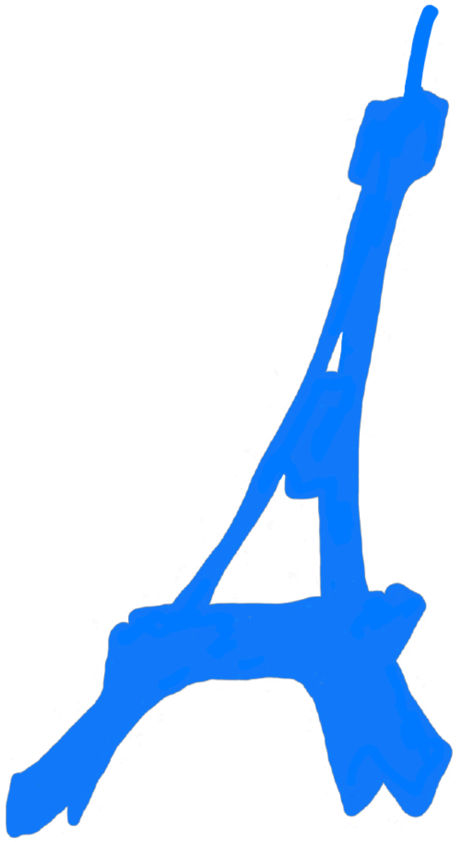
A Glimpse of Numerical Analysis in Computational Chemistry : Some Recent Mathematical Results



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EMC²
Extreme-scale Mathematically-bas
Computational Chemistry

Many problem in science take the form

Find U in X such that:

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e.g. Hartree Fock of Kohn-Sham

Find M orbitals $(\phi_1^0, \ldots, \phi_M^0)$ with corresponding lowest eigenvalues $\lambda_1^0, \ldots, \lambda_M^0$, such that

$$\mathcal{H}^0 \phi_i^0 = \lambda^0 \phi_i^0, \quad i = 1, \ldots, M,$$

where

$$\mathcal{H}^0 = \mathcal{H}_{[\rho^0]} = -\frac{1}{2}\Delta + V_{\mathrm{ion}} + V_{\mathrm{coul}}(\rho^0) + V_{\mathrm{xc}}(\rho^0)$$

with $\rho^0 = \rho_{[\Phi^0]}$.

Many problem in science take the form

Find U in X such that:

$$F(U) = 0$$

Solving this problem is impossible

hence classically we refer to discretisation

Find U_N in X_N such that:

$$F_N(U_N) = 0$$

Toy problem to start with (Dusson - M.)

Problem presentation: the Gross-Pitaevskii equation

Physical problem: Ground state of a system of bosons at very low temperature.

Two ways of seeing the problem: minimization problem – eigenvalue problem

Minimization problem: Energy functional minimization

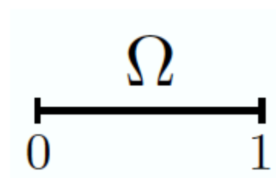
$$I = \inf \left\{ E(v),\ v \in H^1_\#(\Omega),\ \int_\Omega v^2 = 1 \right\} \quad \text{with } \Omega = (0,1)$$

$$\text{where} \quad E(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 + \frac{1}{2}\int_\Omega V v^2 + \frac{1}{4}\int_\Omega v^4, \quad V \in L^p, p > 1$$

Nonlinear eigenvalue problem

$$\begin{cases} (-\Delta + V + u^2)u = \lambda u \\ \int_\Omega u^2 = 1. \end{cases}$$

Setting: 1-Dimensional, Periodic Setting.



Remark: λ is the smallest eigenvalue and is **simple**.

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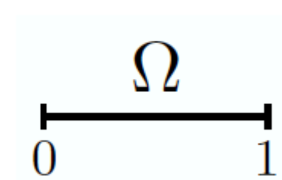

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$U = (u, \lambda)$

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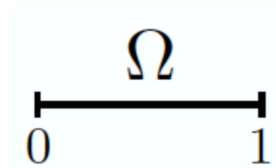

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Resolution method

1- Space discretization: Planewave expansion.
Expansion in Fourier series:

$$u(x) = \sum_k \hat{u}_k e_k(x) \quad \text{where} \quad e_k(x) = e^{2\pi i k.x}$$

Exact space: $X = H^1_{\#}(\Omega)$. Discretized space: $X_N = \text{Span}\{e_k, |k| \leq N, k \in \mathbb{N}\}$.

Discretized problem

$$\forall v_N \in X_N, \int_\Omega \nabla u_N \cdot \nabla v_N + \int_\Omega V u_N v_N + \int_\Omega u_N^3 v_N - \lambda_N \int_\Omega u_N v_N = 0.$$

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$$-\Delta u_N + \Pi_N [V u_N + u_N^3] = \lambda_N u_N$$

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Find U_N in X_N such that:
$F_N(U_N) = 0$

$$-\Delta u_N + \Pi_N[V u_N + u_N^3] = \lambda_N u_N$$

Analysis

$$F_N(u,\lambda) \simeq F_N(u_N,\lambda_N) + DF_N(u_N,\lambda_N)[(u,\lambda) - (u_N,\lambda_N)]$$

$$F_N(u,\lambda) \simeq F_N(u_N,\lambda_N) + DF_N(u_N,\lambda_N)[(u,\lambda)-(u_N,\lambda_N)]$$

so that $u - u_N$ and $\lambda - \lambda_N$ scale like

$$[DF_N(u_N,\lambda_N)]^{-1} F_N(u,\lambda)$$

by using that

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and

$$\|u-u_N\|_{H^1} + |\lambda-\lambda_N| \leq C\|u-\Pi_N u\|_{H^1}.$$

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This is A PRIORI analysis

and

$$\|u - u_N\|_{H^1} + |\lambda - \lambda_N| \le C \|u - \Pi_N u\|_{H^1}.$$

Toy problem to start with (Dusson - M.)

A priori analysis–Convergence results

Notations:

- u: unique positive solution of the exact nonlinear eigenvalue problem
- u_N: a minimizer of the discretized problem such that $(u_N, u)_{L^2} \geq 0$.

Theorem (Cancès, Chakir, Maday)

Under previous assumption, it holds: $\|u_N - u\|_{H^1} \longrightarrow_{N\to+\infty} 0.$
There exists two constants $\beta \in \mathbb{R}_+$ *and* $C \in \mathbb{R}_+$ *such that, for N large enough*

Eigenfunction $\quad \|u_N - u\|_{H^1} \leq C \min_{v_N \in X_N} \|v_N - u\|_{H^1}$ (optimal)

Energy $\quad \beta\|u_N - u\|^2_{H^1} \leq E(u_N) - E(u) \leq C\|u_N - u\|^2_{H^1}$

Eigenvalue $\quad |\lambda_N - \lambda| \leq C \left(\|u_N - u\|^2_{H^1} + \|u_N - u\|_{L^2}\right)$ (improved)

Eigenfunction $\quad \|u_N - u\|^2_{L^2} \leq C\|u_N - u\|_{H^1} \min_{\psi_N \in X_N} \|\psi_{u_N - u} - \psi_N\|_{H^1}$ (quasi-opt.)

where for $w \in X'$, Ψ_w *is the unique solution to the adjoint problem:*
Find $\Psi_w \in u^\perp$ *such that* $\forall v \in u^\perp, \quad \langle (E''(u) - \lambda)\Psi_w, v\rangle_{X',X} = \langle w, v\rangle_{X',X}\,.$

Analysis

Let's go now to

A POSTERIORI analysis

Analysis

instead of

$$F_N(u,\lambda) \simeq F_N(u_N,\lambda_N) + DF_N(u_N,\lambda_N)[(u,\lambda)-(u_N,\lambda_N)]$$

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and $(u_N - u, \lambda_N - \lambda)$ behaves as

$$DF(u, \lambda)^{-1} F(u_N, \lambda_N)$$

using this time the fact that $F(u, \lambda) = 0$.

$$F(u_N,\lambda_N) \simeq F(u,\lambda) + DF(u,\lambda)[(u_N,\lambda_N)-(u,\lambda)]$$

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$$\begin{aligned}
\|u_N - u\|_{H^1} &\le \|(u_N,\lambda_N)-(u,\lambda)\|_{H^1\times\mathbb{R}} \\
&\le \left\|[DF(u,\lambda)]^{-1}F(u_N,\lambda_N)\right\|_{H^1\times\mathbb{R}} \\
&\le \left\|[DF(u,\lambda)]^{-1}\right\|_{\mathcal{L}(H^1\times\mathbb{R},H^{-1}\times\mathbb{R})} \|F(u_N,\lambda_N)\|_{H^{-1}\times\mathbb{R}} \\
&= \left\|[DF(u,\lambda)]^{-1}\right\|_{\mathcal{L}(H^1\times\mathbb{R},H^{-1}\times\mathbb{R})} \|\lambda_N u_N + \Delta u_N - V u_N - u_N^3\|_{H^{-1}}.
\end{aligned}$$

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$$F(u_N, \lambda_N) \simeq F(u, \lambda) + DF(u, \lambda)[(u_N, \lambda_N) - (u, \lambda)]$$

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Residual

Analysis

$$F(u_N,\lambda_N) \simeq F(u,\lambda) + DF(u,\lambda)[(u_N,\lambda_N)-(u,\lambda)]$$

and $(u_N - u, \lambda_N - \lambda)$ behaves as

But this is not the only approximation !!

$$\ldots DF(u,\lambda)^{-1}F(u_N,\lambda_N)$$

using this time the fact that $F(u,\lambda)=0$.

$$\begin{aligned}
\|u_N - u\|_{H^1} &\leq \|(u_N,\lambda_N)-(u,\lambda)\|_{H^1\times I\!R} \\
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Residual

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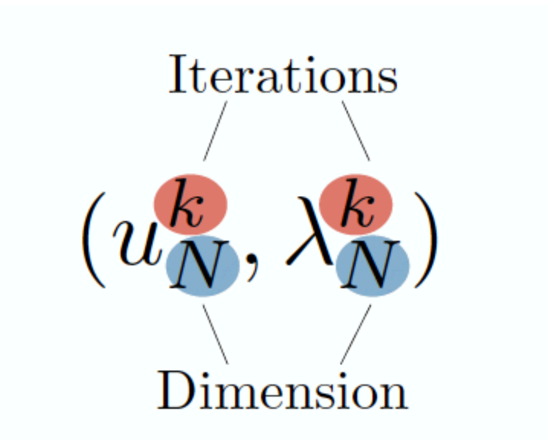
Discretized problem $\forall v_N \in X_N, \int_\Omega \nabla u_N \cdot \nabla v_N + \int_\Omega V u_N v_N + \int_\Omega u_N^3 v_N - \lambda_N \int_\Omega u_N v_N = 0.$

2- Iterative resolution: Algorithm used to solve the equation on X_N:

1. **Initialization:** Well-chosen pair (u_N^0, λ_N^0).
2. **Iterations:** Loop until convergence ($\|u_N^k - u_N^{k-1}\|_{H^1}$ small).
   Linear Problem
   $$\Pi_N(-\Delta \widetilde{u_N^k} + V\widetilde{u_N^k} + (u_N^{k-1})^2 \widetilde{u_N^k}) = \lambda_N^{k-1} u_N^{k-1}.$$
   Normalization $u_N^k = \widetilde{u_N^k} / \|\widetilde{u_N^k}\|_{L^2}$.
   Rayleigh Quotient $\lambda_N^k = \int \nabla(u_N^k)^2 + V(u_N^k)^2 + (u_N^k)^4$.
3. **Output:** Approximate eigenfunction and eigenvalue $(u_N^{k_{out}}, \lambda_N^{k_{out}})$.



Toy problem to start with (Dusson - M.)

First a posteriori bound

Theorem: Guaranteed bound
Under the previous conditions, there exists a unique $(\tilde{u}, \tilde{\lambda})$ in the ball $B((u_N^k, \lambda_N^k), 2\gamma\epsilon)$ such that $F(\tilde{u}, \tilde{\lambda}) = 0$ and

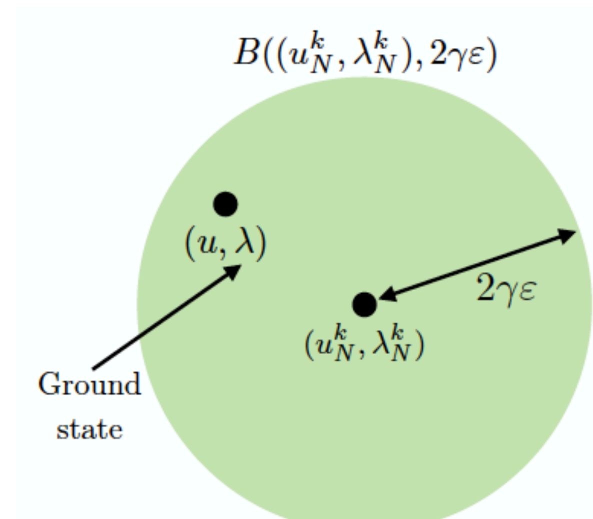
$$\|\tilde{u} - u_N^k\|_{H^1} + |\tilde{\lambda} - \lambda_N^k| \leq 2\gamma \| - \Delta u_N^k + V u_N^k + (u_N^k)^3 - \lambda_N^k u_N^k \|_{H^{-1}} \qquad (1)$$

Theorem: Ground state
There exists a computable condition depending on $\|\tilde{u} - u_N^k\|_{H^1}$, $|\tilde{\lambda} - \lambda_N^k|$, u_N^k, $\lambda_N^k, \mu_N^1, \mu_N^2$ guaranteeing that $(\tilde{u}, \tilde{\lambda})$ is the ground state (u, λ) of our problem.

Key lemma:
If (u, λ) is solution to the nonlinear eigenvalue problem, and is the smallest eigenpair of the linear operator $-\Delta + V + u^2$, then (u, λ) is the ground state.

A posteriori error bound valid under explicit and computable conditions.

Unfortunately too coarse and very restrictive conditions.



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Second a posteriori bound

Residual: $R_N^k = -\Delta u_N^k + V u_N^k + (u_N^k)^3 - \lambda_N^k u_N^k.$

Theorem: Asymptotic error bound
If $\|u - u_N^k\|_{H^1}$ and $|\lambda - \lambda_N^k|$ are small enough, then there exists a computable constant $\alpha > 1$ such that for N and k large enough, the following *a posteriori* error bound holds:

$$\|u - u_N^k\|_{H^1} \leq \alpha \Bigg(\|R_N^k\|_{H^{-1}} + \|(V + 3(u_N^k)^2 - \lambda_N^k - 1)_-\|_{L^\infty} \Bigg[\frac{1}{\beta_N^k} \|\Pi_N R_N^k\|_{H^{-1}} + \frac{2}{\beta_N^k} |\lambda_N^k - \mu_N^1| \|u_N^k - v_N^1\|_{L^2} + \frac{3}{2} \|u_N^k - v_N^1\|_{L^2}^2 \left(1 + \frac{\|2(u_N^k)^2 v_N^1\|_{H^{-1}}}{\beta_N^k}\right) \Bigg] \Bigg)$$

$\alpha = \frac{1}{1-\epsilon(u-u_N^k)}$ where $\epsilon(u - u_N^k) \xrightarrow[\|u-u_N^k\|_{H^1} \to 0]{} 0.$ Asymptotically, α goes to 1.

Corollary: If $\|(V + 3(u_N^k)^2 - \lambda_N^k - 1)_-\|_{L^\infty} = 0$,

$$\|u - u_N^k\|_{H^1} \leq \alpha \|R_N^k\|_{H^{-1}}$$

Depends only on the residual R_N^k.

Better bound...but guaranteed only if the error is small enough.

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more accurate !

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Error balance–Separation of error

Aim

- Analyse the error bound
- Find the origin of the error: space discretization and iterations
- Be able to refine the right parameter at each step
- Get the **best compromise** between space discretization and number of iteration that minimizes the number of computations for a given accuracy.

Two error sources:

- Size of the Fourier space $2N+1$.
- Number of iterations k.

Therefore, we decompose the main residual into **two computable parts**

$$R_{disc} = -\Delta u_N^k + V u_N^k + (u_N^{k-1})^2 u_N^k - \lambda_N^{k-1} u_N^{k-1}$$

$$R_{iter} = (u_N^k)^3 - (u_N^{k-1})^2 u_N^k - \lambda_N^k u_N^k + \lambda_N^{k-1} u_N^{k-1}$$

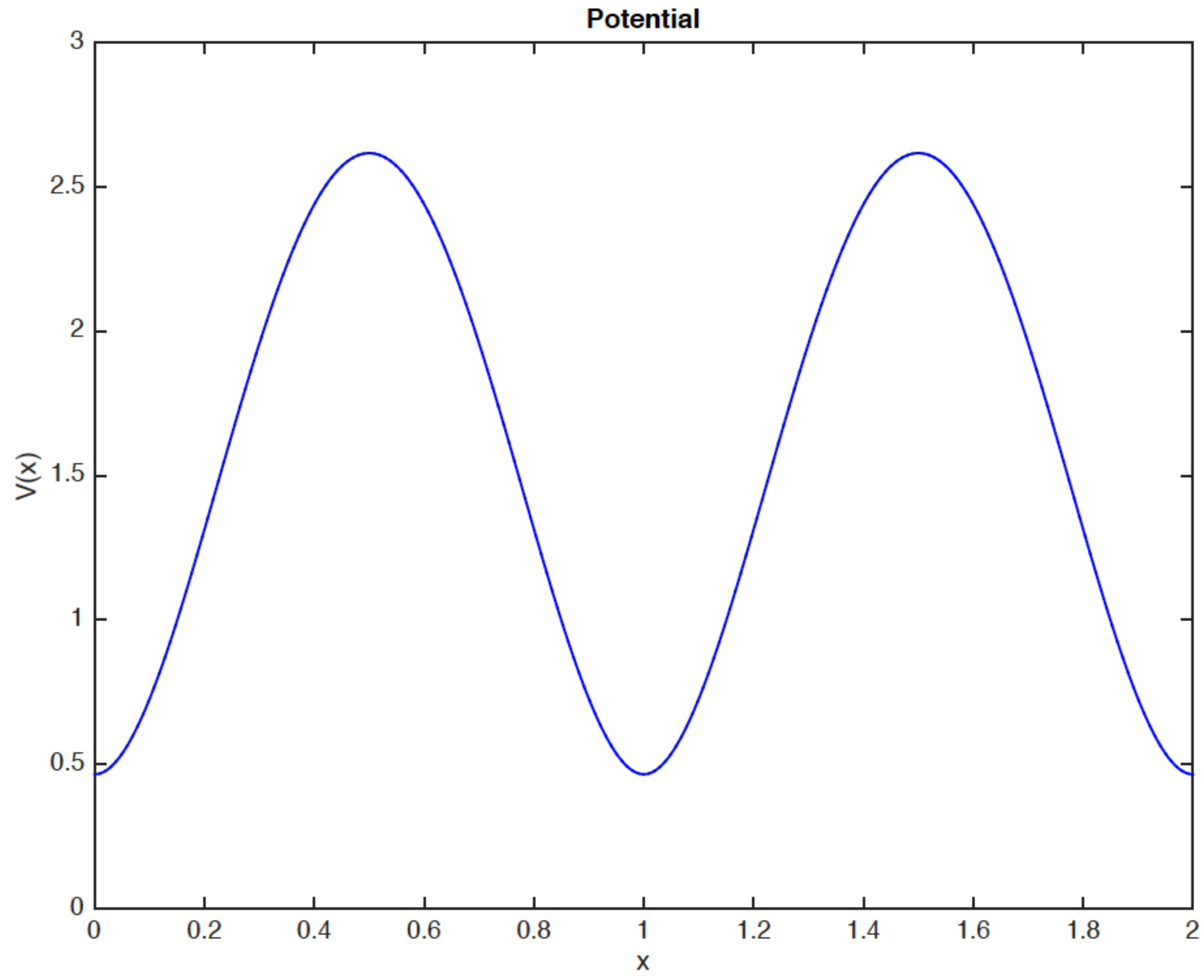
such that

$$R_N^k = R_{disc} + R_{iter}.$$

Toy problem to start with (Dusson - M.)

Numerical simulations: Framework

The Fourier coefficients of the potential V are given by $\widehat{V}_k = -\frac{1}{\sqrt{2\pi}}\frac{1}{|k|^4 - \frac{1}{4}}$,



Toy problem to start with (Dusson - M.)

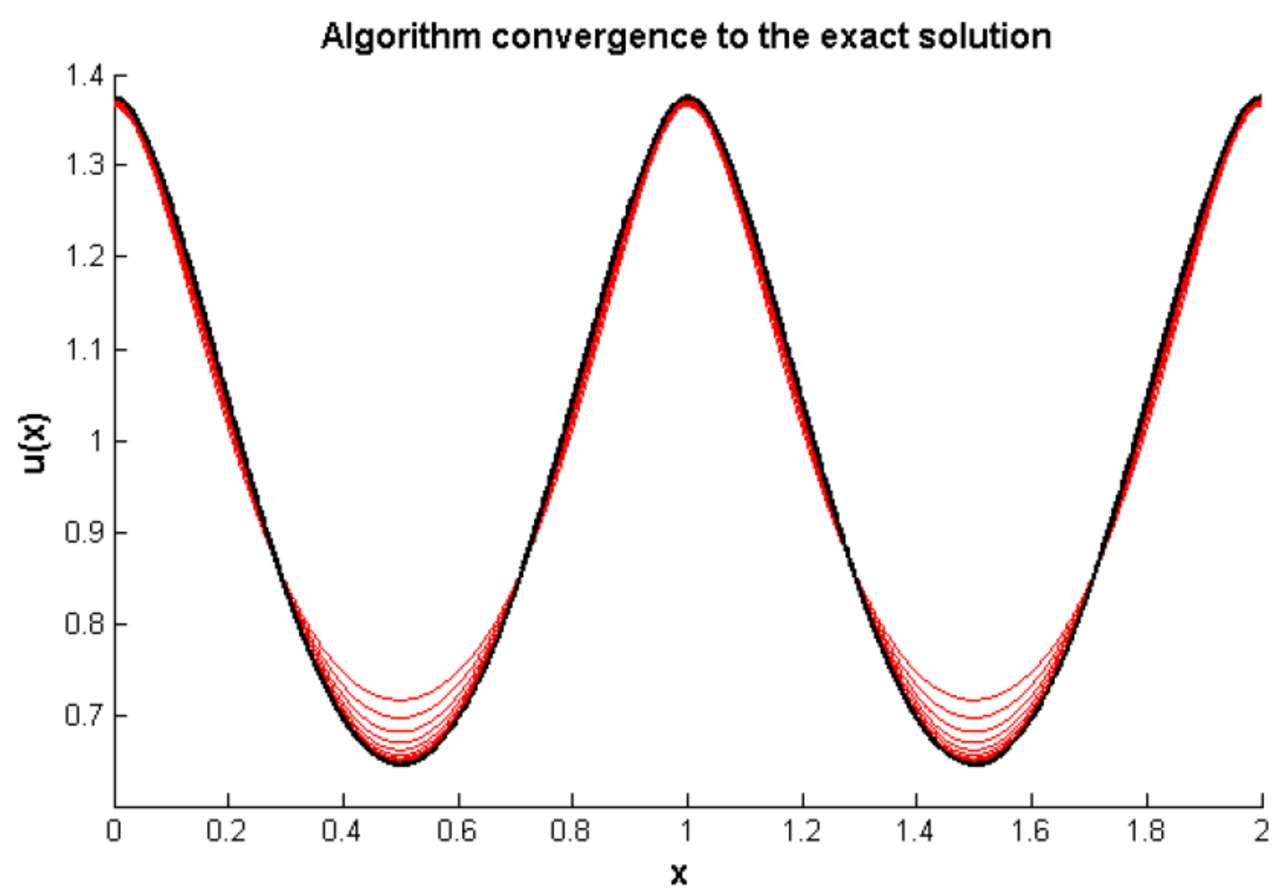
Exact solution

"Exact" solution

- Calculated in a discrete space with N=500.
- Norm of the residual:

$$\|R_N^k\|_{H^{-1}} = 4.10^{-13}$$

Results no more precise than 10^{-13}



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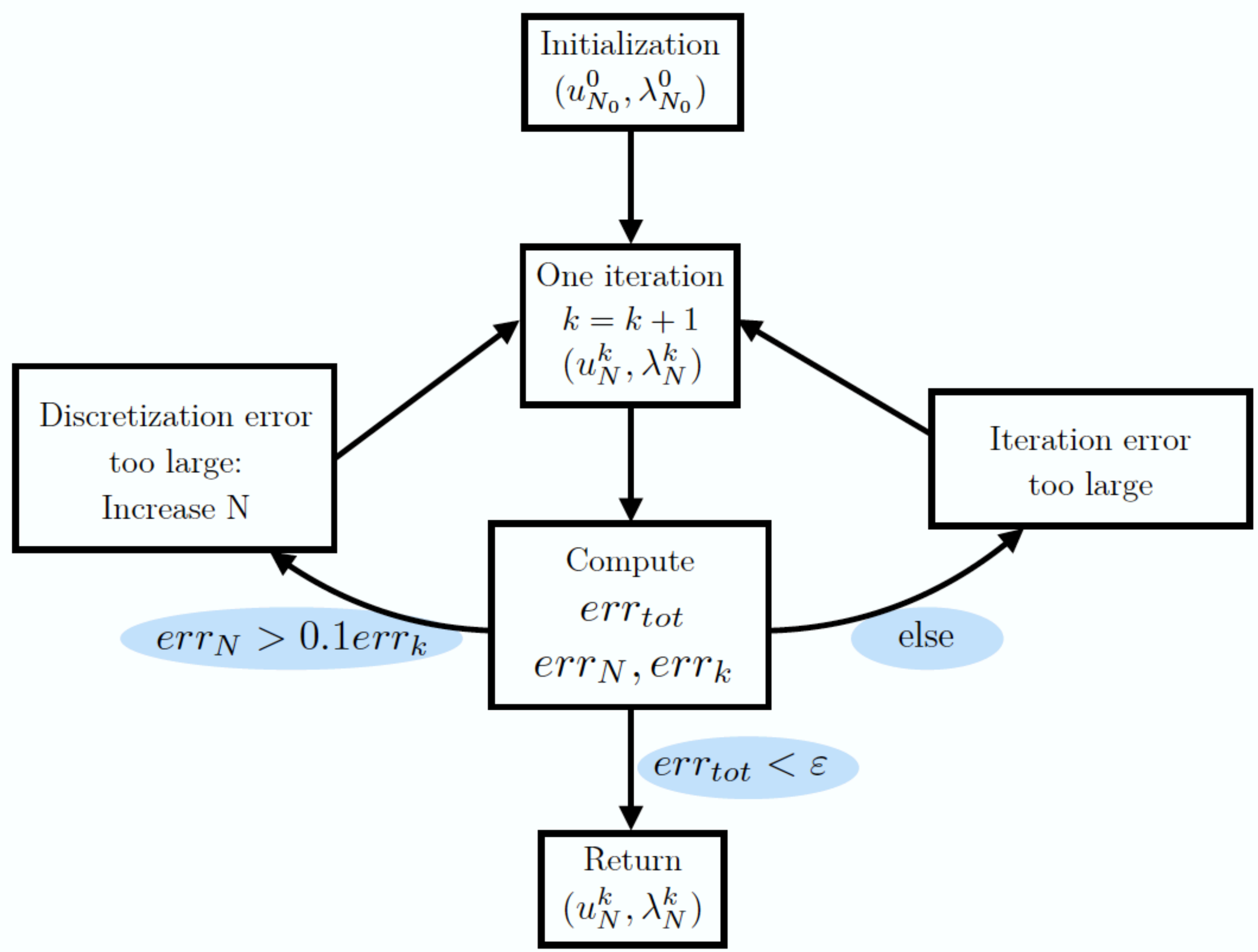
Error balance algorithm

discretization strategy



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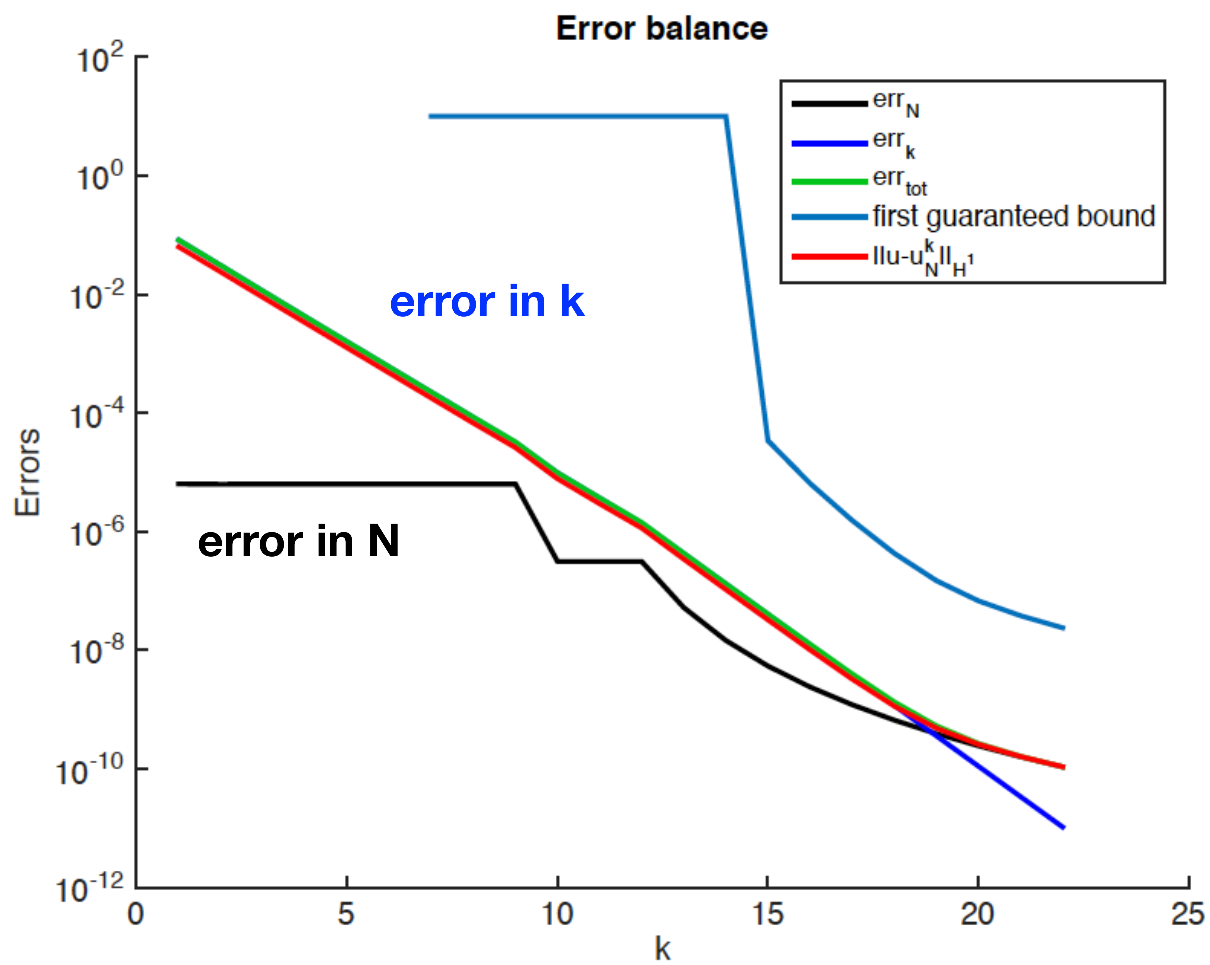
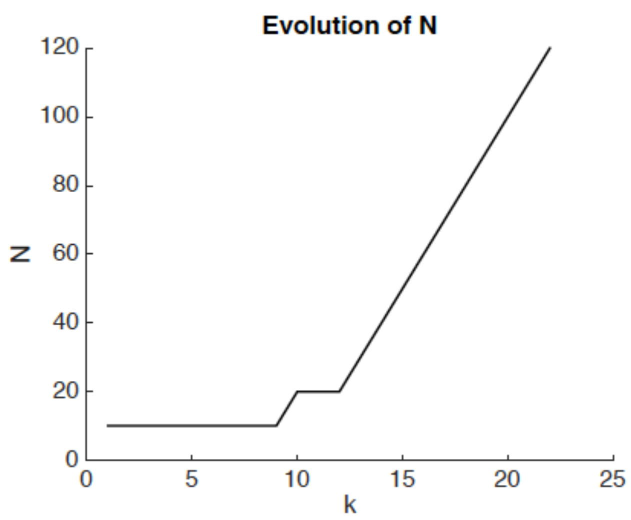
Error balance results





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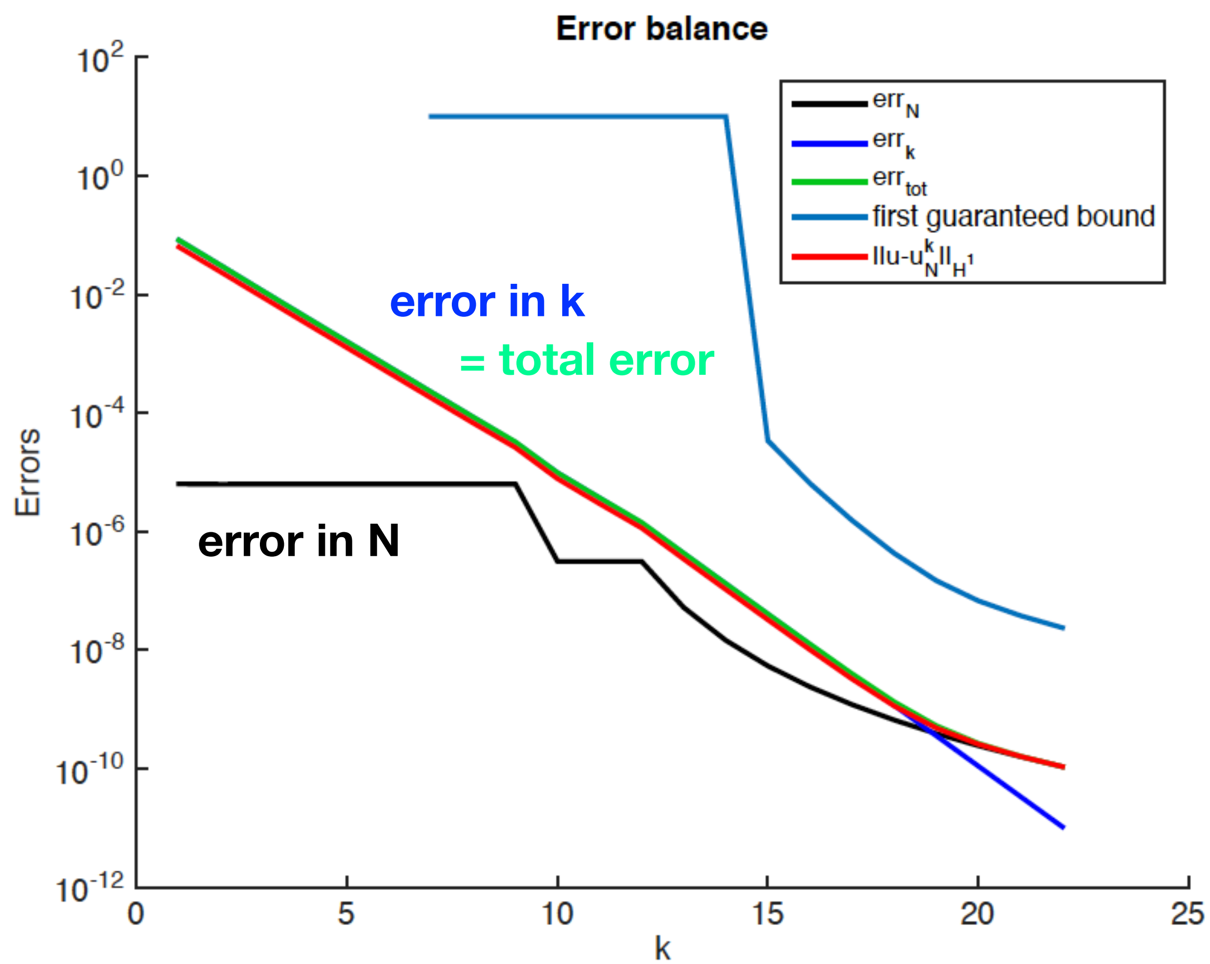
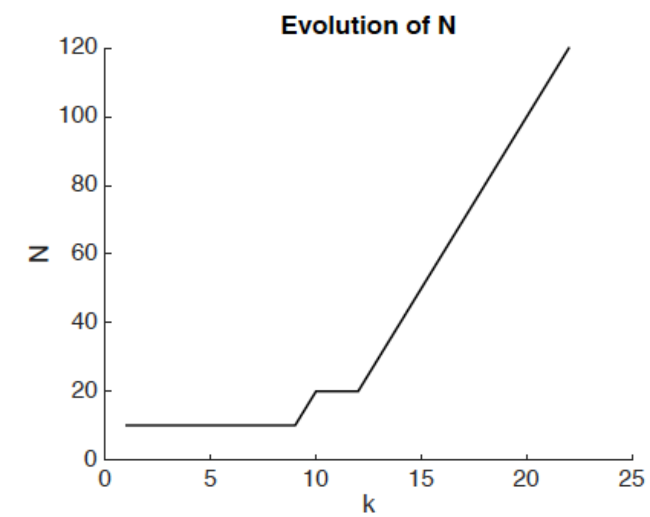
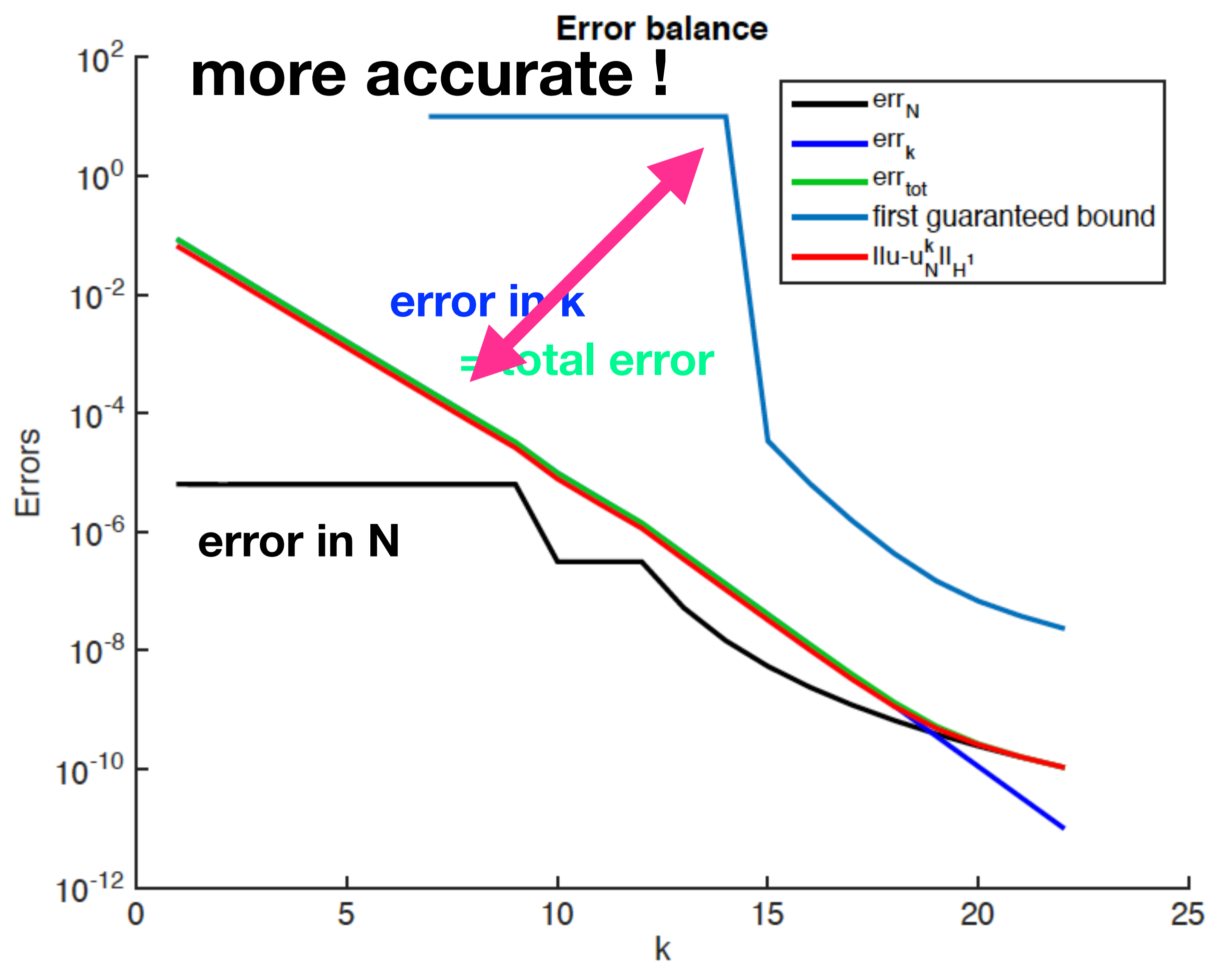
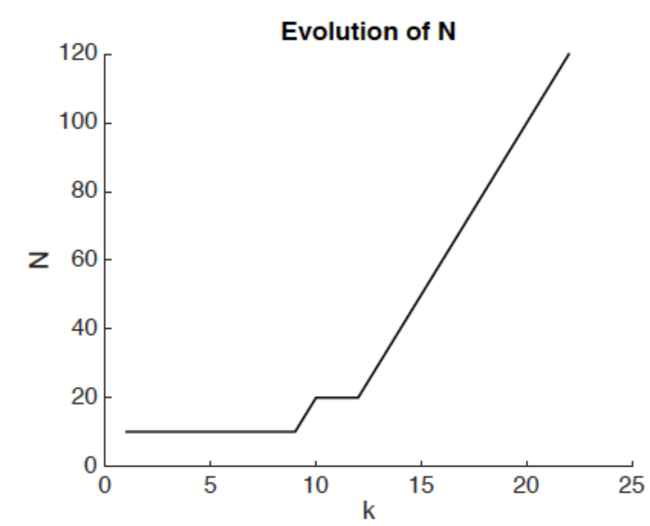




Toy problem to start with (Dusson - M.)

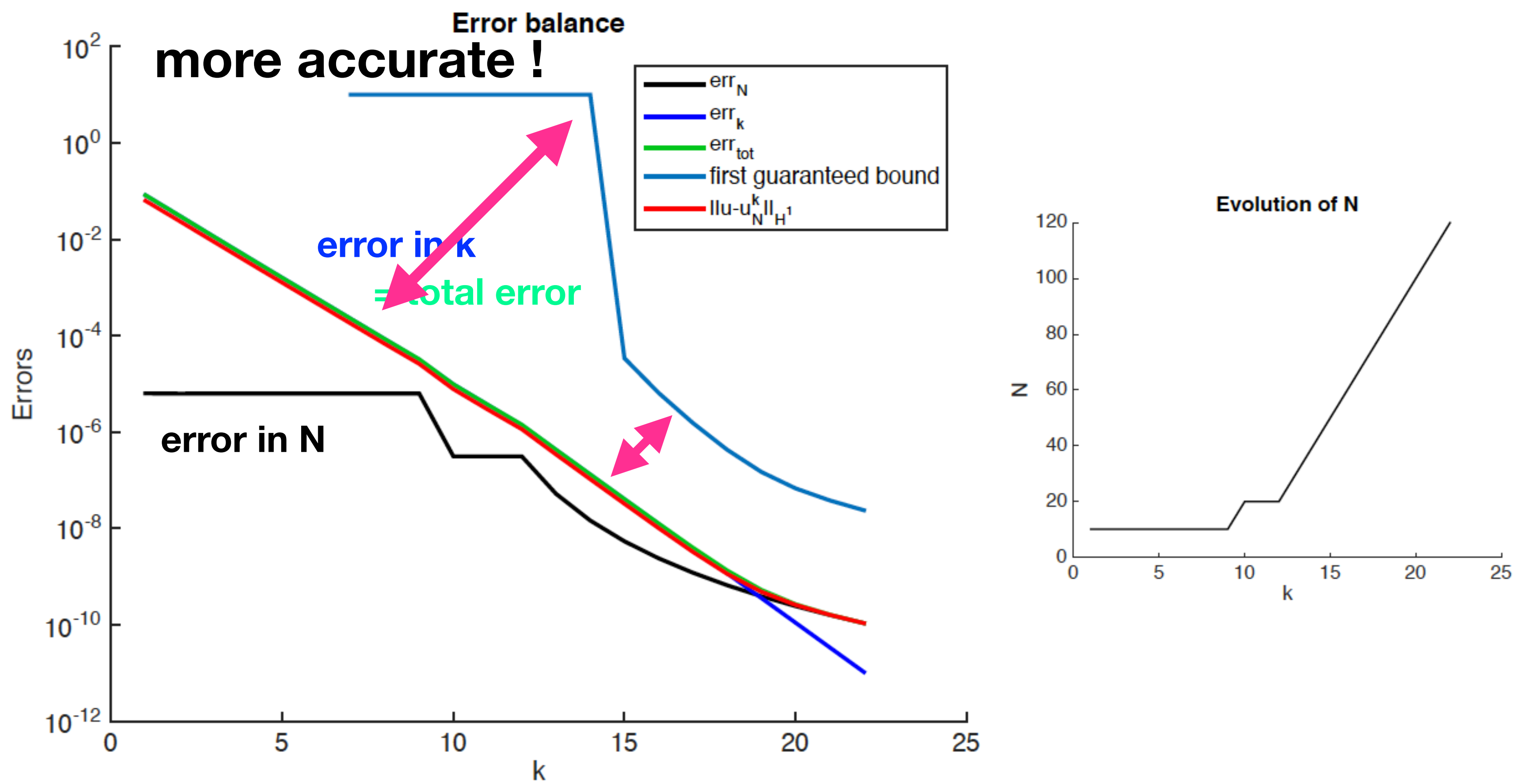
Error balance results





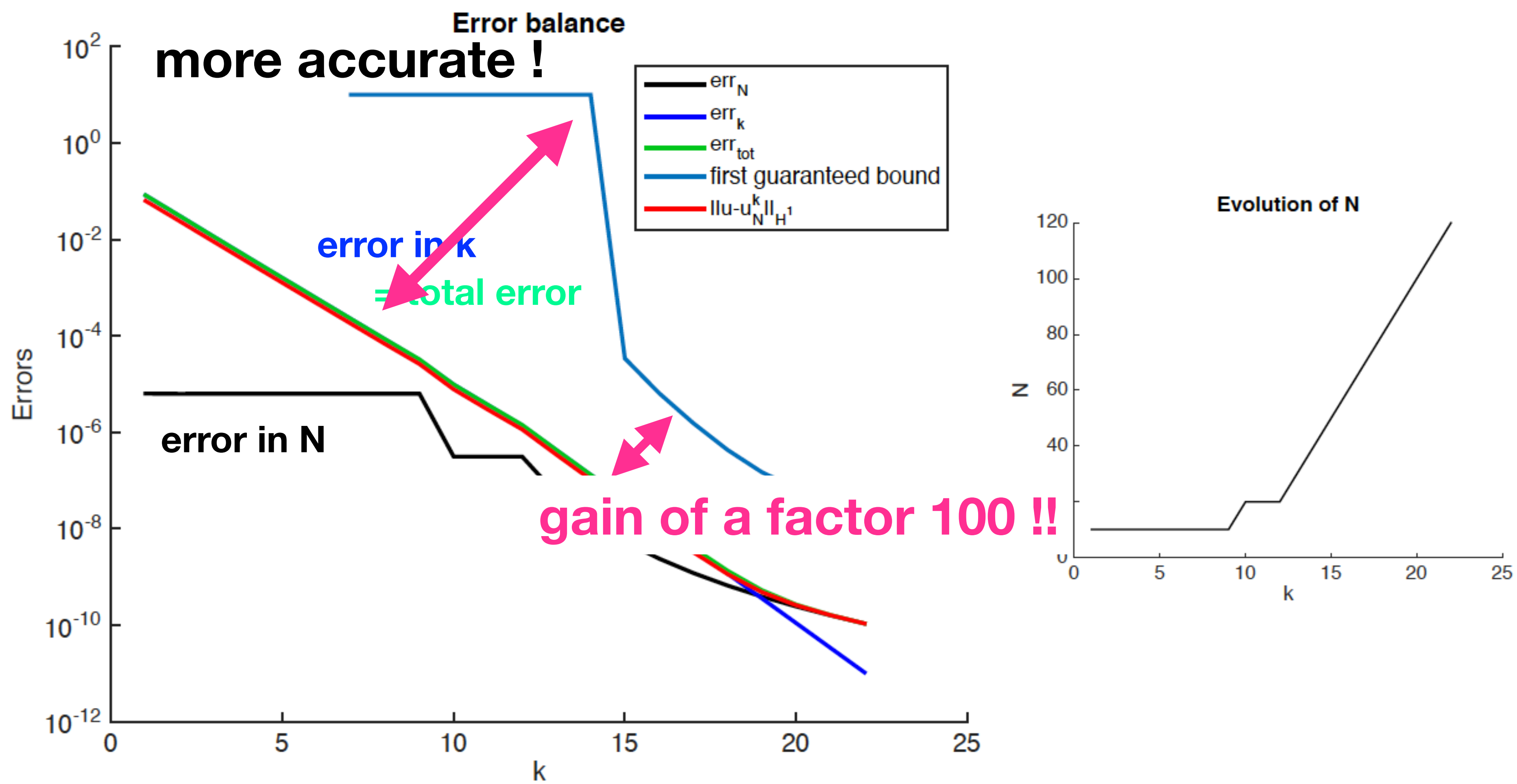
Toy problem to start with (Dusson - M.)

Error balance results



Toy problem to start with (Dusson - M.)

Error balance results



extension to Kohn Sham with

Eric Cances, Genevieve Dusson, Benjamin Stamm and Martin Vohralík
in a series of papers

What’s next ?

Next step

and beyond . . .

We want now to incorporate the error due to the model . . .

Indeed, what is of interest for us is the solution to the full, original, Schrödinger equation. What is the link between Schrödinger and one of the feasible model.

• Kohn Sham, DFT	better correlation models
• Hartree Fock	**post Hartree Fock methods**

Balance the different sources of errors

- model error
- discretization (basis set) error
- resolution error

Balance the different sources of errors

- model error
- discretization (basis set) error
- resolution error

CC with respect to full CI

and more

and more

New basis set

New discretizations : hP-DG taking into account we know where the singularities are located

With Carlo Marcati

New discretizations : hP-DG taking into account we know where the singularities are located

With Carlo Marcati

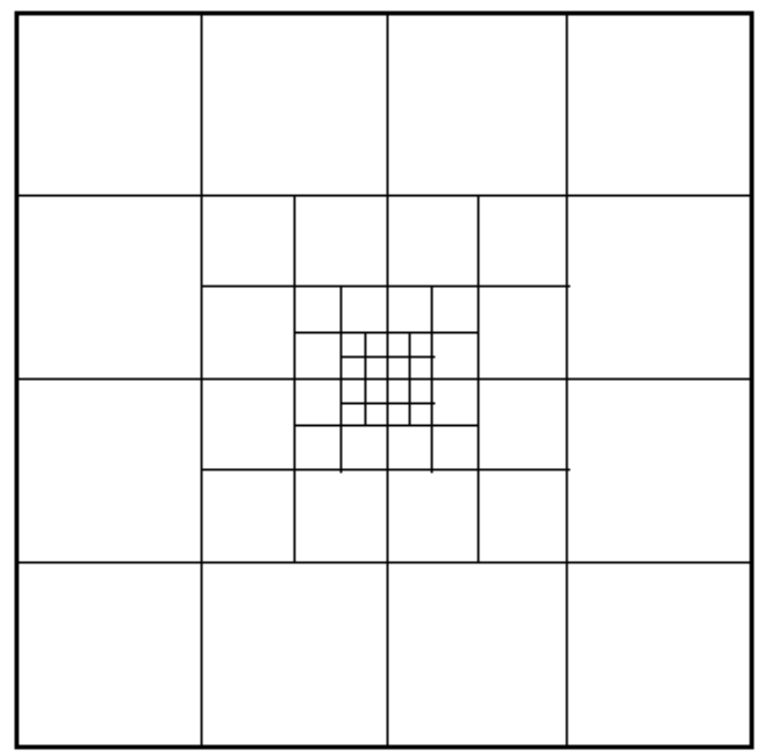
for all $k \in \mathbb{N}$

$$\sum_{|\alpha|=k} \|d(x,\mathfrak{c})^{k-\gamma}\partial^\alpha u\|_{L^2(\Omega)} \le C_u A_u^k k!,$$

New discretizations : hP-DG taking into account we know where the singularities are located

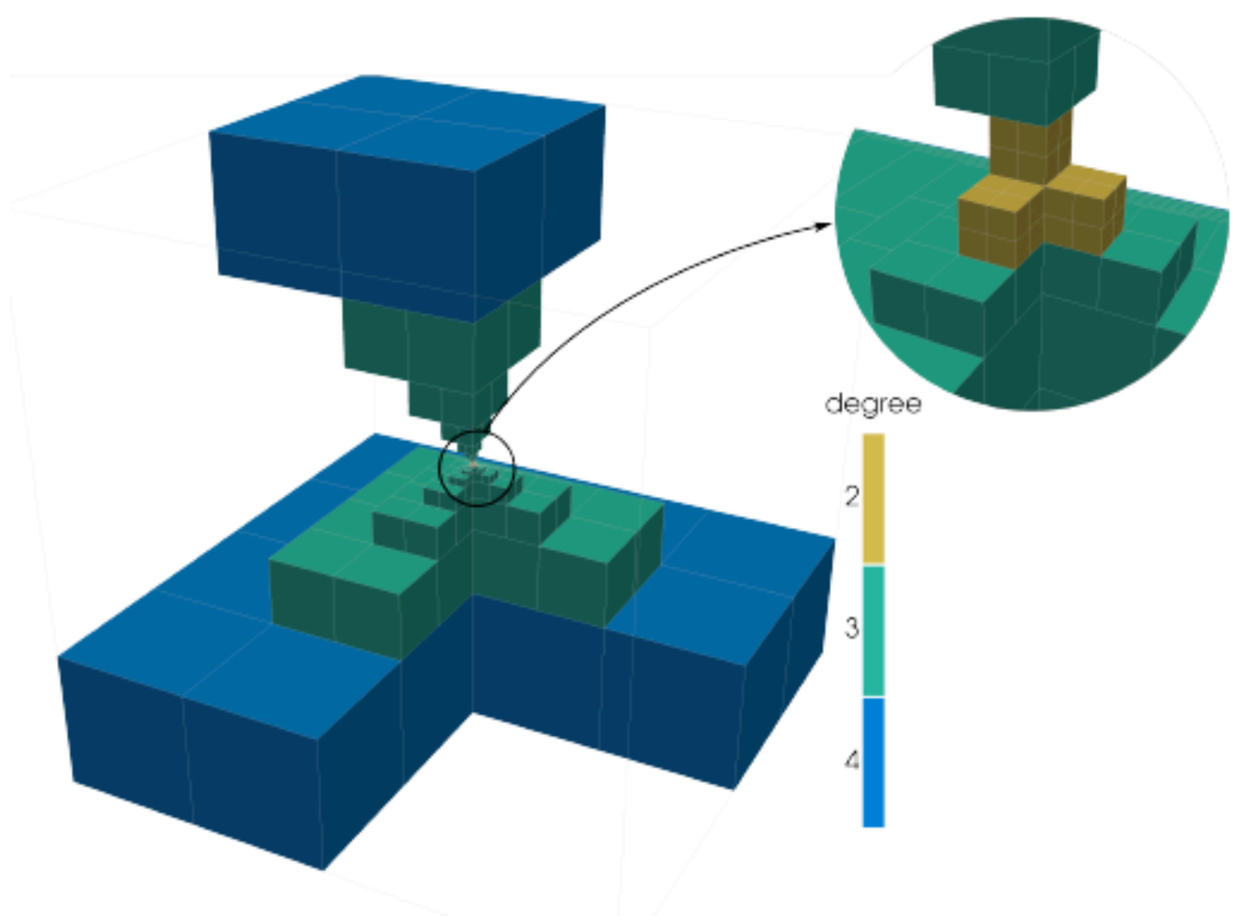
With Carlo Marcati

new discretization with finite element methods



New discretizations : hP-DG taking into account we know where the singularities are located

With Carlo Marcati



New discretizations : hP-DG taking into account we know where the singularities are located

With Carlo Marcati

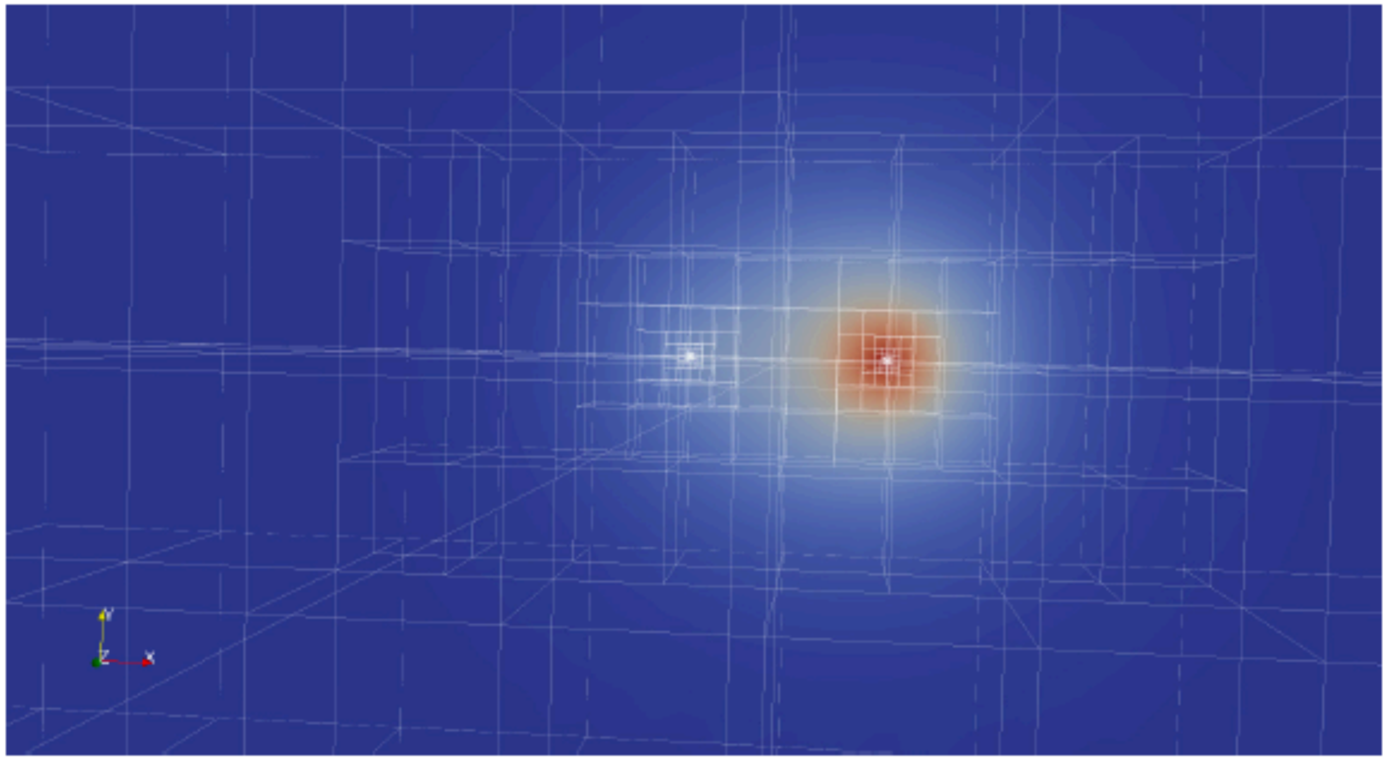


Figure 9.10 – Section of the solution for the HeH^+ molecule, with outline of the three dimensional mesh.

New discretizations : hP-DG taking into account we know where the singularities are located

With Carlo Marcati

Theorem 3. *Let u, λ be the solution to* (4) *and u_δ, λ_δ be the solution to* (11). *Suppose that* (7a), (7b), *and* (81) *hold. Then, for a space X_δ with N degrees of freedom, there exists $b > 0$ such that*

(83) $$\|u - u_\delta\|_{\mathrm{DG}} \leq Ce^{-bN^{1/(d+1)}}$$

and

(84) $$|\lambda - \lambda_\delta| \leq Ce^{-bN^{1/(d+1)}}.$$

Furthermore, if (37) *holds, then,*

(85) $$|\lambda - \lambda_\delta| \leq Ce^{-2bN^{1/(d+1)}}.$$

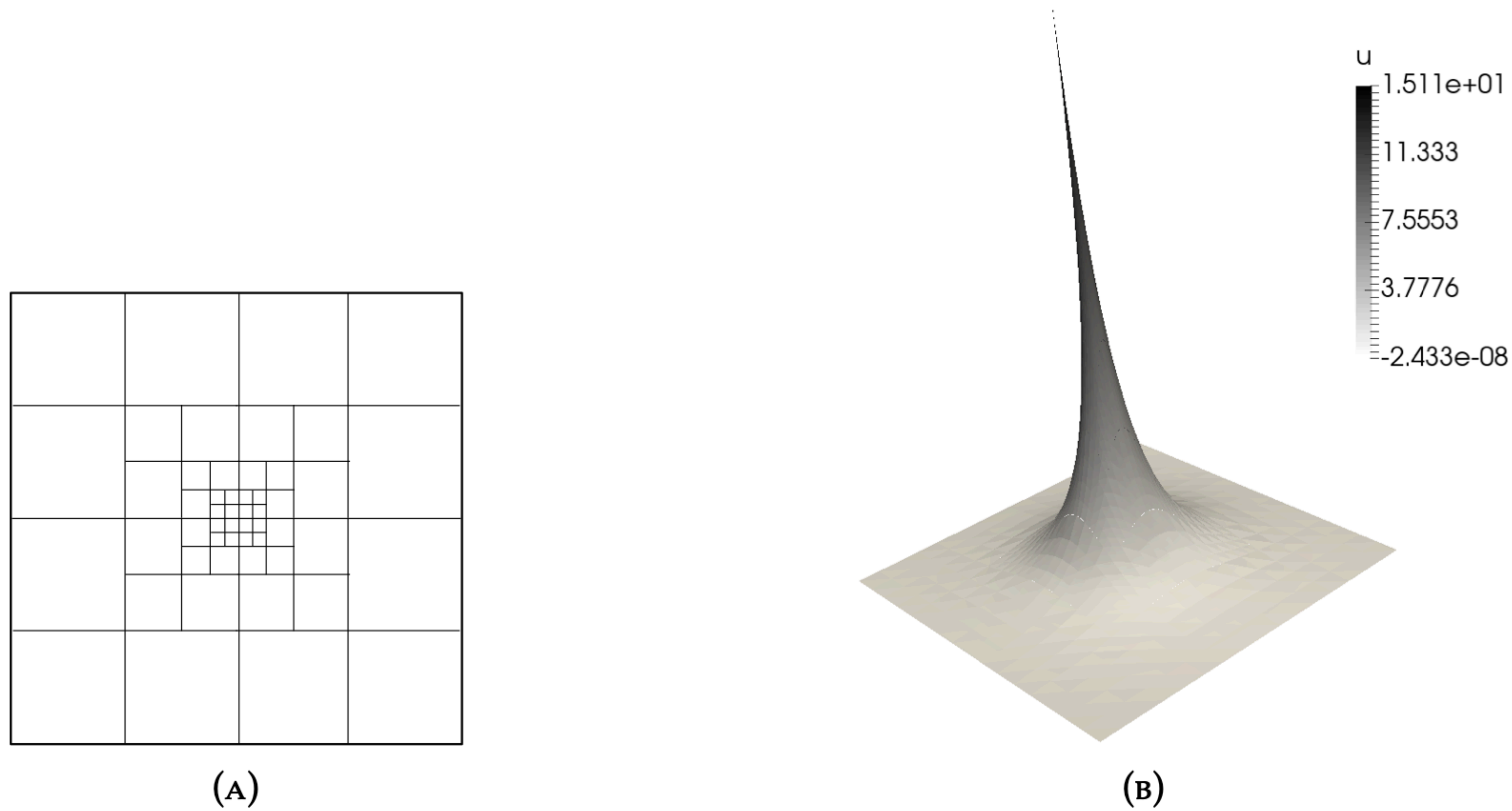
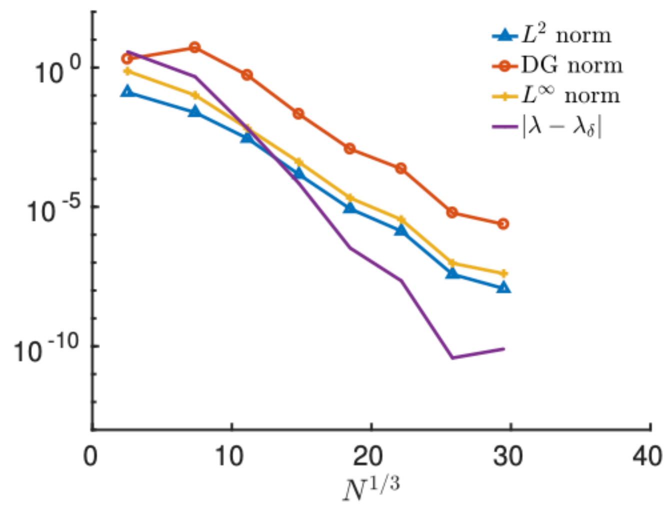
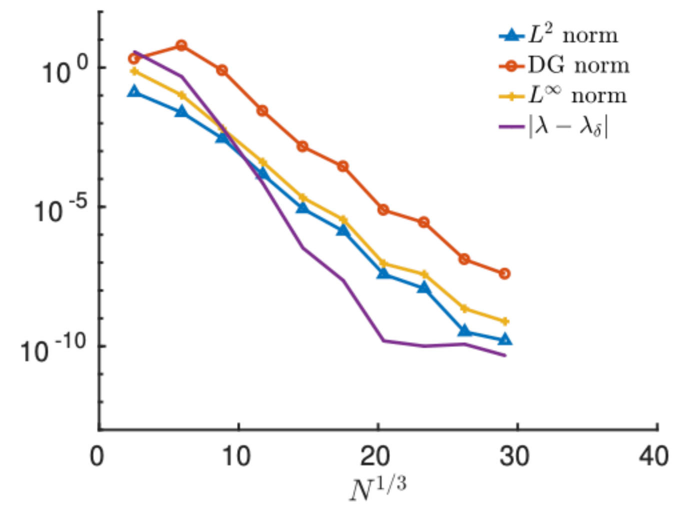


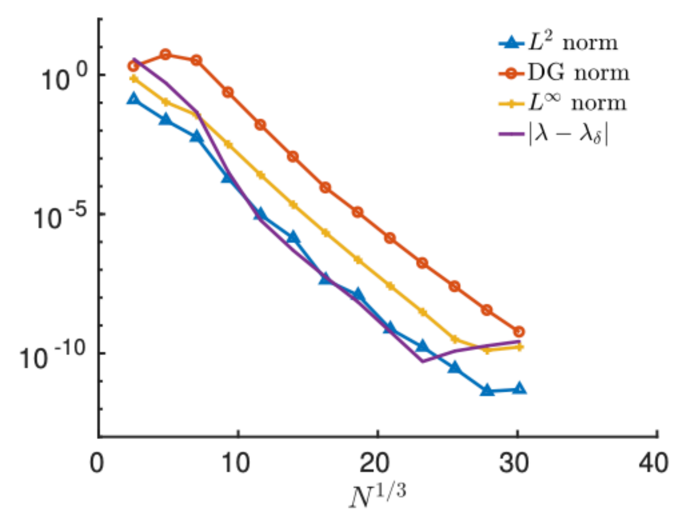
FIGURE 1. Left: mesh for the two dimensional approximation at a fixed refinement step. Right: Numerical solution to (86) with $V(x) = -r^{-3/2}$.


L^2 norm
DG norm
L^∞ norm
$|\lambda - \lambda_\delta|$
10^{0}
10^{-5}
10^{-10}
0
10
20
30
40
$N^{1/3}$

(A)


L^2 norm
DG norm
L^∞ norm
$|\lambda - \lambda_\delta|$
10^{0}
10^{-5}
10^{-10}
0
10
20
30
40
$N^{1/3}$

(B)


L^2 norm
DG norm
L^∞ norm
$|\lambda - \lambda_\delta|$
10^{0}
10^{-5}
10^{-10}
0
10
20
30
40
$N^{1/3}$

(C)

take home message

a priori .. no use

take home message

a priori .. no use but helps !

take home message

a priori .. no use but helps !

a posteriori

take home message

a priori .. no use but helps !

a posteriori.. allows to certify the results with actual figures !

take home message

a priori .. no use but helps !

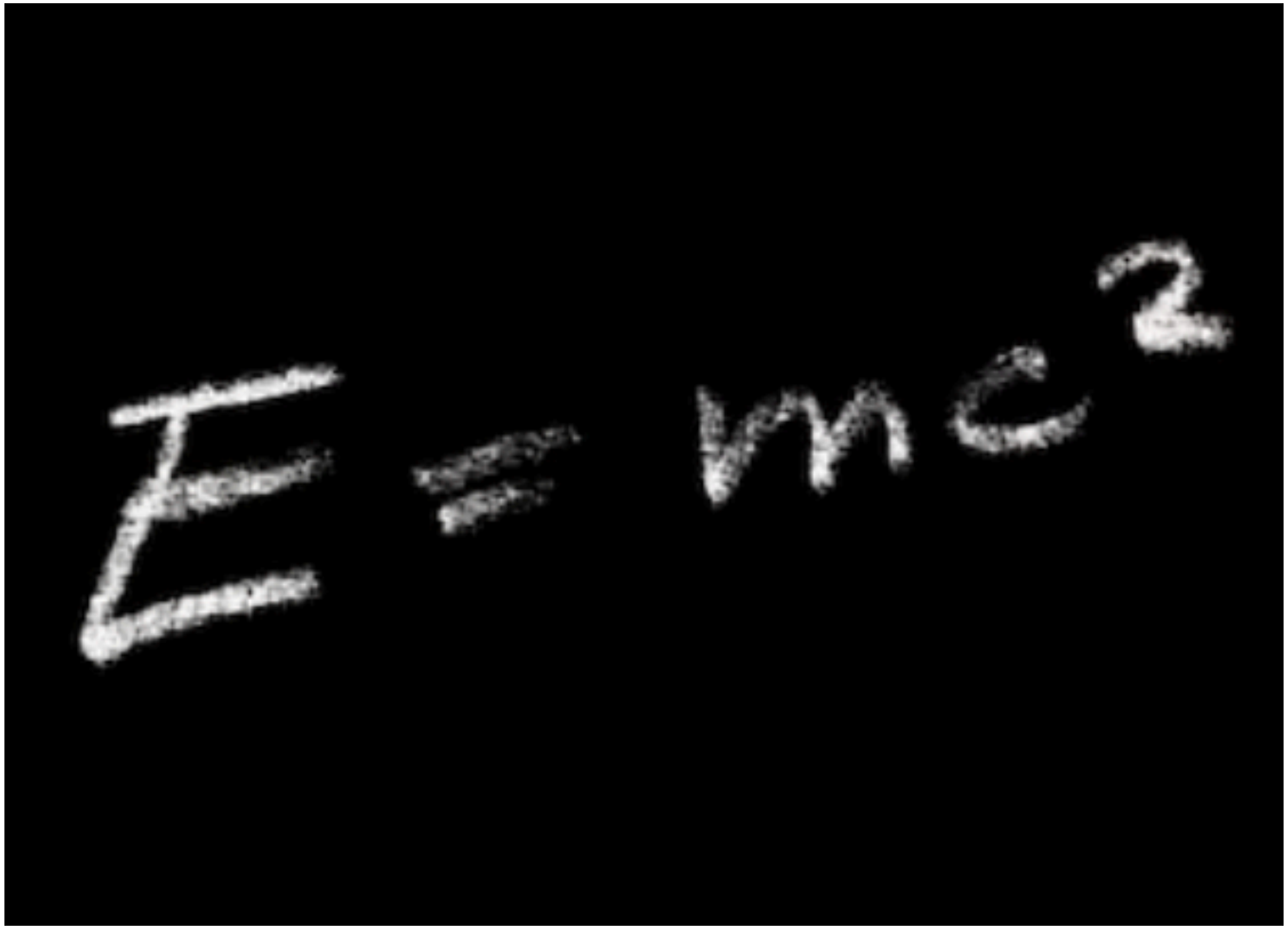
a posteriori.. allows to certify the results with actual figures ! with accuracy

take home message

a priori .. no use but helps !

a posteriori.. allows to certify the results with actual figures ! with accuracy

and even tell what to do to improve the accuracy



EMC2 ERC synergy-project
post doc and PhD Positions
has started last september for 6 years