from data .. only

and a background space Z_N

EIM/GEIM

The Empirical Interpolation Method (EIM)
proposed in 2004 with M. Barrault, N. C. Nguyen and A. T. Patera

This approach allows to determine an "empirical" optimal set of interpolation points and/or set of interpolating functions.

In 2013, with Olga Mula, we have generalized it (GEIM) to include more general output from the functions we want to interpolate : not only pointwize values but also some moments.

recursive (greedy) definition of the functions and the interpolation points if $\mathcal{I}_{n-1}$ is defined by

$$\mathcal{I}_{n-1}(u) = \sum_{i=1}^{n-1} \alpha_i \zeta_i$$

so that

$$\mathcal{I}_{n-1}(u)(x_j) = u(x_j)$$

then

$$\mu_n = \mathrm{argmax}_\mu \|u(\mu) - \mathcal{I}_{n-1}(u(\mu))\|$$

and

$$x_n = \mathrm{argmax}_x |u(x;\mu_n) - \mathcal{I}_{n-1}(u(\mu_n))(x)|$$

The algorithm tells you what points to choose in order to interpolate with functions in $\mathcal{S}$

GEIM

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and

$$\sigma_n = \text{argmax}_\sigma | \sigma[u(\mu_n) - \mathcal{J}_{n-1}(u(\mu_n))] |$$

Formula

$$\sup_{u\in\mathcal{S}}\|u-\mathcal{J}_n[u]\|_{\mathcal{X}} \le (1+\Lambda_n)\sup_{u\in\mathcal{S}}\inf_{v\in X_n}\|u-v\|_{\mathcal{X}},$$

suggests that Λ_n plays an important role in the result and it is therefore important to discuss its behavior as n increases. First of all, Λ_n depends both on the choices of the interpolating functions and interpolation points.

We have proven (YM-Mula-Patera-Yano) that $\Lambda_n = 1/\beta_n$, where

$$\beta_n = \inf_{\varphi\in X_n}\sup_{\sigma\in\mathrm{Span}\{\sigma_0,\ldots,\sigma_{n-1}\}}\frac{\langle\varphi,\sigma\rangle_{\mathcal{X},\mathcal{X}'}}{\|\varphi\|_{\mathcal{X}}\|\sigma\|_{\mathcal{X}'}}.$$

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GEIM interpreted as an oblic projection …

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Λ_n

optimal placement of the sensors

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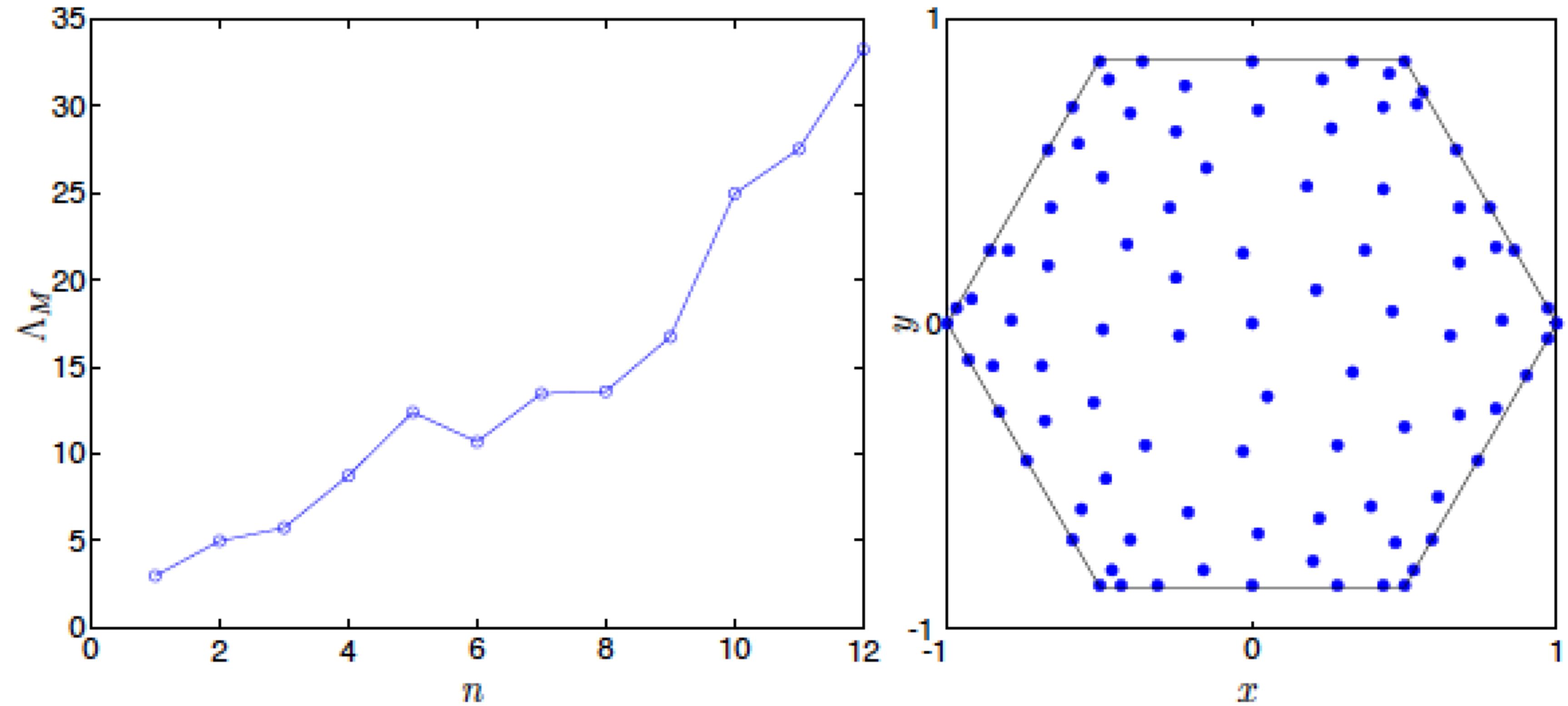


Figure 3: (a) Variation of Lebesgue constant, Λ_M with n where $M = \frac{1}{2}(n+1)(n+2)$, and (b) distribution of magic points, for Ω_{hex}.

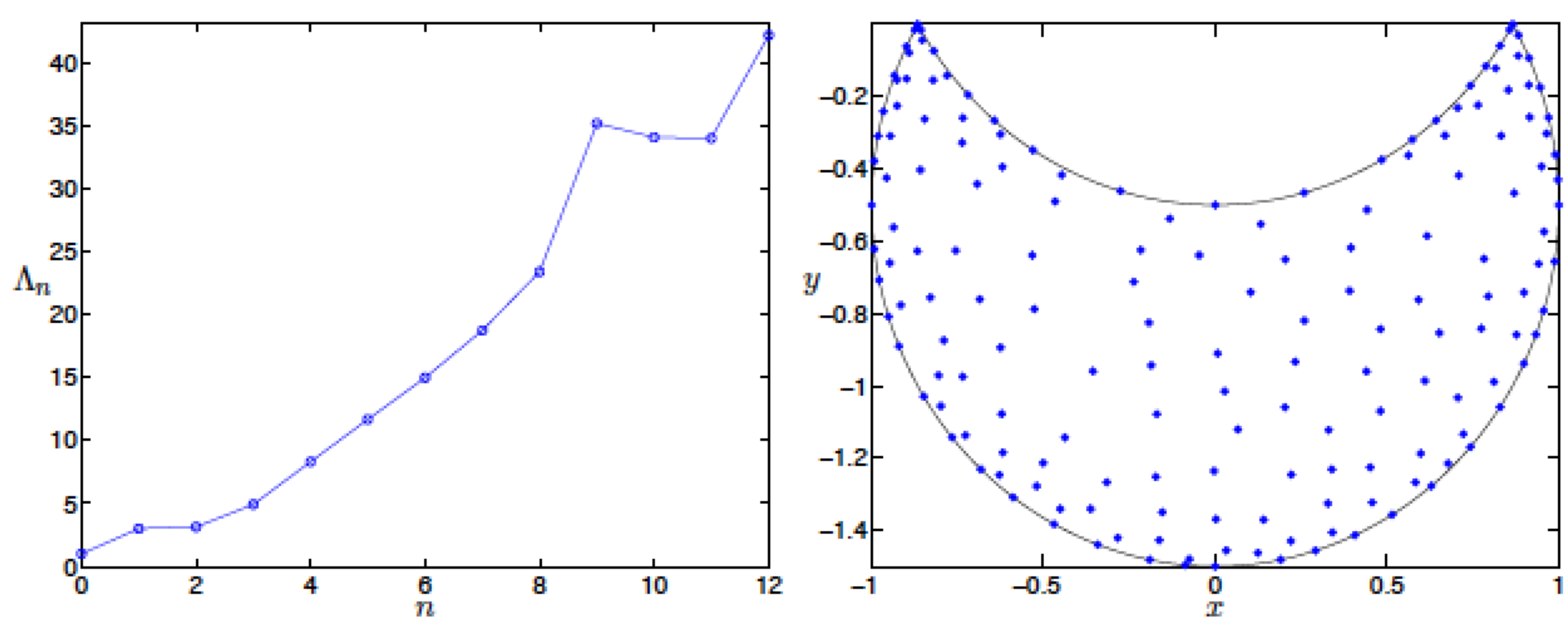
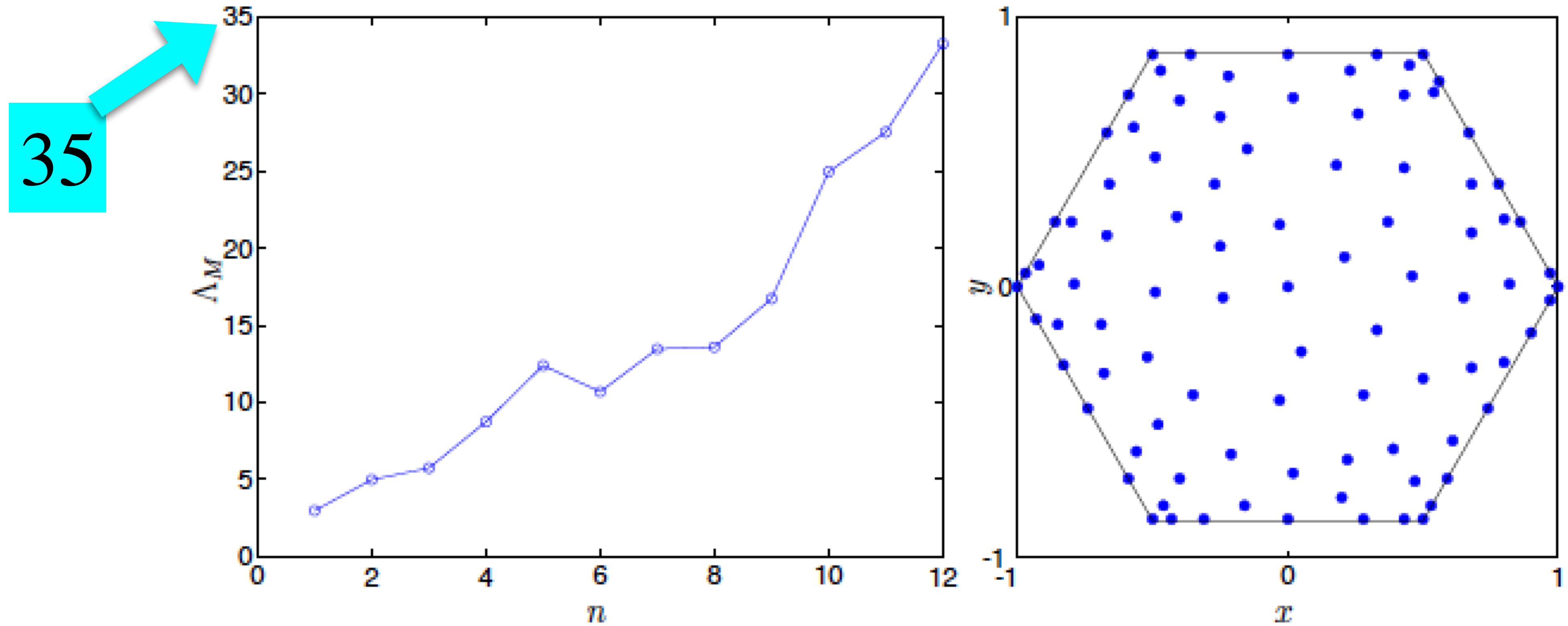


Figure 4: Results for a "lunar croissant" domain Ω_{cro}: (a) variation of the Lebesgue constant Λ_n with n, and (b) distribution of magic points for $n = 12$.



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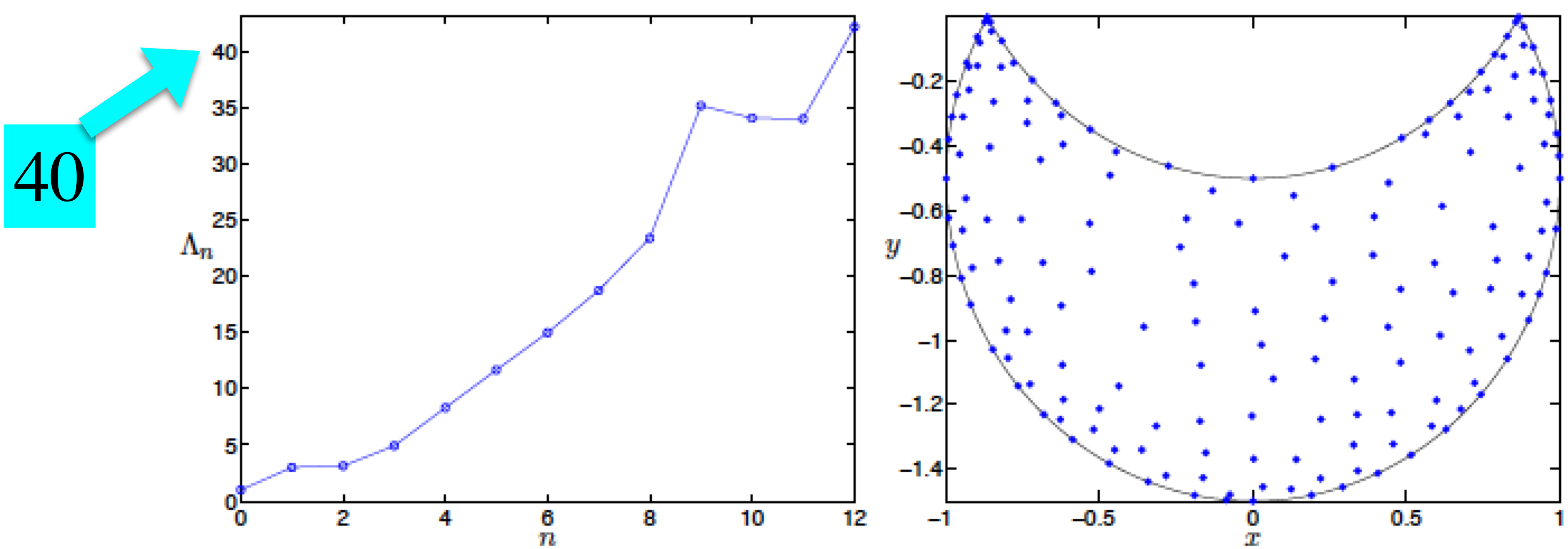
Lebesgue constant for EIM — polynomial degree 12



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- and R. A. DeVore, G. Petrova, and P. Wojtaszczyk,

to analyse the convergence properties of our algorithm

In a nutshell, in the case where we have a Hilbert framework, our result states that

Theorem (with O. Mula and G. Turinici)
If $(\Lambda_n)_{n=1}^{\infty}$ is a monotonically increasing sequence then

i) if $d_n \leq C_0 n^{-\alpha}$ for any $n \geq 1$, then $\tau_n \leq C_0 \tilde{\beta}_n n^{-\alpha}$, with

$$\tilde{\beta}_n := 2^{3\alpha+1}\Lambda_n^2, \quad \text{if } n \geq 2.$$

ii) if $d_n \leq C_0 e^{-c_1 n^{\alpha}}$ for $n \geq 1$ and $C_0 \geq 1$, then $\tau_n \leq C_0 \tilde{\beta}_n e^{-c_2 n^{-\alpha}}$, with

$$\tilde{\beta}_n := \sqrt{2}\Lambda_n, \quad \text{if } n \geq 2.$$

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- and R. A. DeVore, G. Petrova, and P. Wojtaszczyk,

to analyse the convergence properties of our algorithm

In a nutshell, in the case where we have a Hilbert framework, our result states that

Theorem (with O. Mula and G. Turinici)

If $(\Lambda_n)_{n=1}^{\infty}$ is a monotonically increasing sequence then

i) if $d_n \leq C_0 n^{-\alpha}$ for any $n \geq 1$, then $\tau_n \leq C_0 \tilde{\beta}_n n^{-\alpha}$, with

Kolmogorov n-width

$$\tilde{\beta}_n := 2^{3\alpha+1} \Lambda_n^2,$$

actual deviation

ii) if $d_n \leq C_0 e^{-c_1 n^{\alpha}}$ for $n \geq 1$ and $C_0 \geq 1$, then $\tau_n \leq C_0 \tilde{\beta}_n e^{-c_2 n^{-\alpha}}$, with

$$\tilde{\beta}_n := \sqrt{2} \Lambda_n, \quad \text{if } n \geq 2.$$

Numerical results

We consider $u\left((x_1, x_2); (\mu_1, \mu_2)\right) \equiv \left((x_1 - \mu_1)^2 + (x_2 - \mu_2)^2\right)^{-1/2}$ for $x \in]0,1[^2$ and $\mu \in [-1, -0.01]^2$

M	$\varepsilon^*_{M,\max}$	$\overline{\rho}_M$	Λ_M	$\overline{\eta}_M$
8	8.30 E-02	0.68	1.76	0.17
16	4.20 E-03	0.67	2.63	0.1.
24	2.68 E-04	0.49	4.42	0.28
32	5.64 E-05	0.48	5.15	0.20
40	3.66 E-06	0.54	4.98	0.60
48	6.08 E-07	0.37	7.43	0.29

Note that we have here approximated the full set of $u\left((x); \mu\right)$ with a few of them $u\left((x); (\mu)\right) \simeq \sum_{i=1}^{M} \alpha_i u\left((x); \mu^i\right)$

NUMERICAL RESULTS

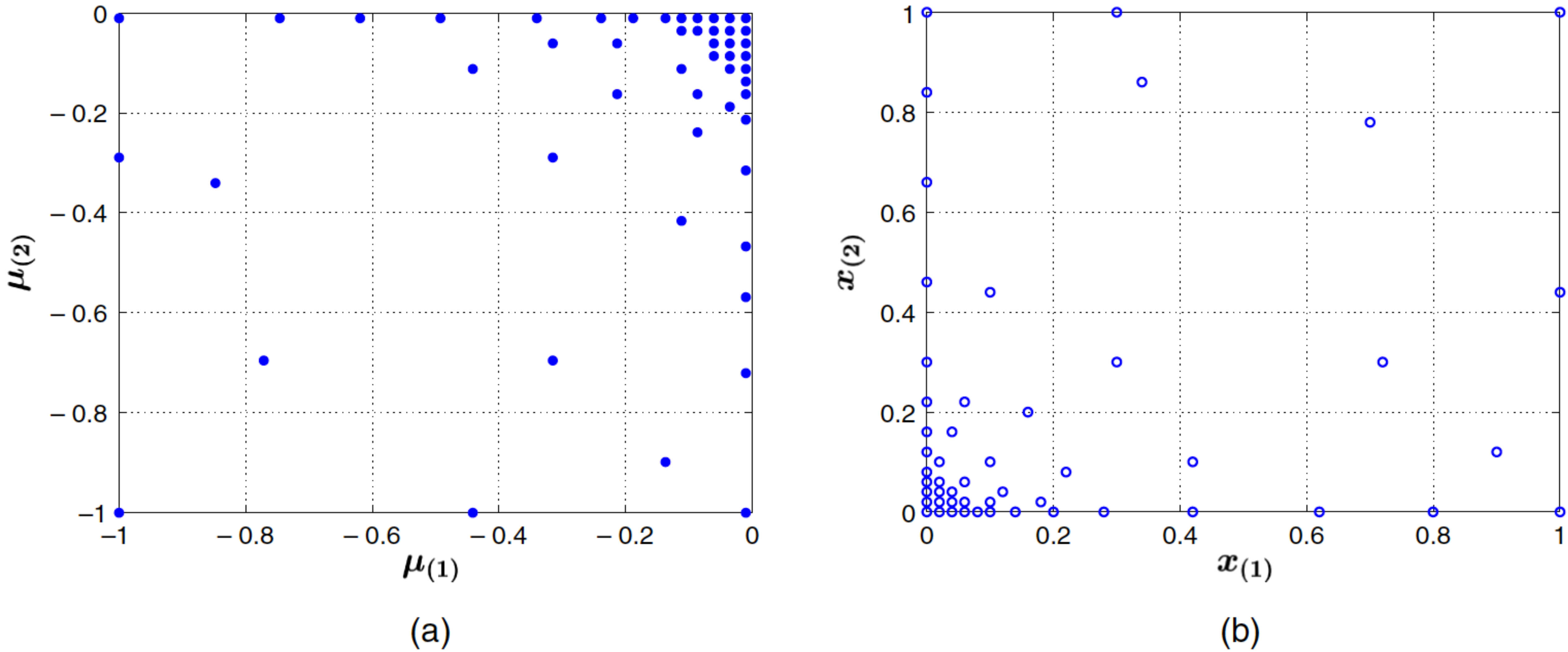

Figure: (a) Parameter sample set S_M^g, $M_{\max} = 51$, and (b) interpolation points x_m, $1 \leq m \leq M_{\max}$.

An application

Electronic Schrödinger equation

$$H\Psi = E\Psi$$

$H = T + V_{ne} + V_{ee}$

$T = \sum_{i=1}^{N} -\frac{1}{2}\nabla_i^2$

$V_{ne} = \sum_{i=1}^{N} v_{ne}(r_i)$, with, typically, $v_{ne}(r) = -\sum_A Z_A/|r - R_A|$

$V_{ee} = \sum_{i=1}^{N} 1/|r_i - r_j|$

Ψ is antisymmetric

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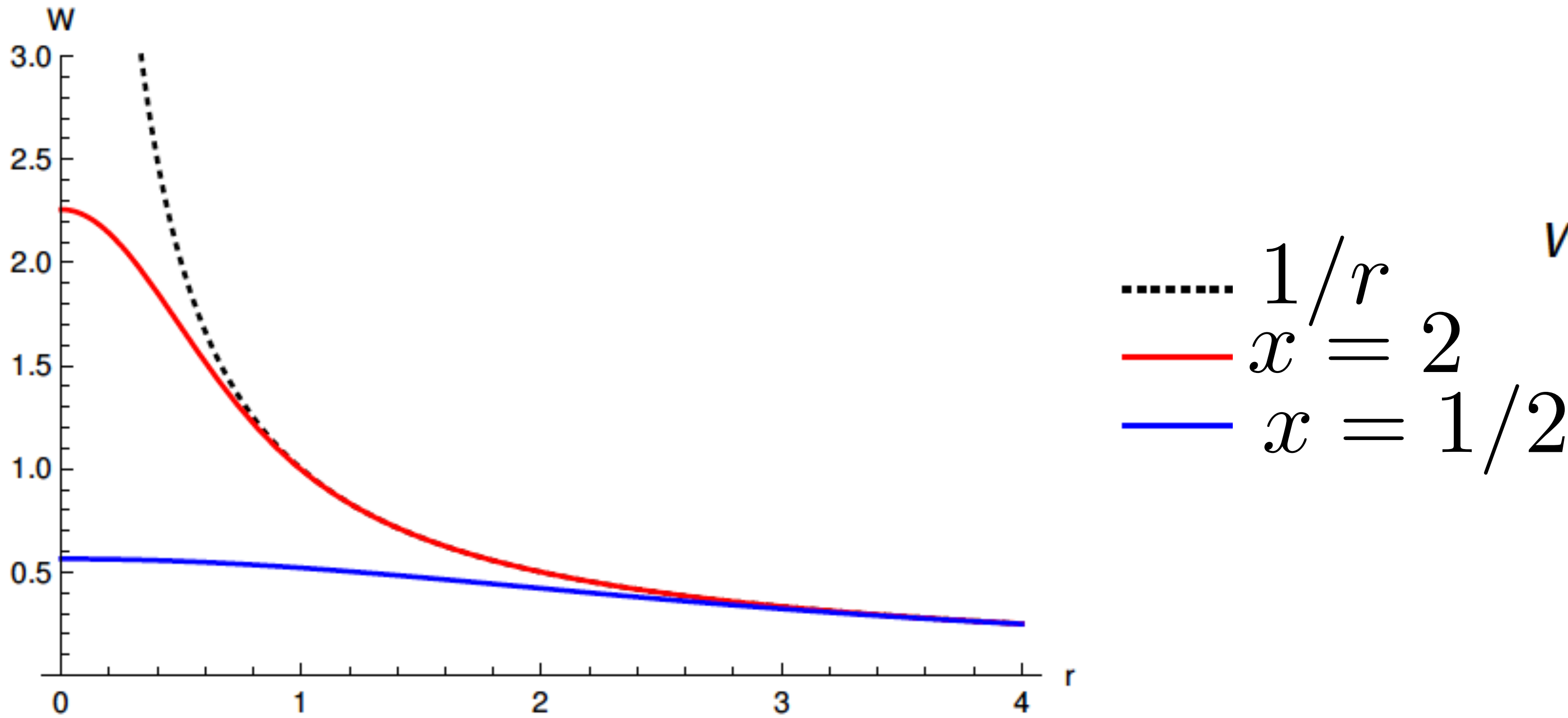
The proposed idea is to change the interaction

Avoid the singularity V_{ee}

joint work with E. Polack, J. Karwowski and A. Savin.

$$\frac{1}{r} \to w = \frac{\mathrm{erf}(xr)}{r}$$



$$w \approx \begin{cases} x & r < 1/x \\ 1/r & r > 1/x \end{cases}$$

μ	w
0	0
∞	$1/r$

Avoid the singularity $V_{ee}(x) = \sum_{i,j=1}^{N} \frac{\mathrm{erf}(x|r_i - r_j|)}{|r_i - r_j|}$

$$H(x) = T + V_{ne} + V_{ee}(x)$$

The idea is thus to approximate this simpler system for finite values of x and derive the energy *E(* x *)* or other quantities like excited states.
Then the idea is to extrapolate at infinity

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Due to the behavior of $E(x)$ for large x, namely proportional to x^{-2}, and the linear behavior with x when it approaches zero, we choose as basis $(1+ax^2)^{-1}$, with $a \in [1, 50]$.

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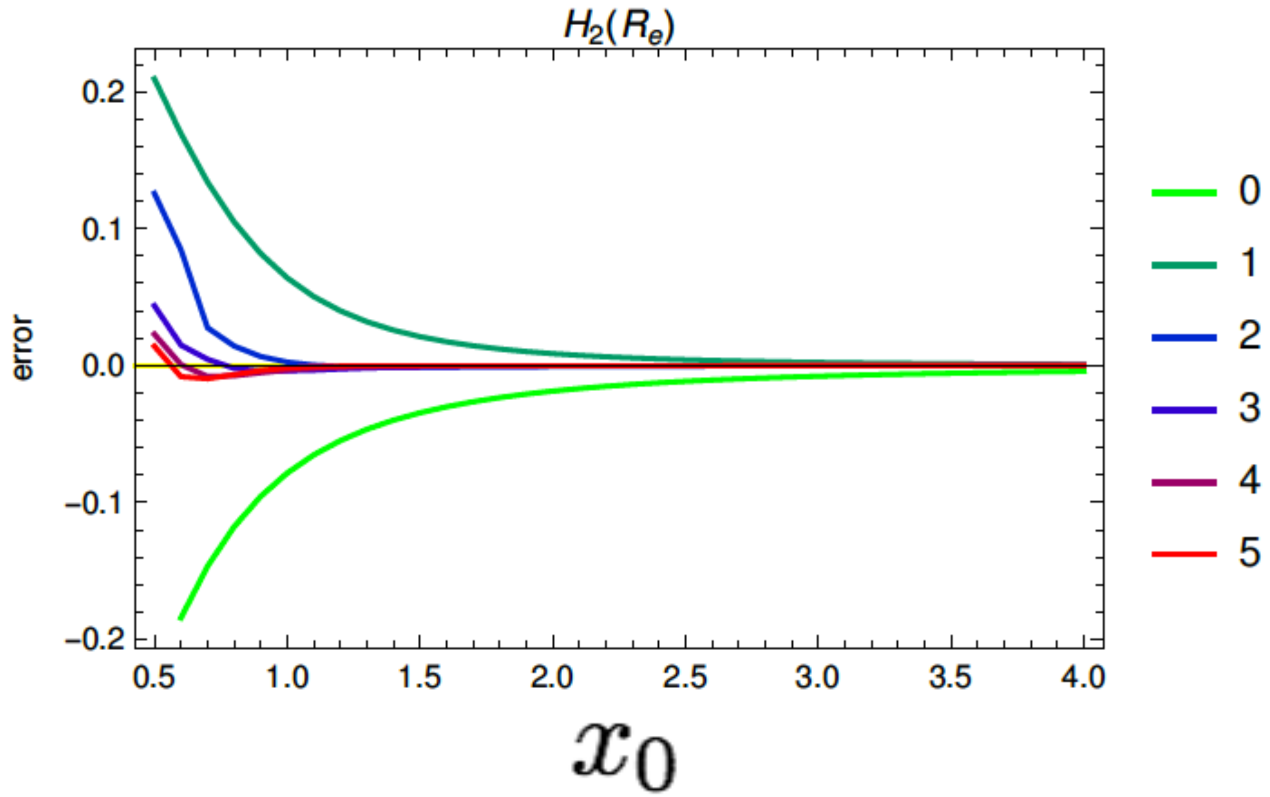
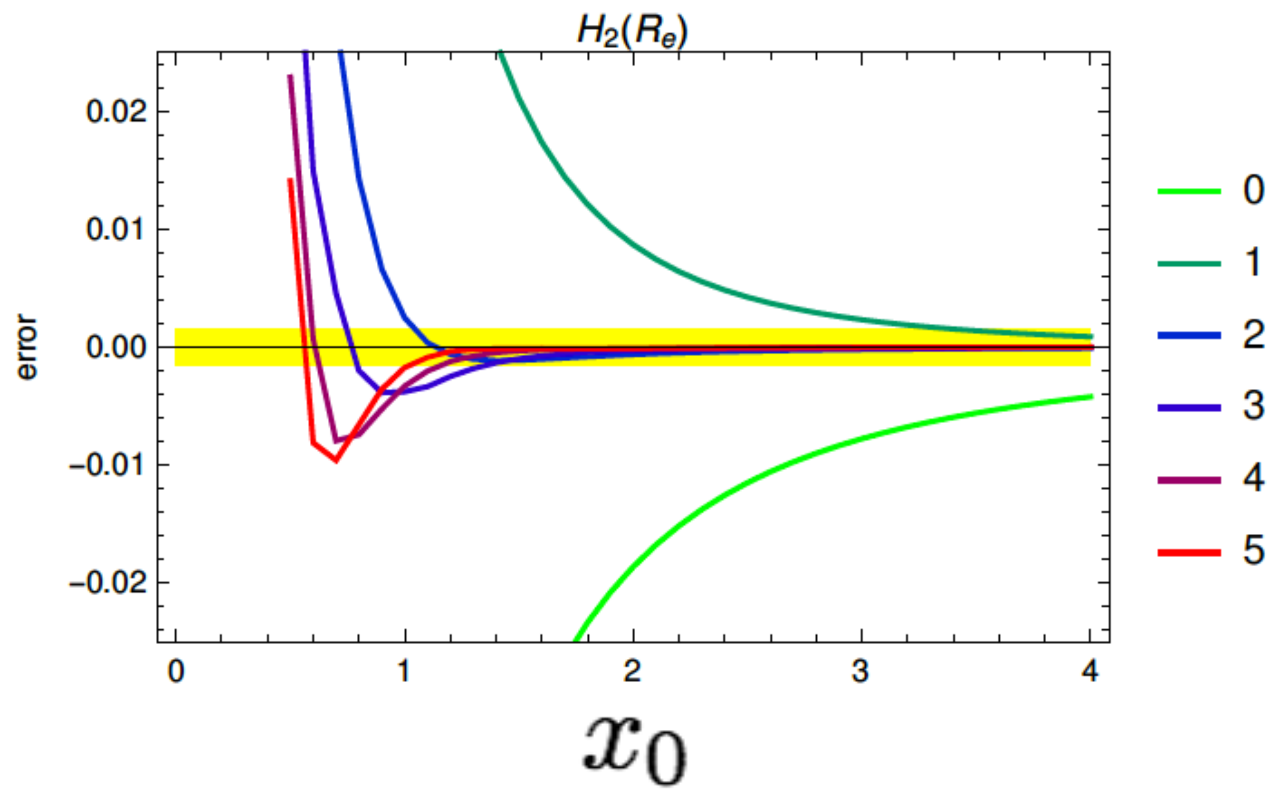
Classical ?
but what are the interpolation nodes?

The interpolation/extrapolation nodes are chosen by a greedy procedure between 0 and a maximum value x_0. This one is chosen so that the computation of $E(x)$ is "easy" for $0 < x \leq x_0$.

Results : General behavior on the hydrogen molecule





Errors (in hartree) made by using extrapolation method, to approximate the total electronic energy of the hydrogen molecule using an increasingly in size basis set and associated set of interpolation points, as a function of the largest interpolation point used, μ_0. The yellow background covers the region where the error is smaller than chemical accuracy (1 kcal/mol).

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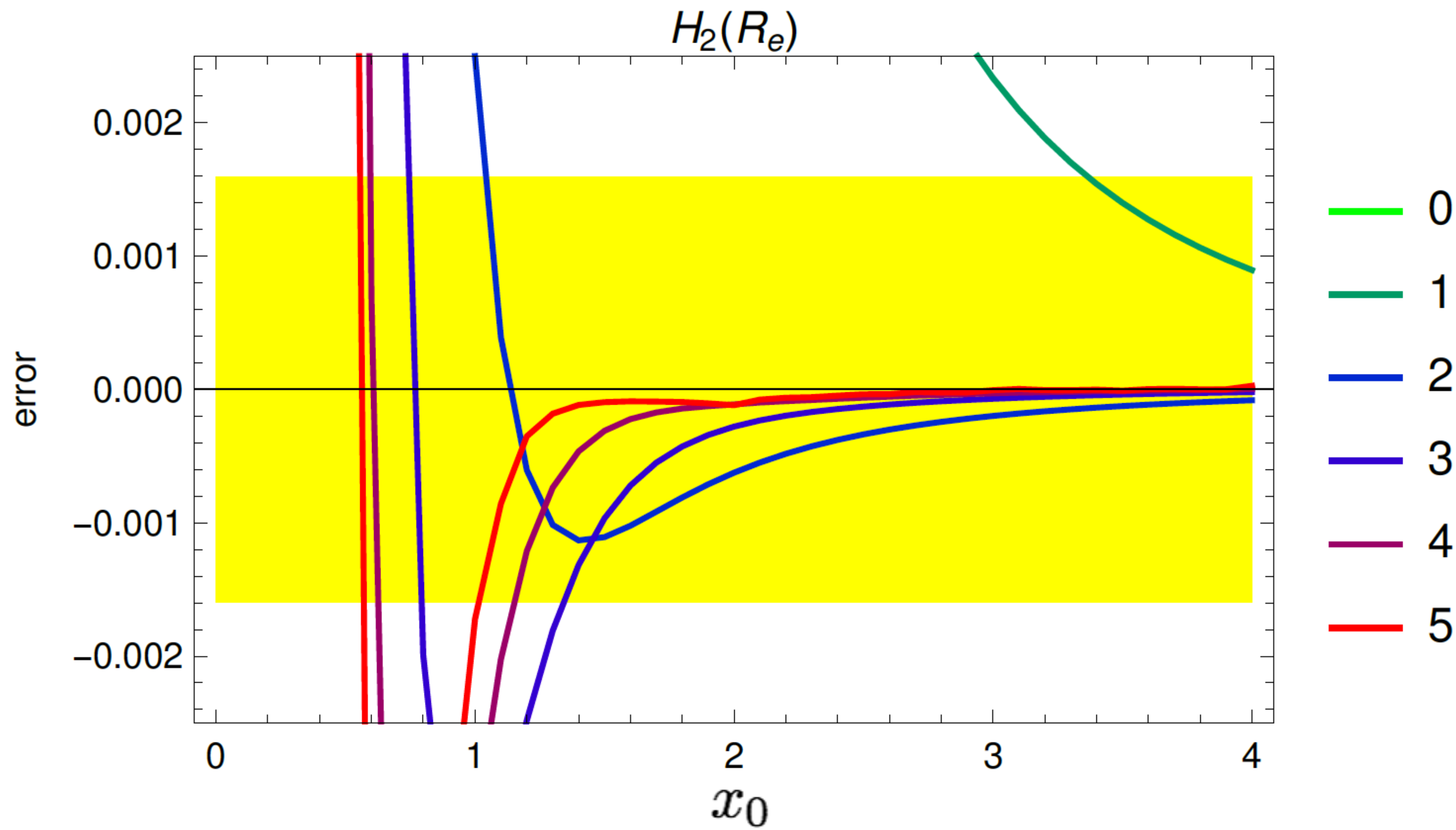

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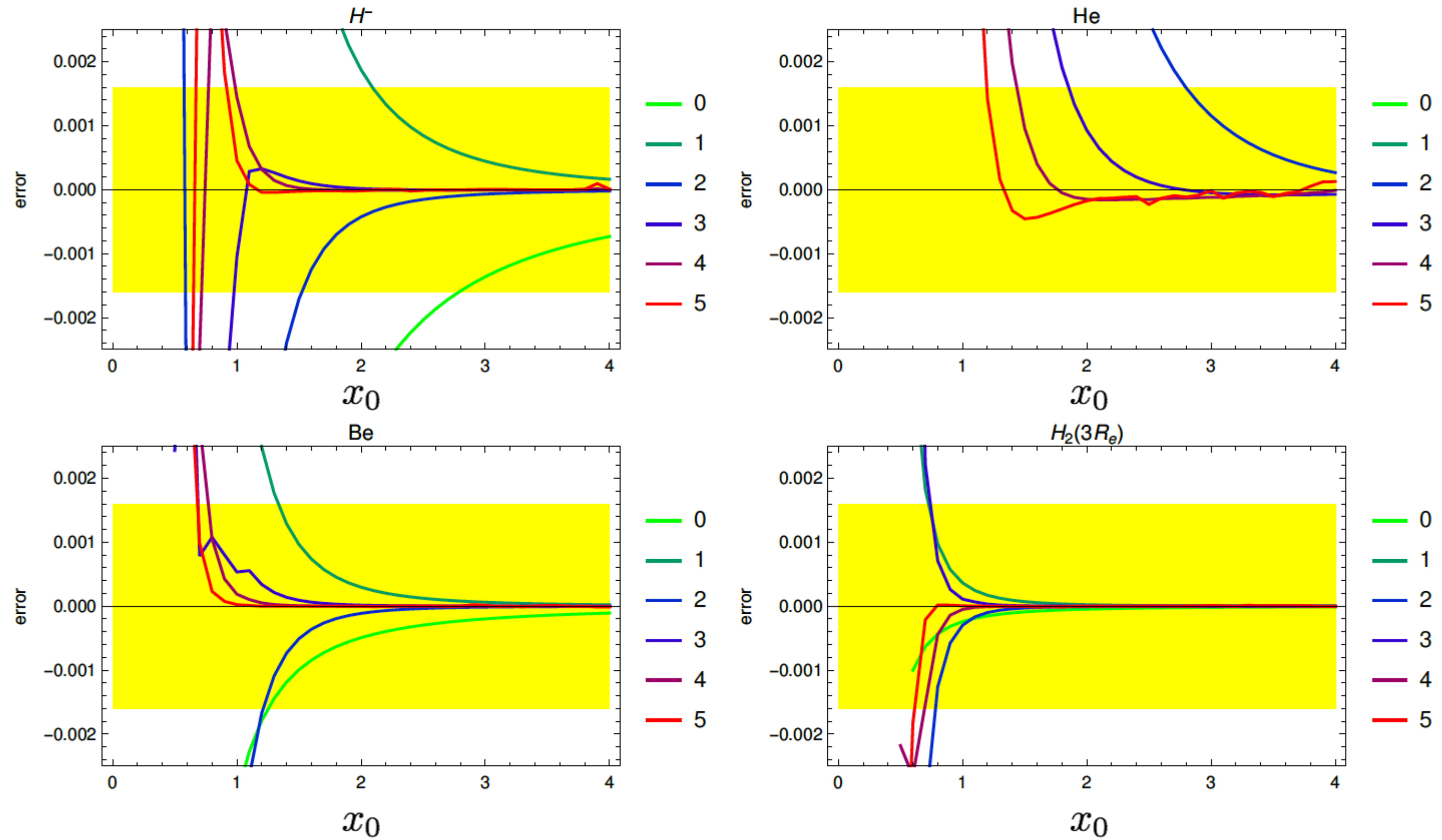
Results : other examples



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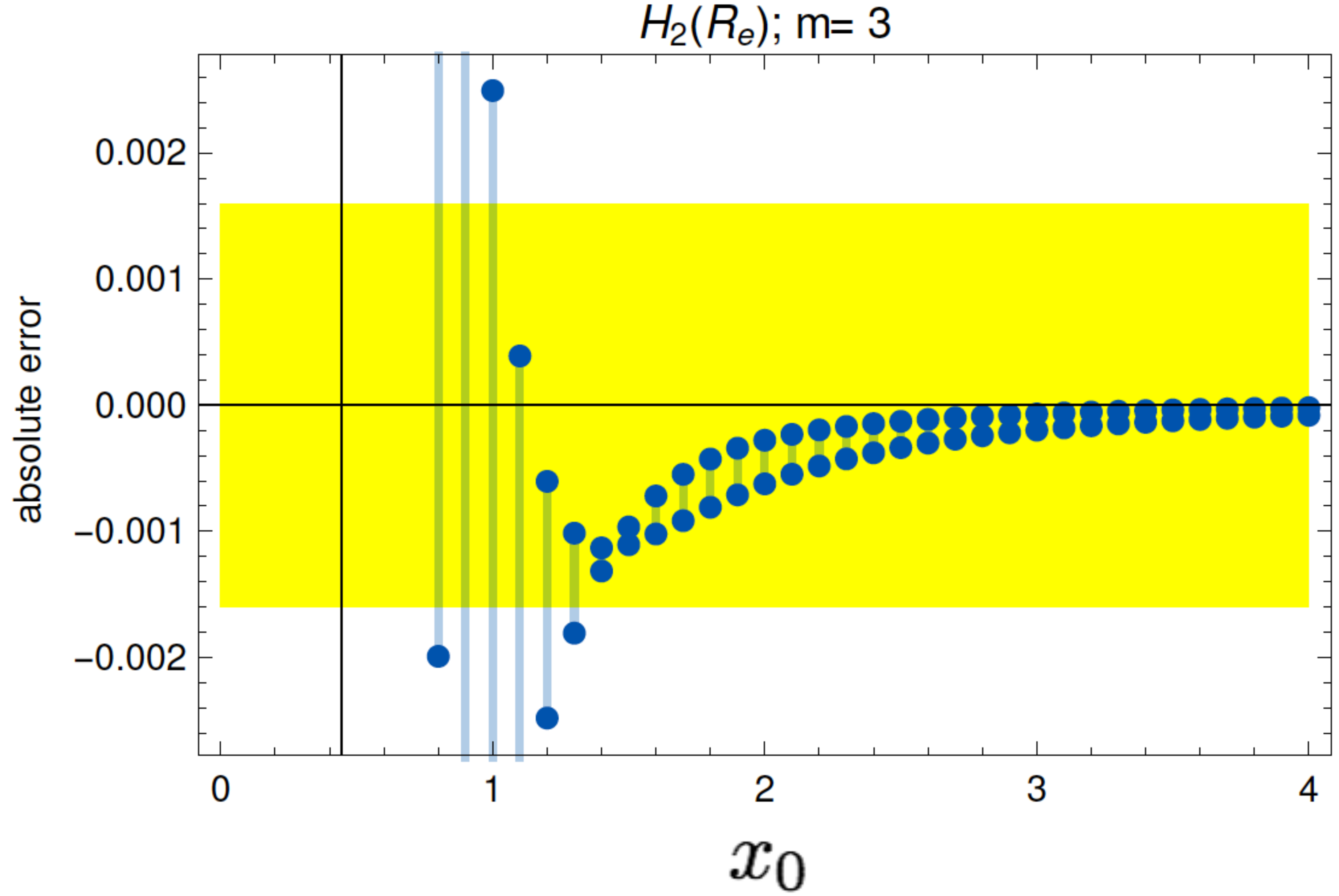
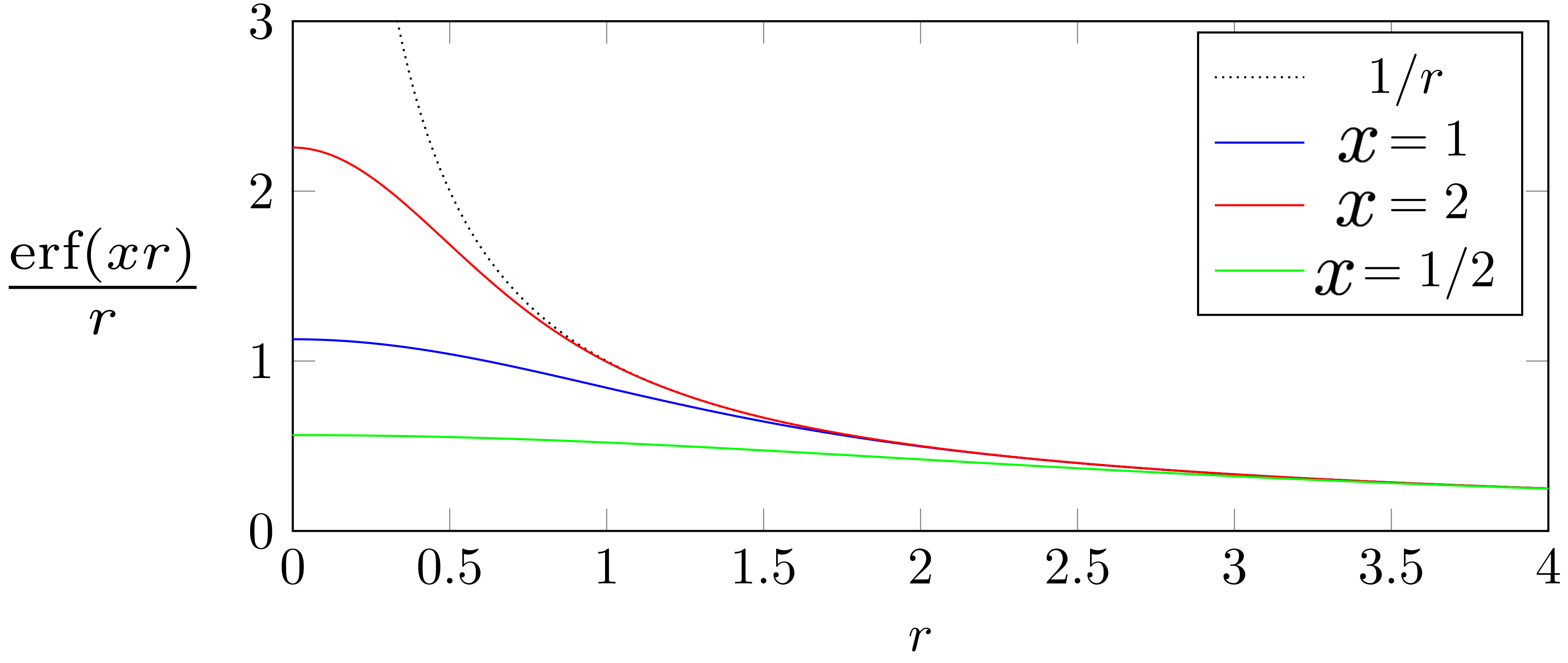
Results : empirical error bars



Remember the mollifier for different values of x



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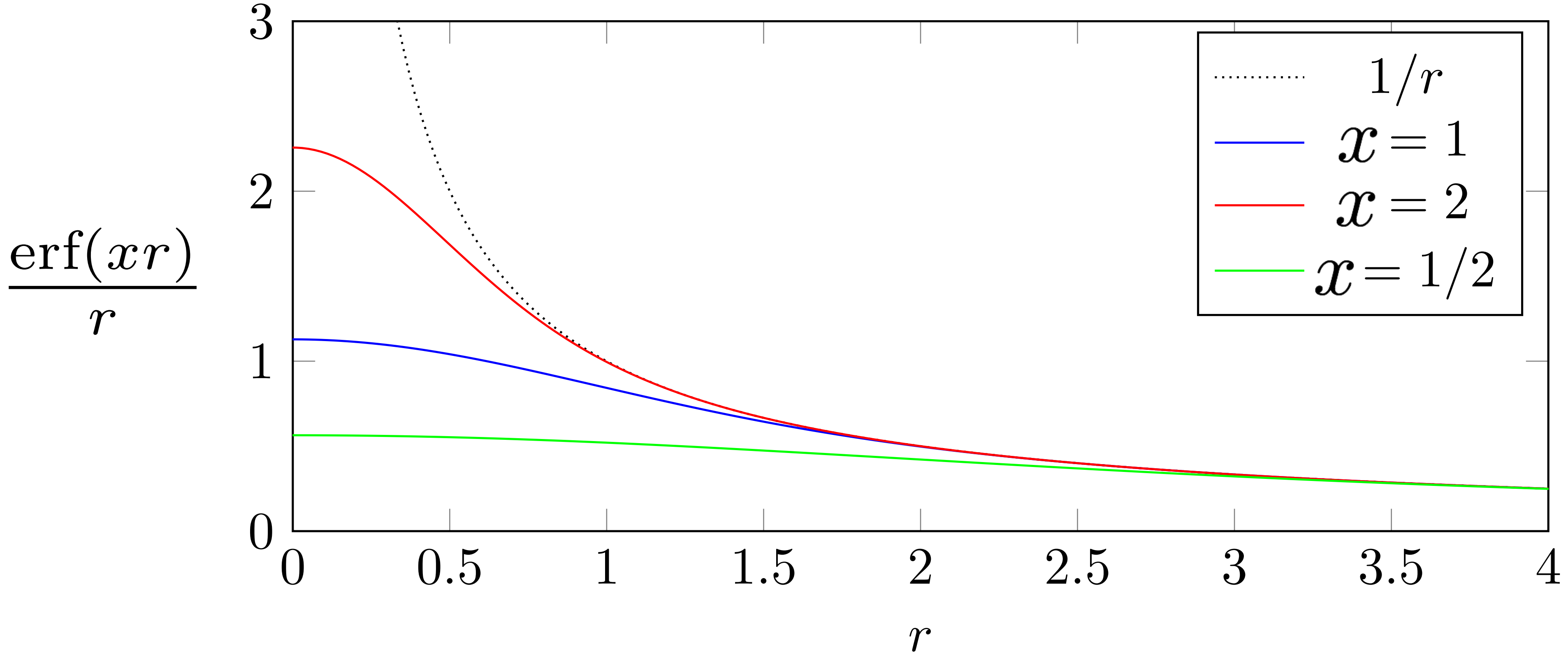
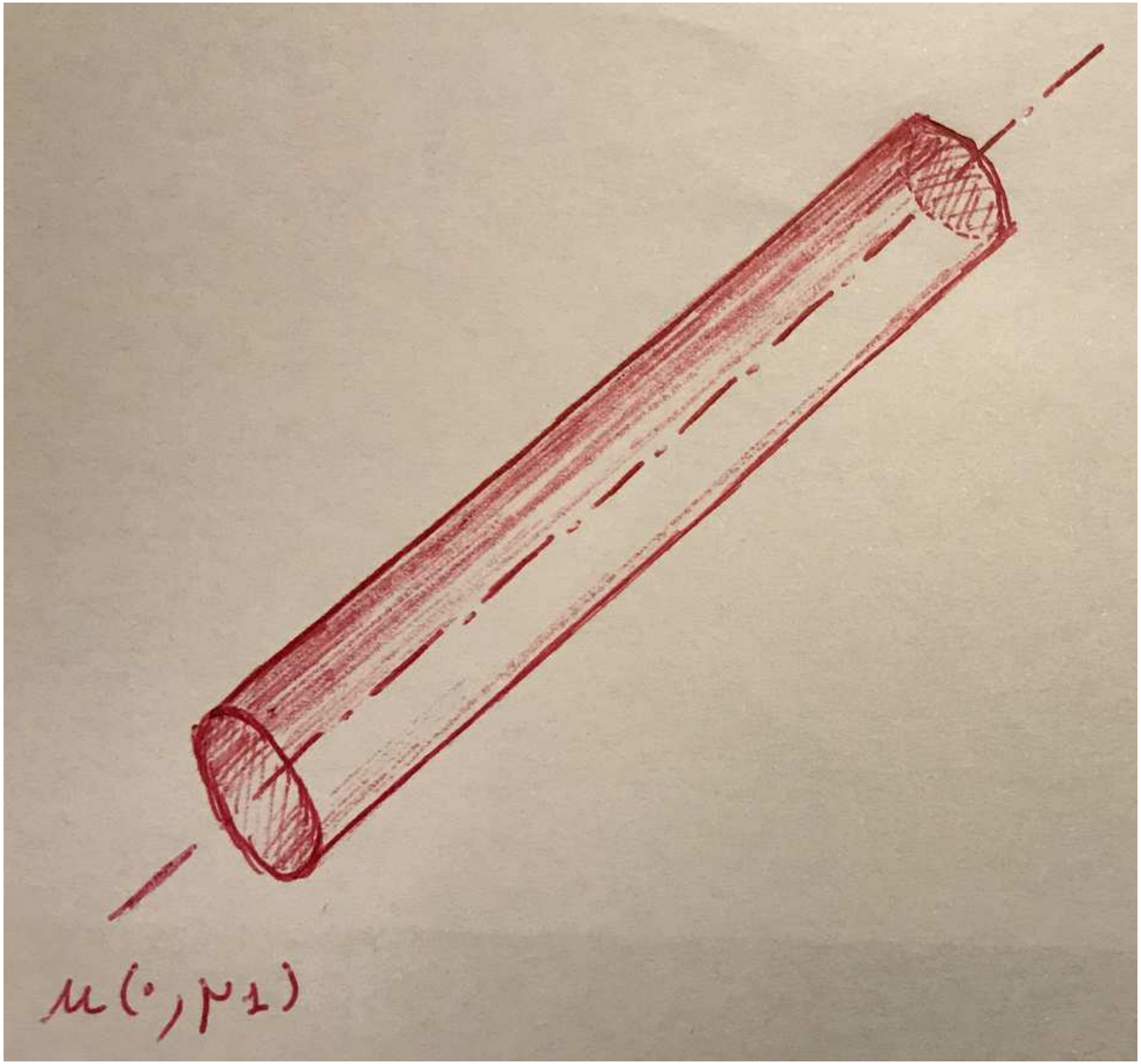


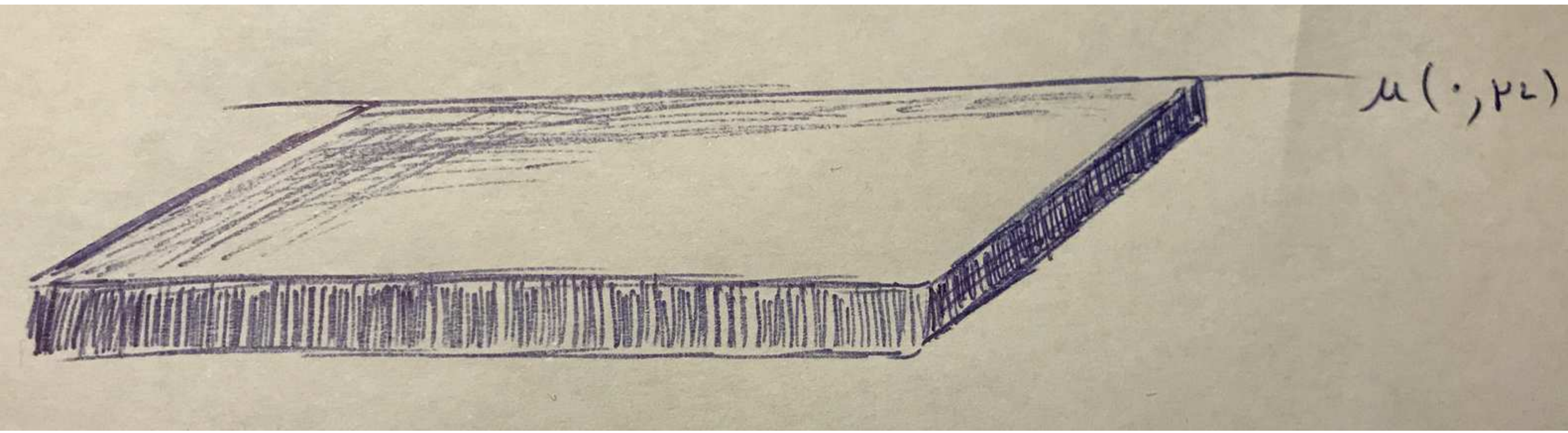
For $x = 1$ or $x = 2$ the solutions are more easy to compute.. requires a smaller basis set

What if the data are polluted with noise

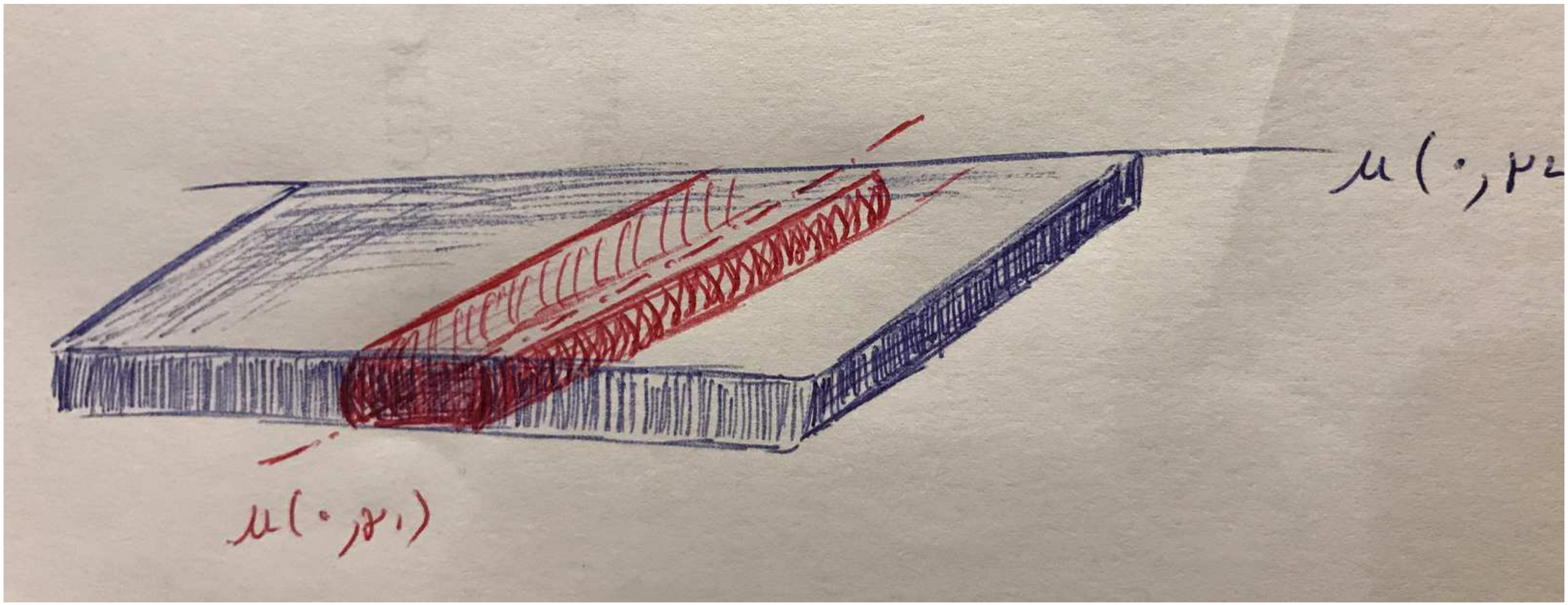
We want now to use the fact that In the previous approaches, we have mainly used the fact that X_N has good approximation properties



This is the part of X_1 of interest



This is the part of X_2 of interest



And this is actually where we should be looking at

$$X_1 \cap X_2$$

How can we do this ?

Remember the recursive formula

Remember the recursive formula

$$\mathcal{I}_M[u(.,\mu)] = \mathcal{I}_{M-1}[u(.,\mu)] + \frac{u(x_M,\mu) - \mathcal{I}_{M-1}[u(.,\mu)](x_M)}{u(x_M,\mu_M) - \mathcal{I}_{M-1}[u(.,\mu_M)](x_M)} \Big[[u(.,\mu_M) - \mathcal{I}_{M-1}[u(.,\mu_M)] \Big]$$

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$$q_M = \frac{[u(.,\mu_M) - \mathcal{I}_{M-1}[u(.,\mu_M)]]}{u(x_M,\mu_M) - \mathcal{I}_{M-1}[u(.,\mu_M)](x_M)}$$

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and remark q_M is order 1, so that

$$\mathcal{I}_M[u(.,\mu)] = \mathcal{I}_{M-1}[u(.,\mu)] + \Big[u(x_M,\mu) - \mathcal{I}_{M-1}[u(.,\mu)](x_M)\Big] q_M(.)$$

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hence, we can write

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$$\mathcal{I}_M[u(.,\mu)] = \sum_n \alpha_n q_n(.)$$

where the α_n are going to zero as $n \to \infty$

with every q_n of order 1.

So we want to use this information that

the α_n are going to zero as $n \to \infty$

This gives rise to the Constrained Stabilized (G)EIM

from J.P. Argaud, B. Bouriquet, H. Gong, Y. Maday, O. Mula (*)

(*) in *Stabilization of (G)EIM in presence of measurement noise: application to nuclear reactor physics*

Constrained Stabilized EIM

We write

$$u_N = \sum_n \alpha_n q_n$$

so as to solve

$$\min_{\alpha_n} \sum_i |u_N(x_i) - u(x_i)|^2$$

under the constraint that

$$|\alpha_n| \leq \varepsilon_n$$

Constrained Stabilized GEIM

We write

$$u_N = \sum_n \alpha_n q_n$$

so as to solve

$$\min_{\alpha_n} \sum_i |\sigma_i(u_N) - \sigma_i(u)|^2$$

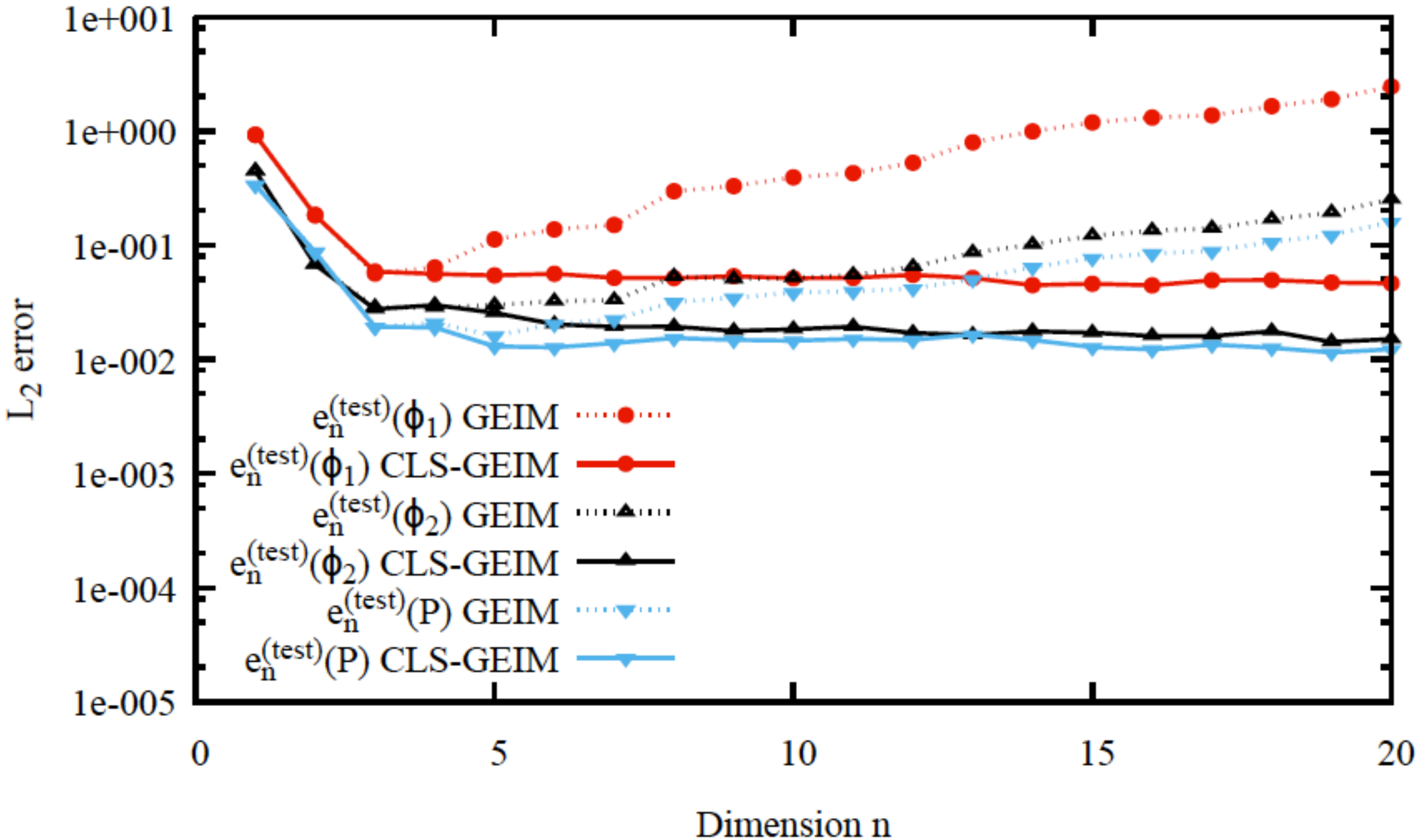
under the constraint that

$$|\alpha_n| \leq \varepsilon_n$$

The main interest is with noisy data

Assume that $u(x_i)$ (or the $\sigma_i(u)$) are polluted with some (random) noise η_i

The the CS approximation allows to minimize the effect of the noise



1e+001
1e+000
1e-001
1e-002
1e-003
1e-004
1e-005
0
5
10
15
20
Dimension n
L2 error
e_n^(test)(ϕ1) GEIM
e_n^(test)(ϕ1) CLS-GEIM
e_n^(test)(ϕ2) GEIM
e_n^(test)(ϕ2) CLS-GEIM
e_n^(test)(P) GEIM
e_n^(test)(P) CLS-GEIM

The data are polluted with noise

$$\forall i = 1, \ldots, n,\ \sigma_i(\mathcal{J}_n[u]) = \sigma_i(u) + \varepsilon_i$$

this leads to a polluted reconstruction

$$\mathcal{J}_n[u,\varepsilon] = \sum_{j=1}^{n} \tilde{\beta}_j\ \varphi_j,\ \text{such that}\ \ \forall i = 1, \ldots, n,\ \sigma_i(\mathcal{J}_n[u,\varepsilon]) = \sigma_i(u) + \varepsilon_i$$

And of course now, the error, scales like

$$\|u - \mathcal{J}_n[u,\varepsilon]\|_{\mathcal{X}} \leq (1 + \Lambda_n) \inf_{v_n \in X_n} \|u - v_n\|_{\mathcal{X}} + \Lambda_N \max_{i=1,\ldots,n} |\varepsilon_i|$$

This is what we see here

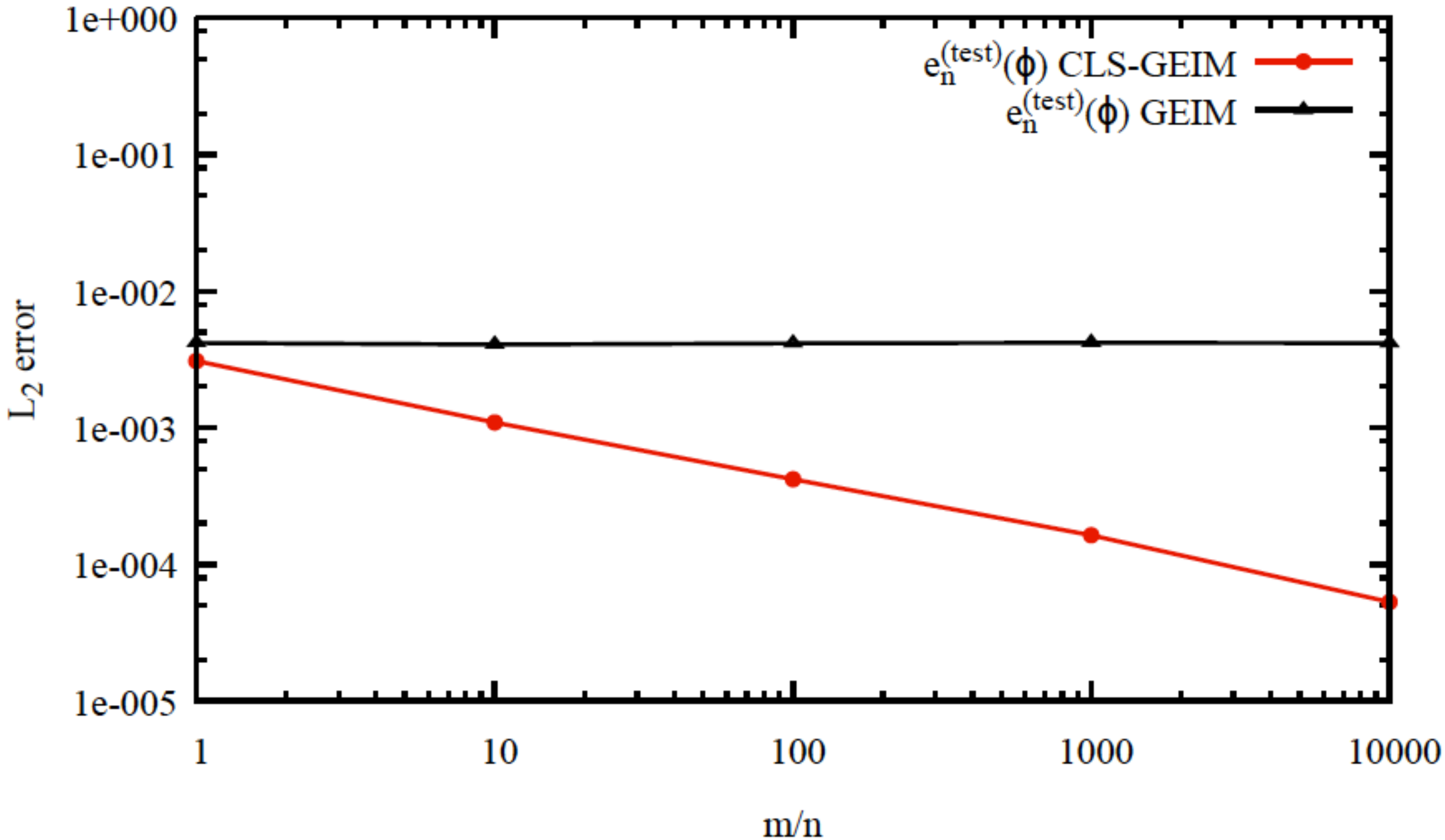


Fig. 12: CS-GEIM with different n/m ratio, the input noise level is 10^{-2}, with the function $g(x,\mu) \equiv ((x_1-\mu_1)^2+(x_2-\mu_2)^2)^{-1/2}$, the error converges with $\sim n^{-\frac{1}{2}}$.

Now a mixed of data and model ...

Incorporating the model error : Parametrized-Background Data-Weak (PBDW) formulation with A.T. Patera, J. D. Penn and M. Yano

The PBDW formulation integrates a parametrized mathematical model and M experimental observations associated with the configuration $\mathcal{C}$ to estimate the true field $u^{true}[\mathcal{C}]$ as well as any desired output $l^{out}(u^{true}[\mathcal{C}]) \in C$ for given output functional l^{out}.

We first introduce a sequence of background spaces that reflect our (prior) best knowledge,

$$\mathcal{Z}_1 \subset \cdots \subset \mathcal{Z}_{N_{max}} \subset \mathcal{U};$$

here the second ellipsis indicates that we may consider the sequence of length N_{max} as resulting from a truncation of an infinite sequence. Our goal is to choose the background spaces such that

$$\lim_{N\to\infty} \inf_{w\in\mathcal{Z}_N} \|u^{\text{true}}[\mathcal{C}] - w\| \leq \epsilon_{\mathcal{Z}} \quad \forall \mathcal{C} \in \mathcal{S},$$

In words, we choose the background spaces such that the most dominant physics that we anticipate to encounter for various system configurations is well represented for a relatively small N.

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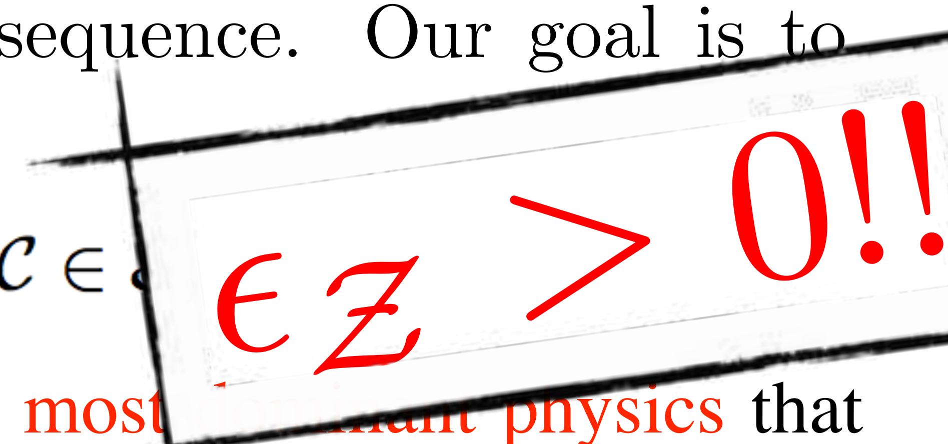

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We now characterize our data acquisition procedure. Given a system in configuration $\mathcal{C} \in \mathcal{S}$, we assume our observed data $y^{\rm obs}[\mathcal{C}] \in \mathbb{C}^M$ is of the form,

$$\forall m = 1, \ldots, M, \quad y_m^{\rm obs}[\mathcal{C}] = \ell_m^{\rm o}(u^{\rm true}[\mathcal{C}])$$

here $y_m^{\rm obs}[\mathcal{C}]$ is the value of the m-th observation, $\ell_m^{\rm o} \in \mathcal{U}'$

We first associate with each observation functional $\ell_m^o \in \mathcal{U}'$ an observable function,

$$\forall m = 1, \ldots, M, \quad q_m = R_{\mathcal{U}} \ell_m^{\text{o}},$$

the Riesz representation of the functional [1]. We then introduce hierarchical *observable spaces*,

$$\forall M = 1, \ldots, M_{\max}, \ldots, \quad \mathcal{U}_M = \operatorname{span}\{q_m\}_{m=1}^M;$$

We may now state the PBDW estimation statement: given a physical system in configuration $\mathcal{C} \in \mathcal{S}$, find $(u_{N,M}^*[\mathcal{C}] \in \mathcal{U}, z_{N,M}^*[\mathcal{C}] \in \mathcal{Z}_N, \eta_{N,M}^*[\mathcal{C}] \in \mathcal{U})$ such that

$$(u_{N,M}^*[\mathcal{C}], z_{N,M}^*[\mathcal{C}], \eta_{N,M}^*[\mathcal{C}]) = \underset{\substack{u_{N,M} \in \mathcal{U} \\ z_{N,M} \in \mathcal{Z}_N \\ \eta_{N,M} \in \mathcal{U}}}{\arg\inf} \|\eta_{N,M}\|^2 \tag{2}$$

subject to

$$\begin{aligned} (u_{N,M}, v) &= (\eta_{N,M}, v) + (z_{N,M}, v) \quad \forall v \in \mathcal{U}, \\ (u_{N,M}, \phi) &= (u_M^{\text{obs}}[\mathcal{C}], \phi) \quad \forall \phi \in \mathcal{U}_M. \end{aligned}$$

We may readily derive the associated (reduced) Euler-Lagrange equations as a saddle problem given a physical system in configuration $\mathcal{C} \in \mathcal{S}$, find $(\eta_{N,M}^*[\mathcal{C}] \in \mathcal{U}_M, z_{N,M}^*[\mathcal{C}] \in \mathcal{Z}_N)$ such that

$$\begin{aligned} (\eta_{N,M}^*[\mathcal{C}], q) + (z_{N,M}^*[\mathcal{C}], q) &= (u_M^{\text{obs}}[\mathcal{C}], q) \quad \forall q \in \mathcal{U}_M, \\ (\eta_{N,M}^*[\mathcal{C}], p) &= 0 \quad \forall p \in \mathcal{Z}_N, \end{aligned} \tag{3}$$

and set

$$u_{N,M}^*[\mathcal{C}] = \eta_{N,M}^*[\mathcal{C}] + z_{N,M}^*[\mathcal{C}]. \tag{4}$$

Algebraic Form: Offline-Online Computational Procedure

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^H & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\eta}^*[\mathcal{C}] \\ \mathbf{z}^*[\mathcal{C}] \end{pmatrix} = \begin{pmatrix} y^{\text{obs}}[\mathcal{C}] \\ 0 \end{pmatrix},$$

where

$$\mathbf{A} \equiv Q^\dagger U Q = LQ \in \mathbb{C}^{M \times M}$$
$$\mathbf{B} \equiv Q^\dagger U Z = LZ \in \mathbb{C}^{M \times N},$$

So now let us assume that the data are polluted with noise

and propose a CS version of the PBDW approximation

There are two ways : the **Tikhonov** and Ivanov approaches

$$\min\Big[\kappa\|\eta_{N,M}\|^2 + \sum_m |\ell^o_m(u^{\text{true}}) - \ell^o_m(u_{N,M})|^2\Big]$$

under the constraints that

- $\eta_{N,M}$ belongs to $\mathcal{U}_M$
- $u_{N,M} = z_{N,M} + \eta_{N,M}$
- $z_{N,M} \in \mathcal{Z}_N$, $z_{N,M} = \sum_n \alpha_n q_n$
- $|\alpha_n| \leq \varepsilon_n$

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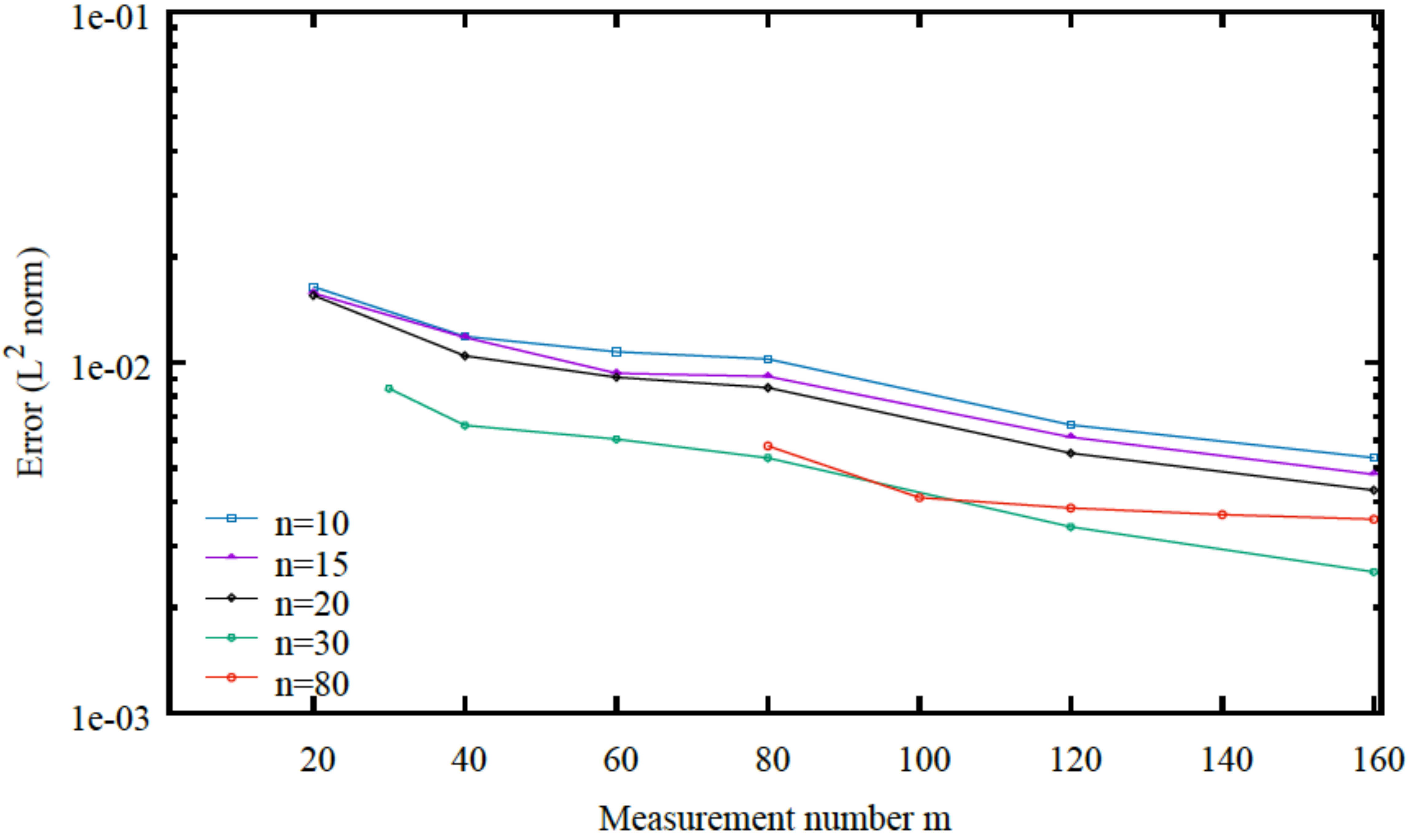
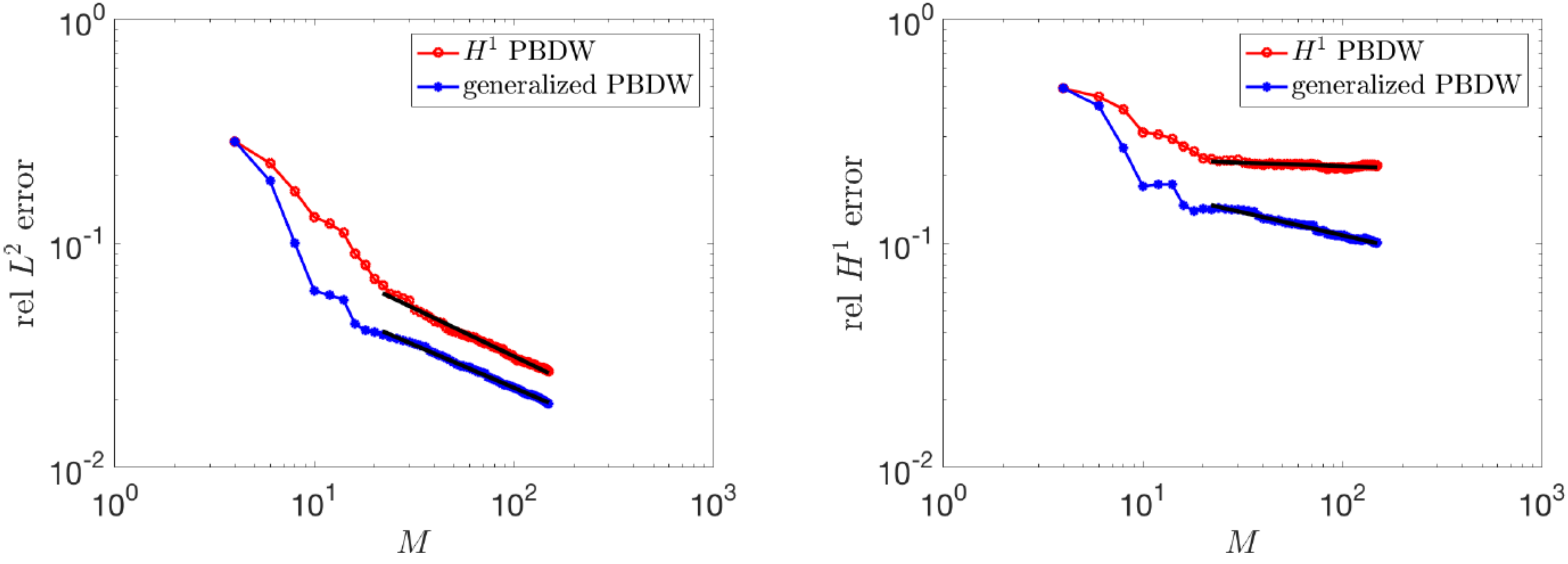
- $|\alpha_n| \leq \varepsilon_n$
- $\forall m, |\ell^o_m(u^{\text{true}}) - \ell^o_m(u_{N,M})| \leq \text{noise}$



Ivanov with noise level is 10^{-2} (in collaboration with Gong and Mula)



Tikhonov with noise level is 10^{-1} (in collaboration with Taddei)

How do we have a hand on $u(., \mu)$?

through a parameter dependent PDE

For some μ in a chosen parameter set $\mathcal{D}$:

$$\mathcal{L}(u(., \mu); \mu) = 0$$

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EIM is actually one very important tool for the efficient implementation of nonlinear problems.

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Once we have such a candidate X_N

We can solve a new PDE

- either by a Galerkin method, or another discrete approach
- the error between the exact solution and the Galerkin approximation is then “optimal”
- optimal meaning that it has the size

$$\sup_{u \in \mathcal{S}} \inf_{v_n \in X_n} \|u - v_n\|_X.$$

Question : is that small enough ?

A Posteriori Analysis

Numerical analysis can be developed and provide a computable estimator : $\varepsilon_n(\mu)$

$$\varepsilon_n(\mu) \equiv \|u(\mu) - u_n(\mu)\|$$

… when such an a posteriori estimator is available you can get an other approach to SVD/POD

Greedy algorithm

The POD/SVD is expensive since it is based on the preliminary evaluations of many solutions $u(\mu)$ that scan $\mathcal{S}$ well enough

The greedy algorithm builds the space recursively

Greedy

Start with one parameter value and compute

$$u(\mu_1)$$

This gives a first space X_1

and a first Galerkin method

and a first a posteriori estimator $\varepsilon_1(\mu)$

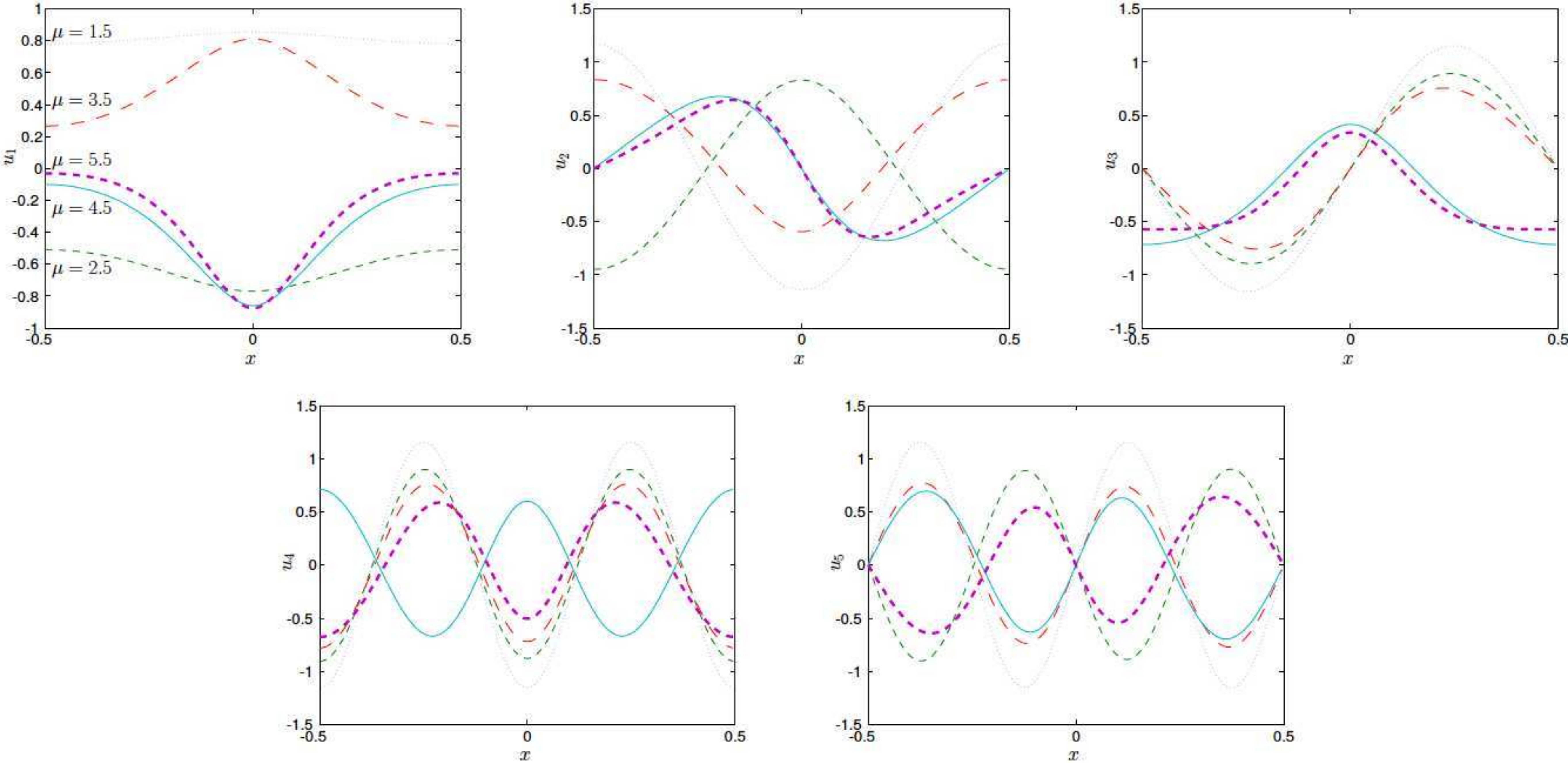
$$\mu_2 = \mathrm{argmax}_\mu \varepsilon_1(\mu)$$

then the solution $u(\mu_2)$ is computed

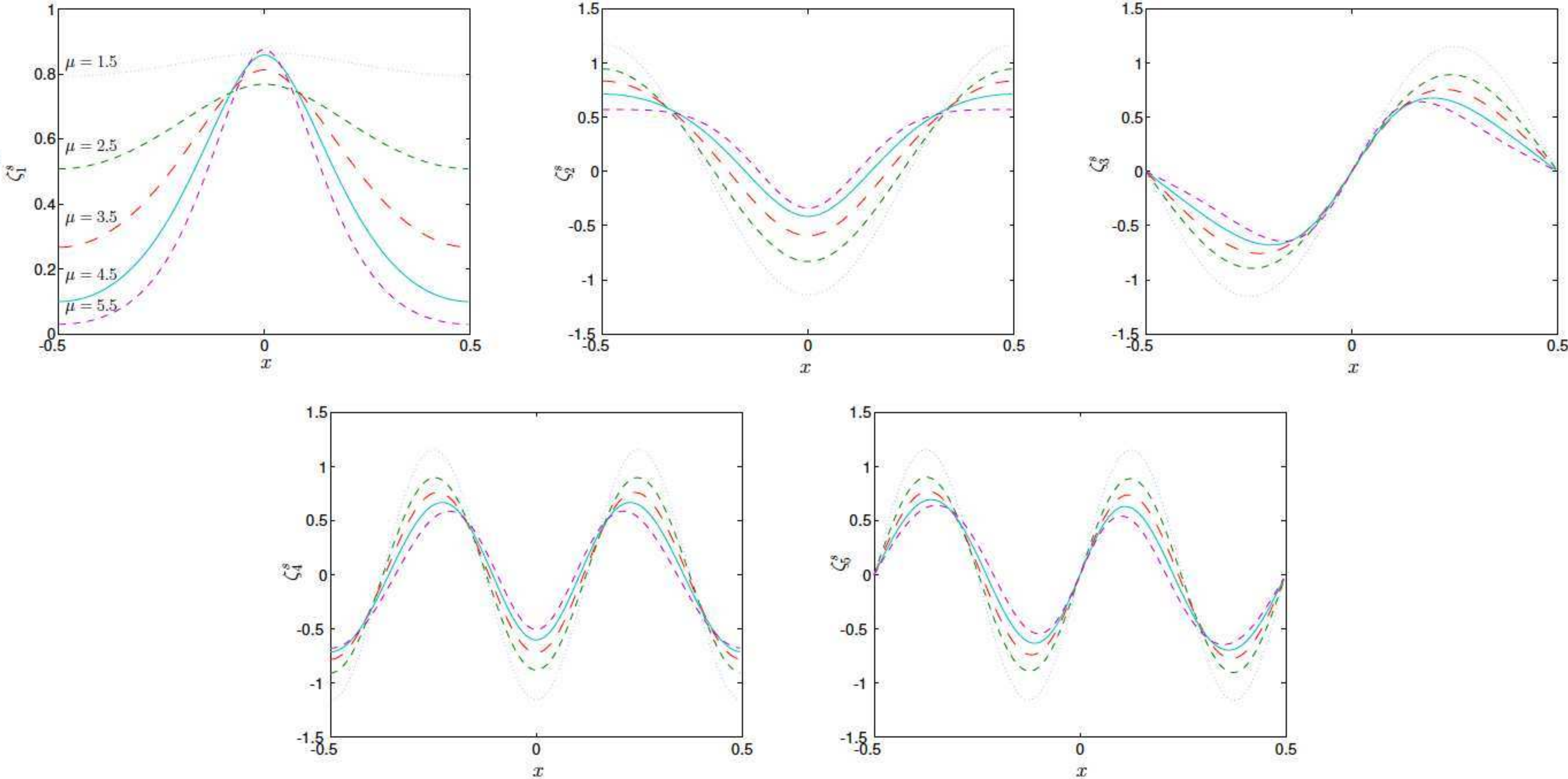
.. this gives a second space X_2 ...

and a second a posteriori estimator

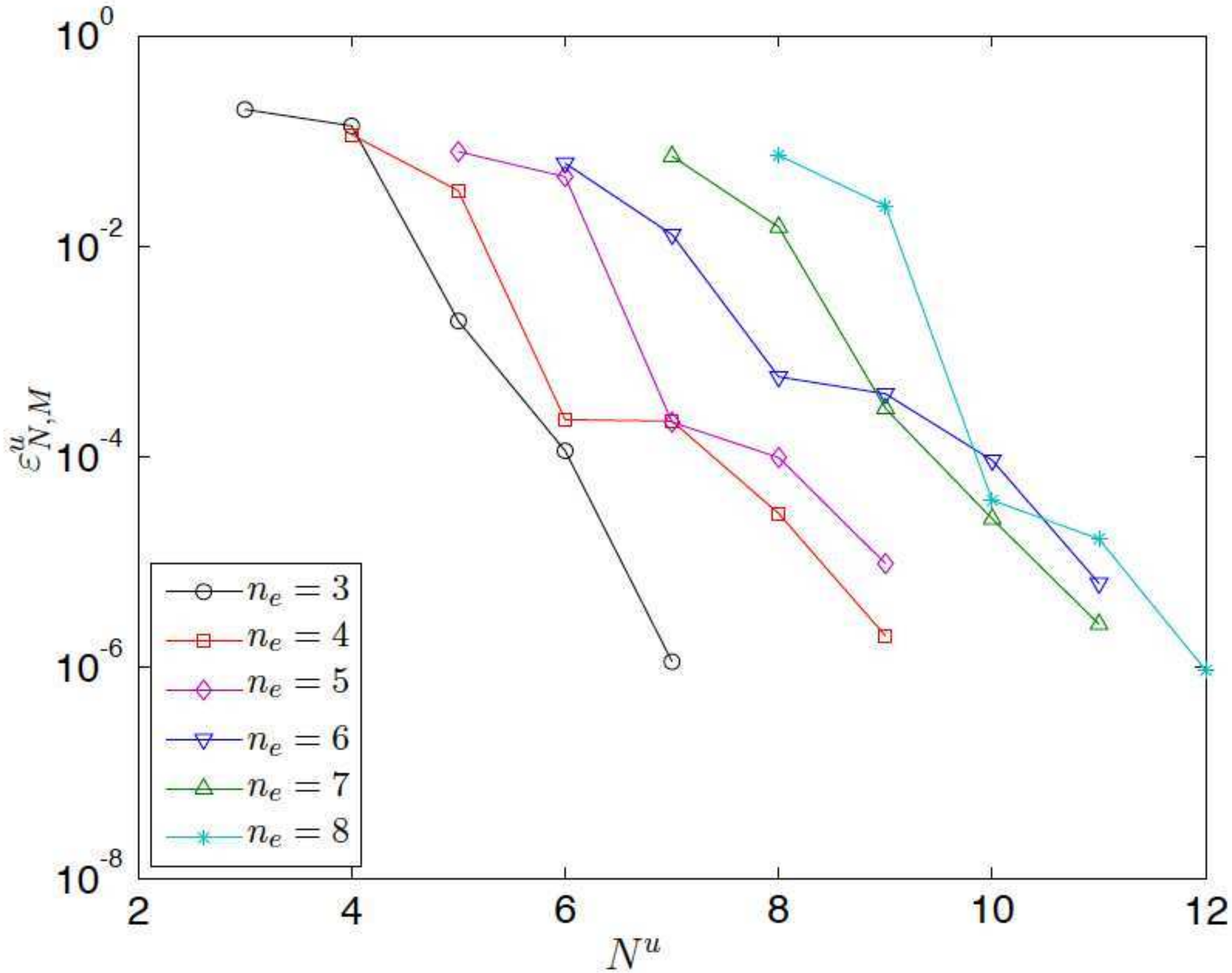
Application to Kohn-Sham : the wave functions



Solutions of $\hat{\mathbf{u}}(\mu)$ at $\mu = 1.5, 2.5, 3.5, 4.5$ and 5.5, before the alignment process.



$\hat{\zeta}^s$ at $\mu = 1.5, 2.5, 3.5, 4.5$ and 5.5, after the alignment process.



] Convergence of the reduced basis error $\varepsilon^u_{N,M}$ for $3 \leq n_e \leq 8$. The μ range is $[1.5, 5.5]$.

Feasibility and Competitiveness of a Reduced Basis Approach for Rapid Electronic Structure Calculations in Quantum Chemistry

E. Cancès, C. Le Bris, Y. Maday, N.C. Nguyen, A.T. Patera, and G.S.H. Pau

Hartree Fock model

Variation of the reduced-basis error

N	18	19	20	21	36	38	40	42
$e^{\boldsymbol{\Phi}}$	1.2407E − 01	6.5046E − 03	1.0888E − 03	5.4543E − 03	1.6311E − 04	2.0232E − 05	6.6913E − 05	1.7891E − 05
e^{E}	8.3389E − 05	5.3251E − 06	1.1965E − 06	1.4195E − 07	9.8293E − 11	1.6531E − 12	3.9346E − 12	3.1278E − 12
e^{ortho}	1.2407E − 01	7.5226E − 03	1.901E − 03	8.0144E − 03	1.167E − 04	1.1855E − 05	7.393E − 05	1.6658E − 05

we consider the reaction between the ion F^- and the methane molecule $CH_4 : F^- + CH_4 \rightarrow CH_3F^- + H$

Here the number of pair of electrons is $n_e = 9$.

A reduced basis method applied to the Restricted Hartree–Fock equations

Yvon Maday [a,b], Ulrich Razafison [a]

Conclusion

We have presented various use of the reduced framework

These approaches are already useful per se

- EIM
- GEIM
- PBDW
- Reduced basis …

Conclusion

We have presented various use of the reduced framework

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- EIM
- GEIM
- PBDW
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- by some values of $u(.,\mu)$ at some points in Ω
- by some outputs of $u(.,\mu)$
- through a parameter dependent PDE

or a mix of the above

Conclusion

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Conclusion

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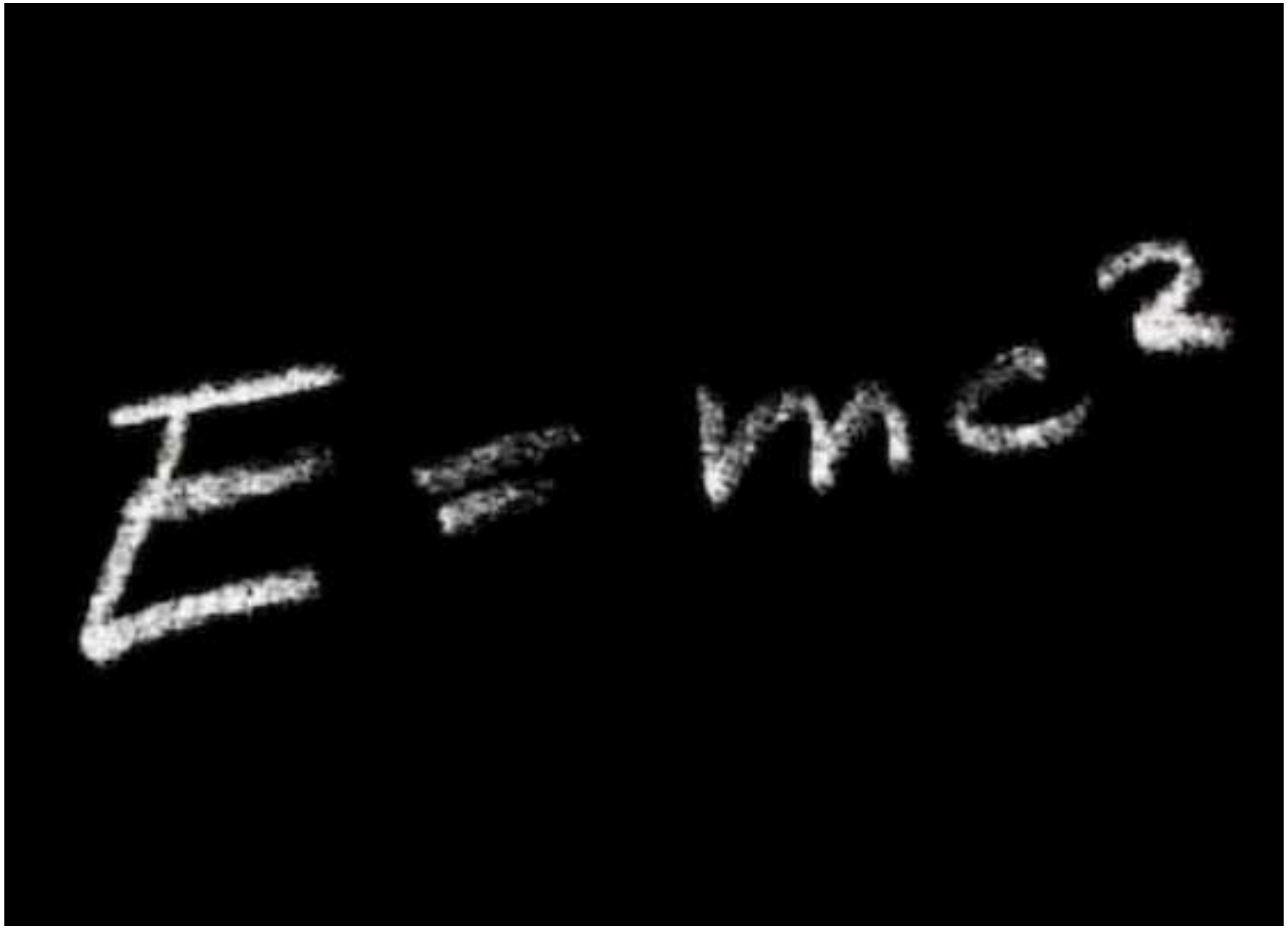
Important I think with further data assimilation tools…

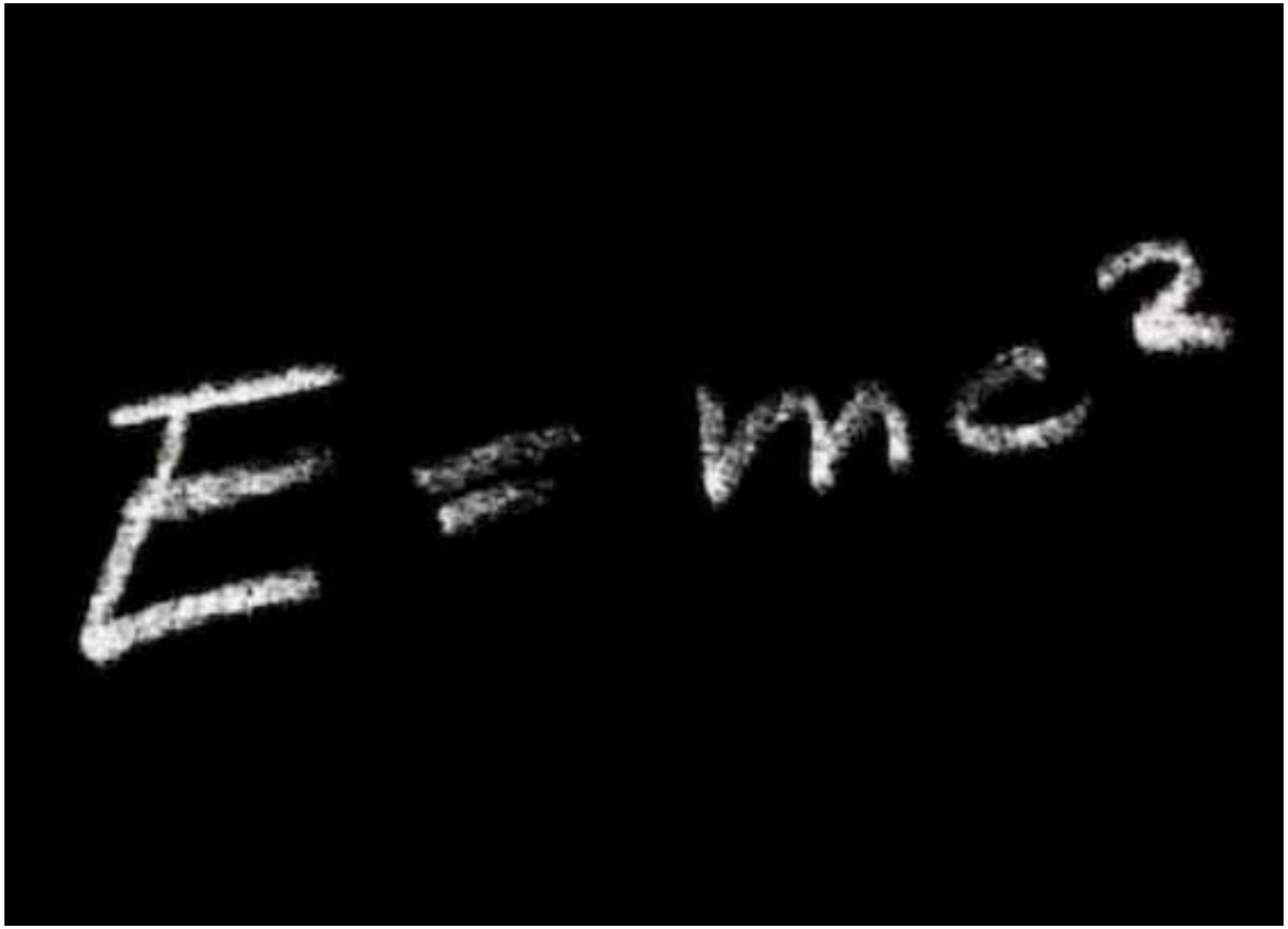
Collaboration with

- A. T. Patera, MIT

- J.-P. Argaud, B. Bouriquet, EDF
- A. Buffa, Pavia
- R. Chakir, IFSTAR
- Y. Chen, Brown
- H. Gong, EDF and UPMC
- Y. Hesthaven, Brown
- E. Løvgren, SIMULA
- O. Mula, G. Turinici, Paris 9
- NC Nguyen, MIT, J.Pen, MIT
- C Prud'homme, Strasbourg
- J. Rodriguez Santiago de Compostella
- E. M. Rønquist, Trondheim
- B. Stamm, Aachen
- M. Yano, Toronto



Extreme-scale Mathematically-based Computational Chemistry (EMC2) porté par Eric Cancès, Laura Grigori, Yvon Maday et Jean-Philip Piquemal



post doc and PhD Positions @ ERC

Thanks

Questions/remarks ??