Two grids approximation of non linear eigenvalue problems

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Density Functional Theory:
Fundamentals and Applications in Condensed Matter Physics

Examples of nonlinear eigenvalue problems

- Mechanics : vibration modes within nonlinear elasticity
- Physics : steady states of Bose-Einstein condensates
- Chemistry and materials science : electronic structure calculations
  - Hartree-Fock model
  - Density Functional Theory

A priori estimates for nonlinear eigenvalue problems

- A. Zhou (Nonlinearity 2004, M2AS 2007)
- E.Cancès, R. Chakir and Y. M. (JSC 2009, arXiv 2010)
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Two grids methods for eigenvalue problems

Introduced by J. Xu and A. Zhou [1]

- Consider the following eigenvalue problem : find λ and u, $\|u\|_{L^2} = 1$ solution of

$$\int \nabla u \nabla v = \lambda \int uv$$

Assume that you have two finite element meshes and two finite element spaces X_H and X_h

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$$\int \nabla u_H \nabla v_H = \lambda_H \int u_H v_H$$

- Solve the fine problem : find $u_h \in X_h$, solution of

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- reconstruct the eigenvalue by Reyleigh quotienty

$$\lambda_h^H = \frac{\int [\nabla u_h^H]^2}{\int [u_h^H]^2}$$

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Error estimates

- $$\|u - u_h^H\|_{H^1} \leq c(h + H^2)$$

- $$|\lambda - \lambda_h^H| \leq c(h^2 + H^4)$$

Two grids methods for non linear problems (V. Girault and J.-L. Lions [2] for Navier Stokes)

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2. Numerical analysis of the Gross-Pitaevskii equation and two grids method

$$\begin{cases} u \in H^1_0(\Omega) \\ -\Delta u + Vu + u^3 = \lambda u \\ \int_\Omega u^2 = 1 \end{cases}$$

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1 - Finite element discretization of the GP equation

$\Omega = (0, L)^d$, $d = 1$, 2 or 3, $\qquad V \in L^2(\Omega)$ and $\mu \geq 0$

We consider the minimization problem

$$I = \inf \left\{ E(v), \; v \in H_0^1(\Omega), \; \int_\Omega v^2 = 1 \right\} \tag{1}$$

where

$$E(v) = \int_\Omega |\nabla v|^2 + \int_\Omega V|v|^2 + \frac{\mu}{2} \int_\Omega |v|^4$$

- (1) has exactly two minimizers u and $-u$
- u is the ground state of the nonlinear eigenvalue problem

$$-\Delta u + Vu + \mu u^3 = \lambda u, \qquad \|u\|_{L^2} = 1$$

- $u \in C^{0,\alpha}(\Omega)$ for some $\alpha > 0$ and $u > 0$ in Ω

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Variational approximation of (1)

Let $(X_\delta)_{\delta>0}$ be a family of finite dimensional subspaces of $H_0^1(\Omega)$ s.t.

$$\min\left\{\|u - v_\delta\|_{H^1},\ v_\delta \in X_\delta\right\} \underset{\delta\to 0^+}{\longrightarrow} 0 \qquad (2)$$

The variational approximation of (1) in X_δ consists in solving

$$I_\delta = \inf\left\{E(v_\delta),\ v_\delta \in X_\delta,\ \int_\Omega v_\delta^2 = 1\right\} \qquad (3)$$

Problem (3) has at least one minimizer u_δ such that $(u_\delta, u)_{L^2} \geq 0$, which satisfies

$$\forall v_\delta \in X_\delta, \quad \int_\Omega \nabla u_\delta \cdot \nabla v_\delta + \int_\Omega V u_\delta v_\delta + \mu \int_\Omega u_\delta^3 v_\delta = \lambda_\delta \int_\Omega u_\delta v_\delta \qquad (4)$$

for some $\lambda_\delta \in \mathbb{R}$. This minimizer is unique for δ small enough.

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A priori error estimates in the linear case ($\mu = 0$)

There exist $0 < c \leq C < \infty$ such that for all $\delta > 0$

$$
\begin{aligned}
\|u_\delta - u\|_{H^1} &\leq C \min_{v_\delta \in X_\delta} \|v_\delta - u\|_{H^1} \\
c\|u_\delta - u\|_{H^1}^2 &\leq E(u_\delta) - E(u) \leq C\|u_\delta - u\|_{H^1}^2 \\
|\lambda_\delta - \lambda| &\leq C\|u_\delta - u\|_{H^1}^2
\end{aligned}
$$

Ref. : I. Babuška and J. Osborn, *Eigenvalue problems*, in : Handbook of numerical analysis. Volume II, (North-Holland, 1991) 641-787

Theorem (Cancès, Chakir, Y.M. 2009). In the nonlinear setting ($\mu > 0$).
There exist $0 < c \leq C < \infty$ and $\delta_0 > 0$ such that for all $0 < \delta \leq \delta_0$,

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|\lambda_\delta - \lambda| &\leq C\|u_\delta - u\|_{H^1}^2 + \mu \left| \int_\Omega u_\delta^2 (u_\delta + u)(u_\delta - u) \right| \quad \text{(Zhou '04)}
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$$\|u_\delta - u\|_{L^2}^2 \leq C\|u_\delta - u\|_{H^1} \min_{\psi_\delta \in X_\delta} \|\psi_{u_\delta - u} - \psi_\delta\|_{H^1}$$

where $\psi_{u_\delta - u} \in u^\perp = \left\{ v \in H_0^1(\Omega) \mid (v, u)_{L^2} = 0 \right\}$ is the unique solution to the adjoint problem

$$\forall v \in u^\perp, \quad \langle (E''(u) - \lambda)\psi_{u_\delta - u}, v \rangle_{H^{-1}, H_0^1} = \langle u_\delta - u, v \rangle_{H^{-1}, H_0^1}$$

Application to $\mathbb{P}_1$ and $\mathbb{P}_2$ finite element discretizations

Let $(\mathcal{T}_h)_h$ be a family of regular triangulations of Ω

- $\mathbb{P}_1$ finite element discretization

$$|\lambda_{h,1} - \lambda| \leq C \left(\|u_{h,1} - u\|_{H^1}^2 + \|u_{h,1} - u\|_{L^2} \right)$$

There exists $h_0 > 0$ and $C \in \mathbb{R}_+$ such that for all $0 < h \leq h_0$,

$$\|u_{h,1} - u\|_{H^1} \leq C\, h \qquad \|u_{h,1} - u\|_{L^2} \leq C\, h^2 \qquad |\lambda_{h,1} - \lambda| \leq C\, h^2$$

- $\mathbb{P}_2$ finite element discretization ($V \in H^1(\Omega)$)

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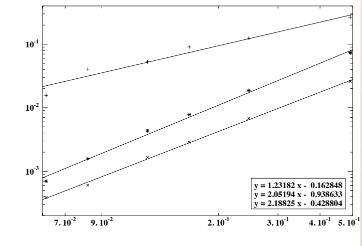
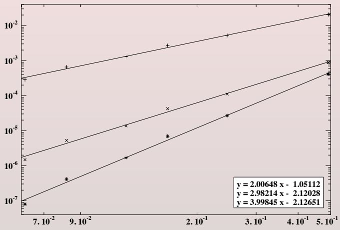
Numerical simulations

$d = 2,\ V(x_1, x_2) = x_1^2 + x_2^2$





Errors $\|u_{h,k} - u\|_{H^1}$ $(+)$, $\|u_{h,k} - u\|_{L^2}$ $(\times)$ and $|\lambda_{h,k} - \lambda|$ $(*)$ for the $\mathbb{P}_1$ ($k = 1$, left) and $\mathbb{P}_2$ ($k = 2$, right) approximations as a function of h in log scales

Eigenvalue problems of the form

$$-\mathrm{div}\,(A\nabla u) + Vu + f(|u|^2)u = \lambda u$$

are dealt with in E.Cancès., R. Chakir and Y. M., *Numerical analysis of nonlinear eigenvalue problems*, JSC 2009

These estimates where improved accuracy is established on the lower order norms are at the basis of a new method on two grids where the nonlinear eigenvalue problem is solved on a coarse mesh and a linear eigenvalue or even a linear problem with right hand side is solved on a fine mesh and optimal results are obtained (both theoretically and numerically)

R. Chakir's thesis

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Two grid method

On a coarse mesh

Non linear eigenvalue problem on a coarse grid X_H
$a(u_H, v) + \int_\Omega f(u_H^2) u_H v = \lambda_H \int_\Omega u_H v, \quad \forall v \in X_H$

On a fine mesh

Problem 1	Problem 2	Problem 3
Linear eigenvalue problem on a fine space X_h	Linear right hand side problem on a fine space X_h	Linear right hand side problem on a fine space X_h
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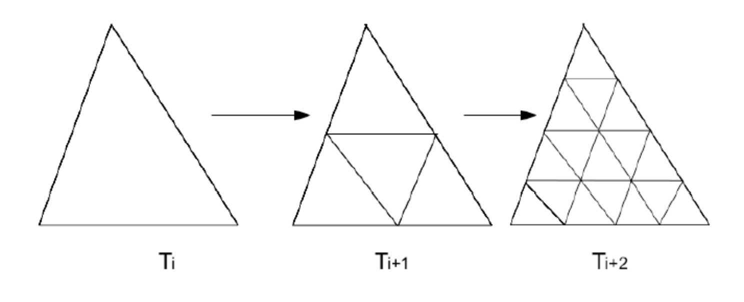
On a coarse mesh

Non linear eigenvalue problem on a coarse grid X_H
$a(u_H, v) + \int_\Omega f(u_H^2) u_H v = \lambda_H \int_\Omega u_H v, \quad \forall v \in X_H$

On a fine mesh

Problem 1	Problem 2	Problem 3
Linear eigenvalue problem on a fine space X_h	Linear right hand side problem on a fine space X_h	Linear right hand side problem on a fine space X_h
$a(u_h^H, v) + \int_\Omega f(u_H^2) u_h^H v = \lambda_h^H \int_\Omega u_h^H v \quad \forall v \in X_h$	$a(\tilde{u}_h^H, v) + \int_\Omega f(u_H^2) \tilde{u}_h^H v = \lambda_H \int_\Omega u_H v \quad \forall v \in X_h$	$a(\overline{u}_h^H, v) = -\int_\Omega f(u_H^2) u_H v + \lambda_H \int_\Omega u_H v \quad \forall v \in X_h.$

Numerical simulations



Numerical simulations fine mesh $= T_4$

$$\|u - u_h\|_{H^1(\Omega_1)} = 0.00647426$$

T_n	Méthode à 2 Grilles			$\|u - u_{H_n}\|_{H^1(\Omega_1)}$
	$\|u - u_{H_n h}\|_{H^1(\Omega_1)}$	$\|u - \tilde{u}_{H_n h}\|_{H^1(\Omega_1)}$	$\|u - \overline{u}_{H_n h}\|_{H^1(\Omega_1)}$	
0	0.00647816	0.00658694	0.00660524	0.118264
1	0.00647449	0.00648174	0.00648297	0.0594255
2	0.00647426	0.00647474	0.00647482	0.0296258
3	0.00647426	0.00647428	0.00647429	0.0144717

$$|\lambda - \lambda_h| = 4.25 \times 10^{-5}$$

T_n	Méthode à 2 Grilles			$\|\lambda - \lambda_{H_n}\|$
	$\|\lambda - \lambda_{H_n h}\_H^1(\Omega_1)$	$\|\lambda - \tilde{\lambda}_{H_n h}\|_{H^1(\Omega_1)}$	$\|\lambda - \overline{\lambda}_{H_n h}\|_{H^1(\Omega_1)}$	
0	3.46×10^{-5}	8.411×10^{-5}	9.69×10^{-5}	1.41×10^{-2}
1	4.05×10^{-5}	5.29×10^{-5}	5.61×10^{-5}	3.58×10^{-3}
2	4.20×10^{-5}	4.50×10^{-5}	4.59×10^{-5}	8.91×10^{-4}
3	4.24×10^{-5}	4.30×10^{-5}	4.33×10^{-5}	2.13×10^{-4}

Numerical simulations fine mesh $= T_4$

$$\|u - u_h\|_{H^1(\Omega_1)} = 0.00647426$$

T_n	Méthode à 2 Grilles			$\|u - u_{H_n}\|_{H^1(\Omega_1)}$
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$$|\lambda - \lambda_h| = 4.25 \times 10^{-5}$$

T_n	Méthode à 2 Grilles			$\|\lambda - \lambda_{H_n}\|$
	$\|\lambda - \lambda_{H_n h}\_H^1(\Omega_1)$	$\|\lambda - \tilde{\lambda}_{H_n h}\|_{H^1(\Omega_1)}$	$\|\lambda - \overline{\lambda}_{H_n h}\|_{H^1(\Omega_1)}$	
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2	4.20×10^{-5}	4.50×10^{-5}	4.59×10^{-5}	8.91×10^{-4}
3	4.24×10^{-5}	4.30×10^{-5}	4.33×10^{-5}	2.13×10^{-4}

Numerical simulations

TABLE: Comparison between the CPU times for the Two Grids Method.

reference time 121.46 sec

T_n	Méthode à 2 Grilles		
	Problème 1	Problème 2	Problème 3
0	14.64 s	7.57 s	7.17 s
1	15.61 s	8.65 s	8.22 s
2	21.08 s	12.78 s	12.27 s
3	39.36 s	34.25 s	33.68 s

2 - Planewave discretization of the periodic GP equation

We now consider the minimization problem

$$I = \inf \left\{ E(v),\ v \in H^1_\#(\Omega),\ \int_\Omega |v|^2 = 1 \right\} \tag{5}$$

where $\Omega = (0, 2\pi)^d$ ($d = 1$, 2 or 3) and where

$$E(v) = \int_\Omega |\nabla v|^2 + \int_\Omega V|v|^2 + \frac{1}{2}\int_\Omega |v|^4,$$

V being a $2\pi\mathbb{Z}^d$-periodic continuous function

Planewave basis sets

For $k \in \mathbb{Z}^d$, we denote by

$$e_k(x) = \frac{e^{ik\cdot x}}{(2\pi)^{d/2}} \qquad\qquad V_N = \left\{ \sum_{|k|\le N} c_k e_k \mid c_{-k} = c_k^* \right\}$$

Spectral approximation

Let u_N be a minimizer of

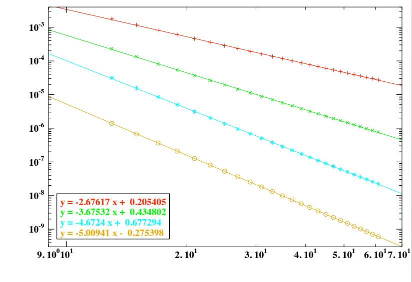
$$I_N = \inf\left\{E(v_N),\ v \in V_N,\ \int_\Omega |v_N|^2 = 1\right\} \qquad \text{s.t. } (u_N, u)_{L^2} \geq 0$$

Theorem (Cancès, Chakir, Y.M. 2009) Assume that $V \in H^\sigma_\#(\Omega)$ for some $\sigma > d/2$. Then $(u_N)_{N\in\mathbb{N}}$ converges to u in $H^{\sigma+2}_\#(\Omega)$ and there exists $0 < c \leq C < \infty$ such that for all $N \in \mathbb{N}$,

$$\begin{aligned}
\|u_N - u\|_{H^s_\#} &\leq \frac{C}{N^{\sigma+2-s}} \qquad \text{for all } -\sigma \leq s < \sigma + 2 \\
c\|u_N - u\|^2_{H^1_\#} &\leq E(u_N) - E(u) \leq C\|u_N - u\|^2_{H^1_\#} \\
|\lambda_N - \lambda| &\leq \frac{C}{N^{2(\sigma+1)}}
\end{aligned}$$

Numerical simulations

$$d = 1,\ V(x) = \sin(|x-\pi|/2)\ (V \in H^{3/2-\varepsilon}_{\#}(0,2\pi))$$



Numerical errors $\|u_N - u\|_{H^1_\#}$ $(+)$, $\|u_N - u\|_{L^2_\#}$ $(\times)$, $\|u_N - u\|_{H^{-1}_\#}$ $(*)$, $|\lambda_N - \lambda|$ $(\circ)$, as functions of $2N+1$ (the dimension of $\widetilde{X}_N$) in log scales

Pseudospectral approximation

Let u_{N,N_g} be a minimizer of

$$I_{N,N_g} = \inf \left\{ E_{N_g}(v_N),\ v \in V_N,\ \int_\Omega |v_N|^2 = 1 \right\} \qquad \text{s.t. } (u_{N,N_g}, u)_{L^2} \geq 0$$

where $N_g \in \mathbb{N} \setminus \{0\}$ (odd for simplicity), $N_g \geq 4N + 1$ and

$$E_{N_g}(v_N) = \int_\Omega |\nabla v_N|^2 + \int_\Omega \mathcal{I}_{N_g}(V)|v_N|^2 + \frac{1}{2}\int_\Omega |v_N|^4$$

$\mathcal{I}_{N_g}$ denoting the interpolation projector on

$$W_{N_g} = \{e_k \mid |k|_\infty \leq (N_g - 1)/2\}$$

The mean field matrix of the above minimization problem is

$$[H_{|v_N|^2}]_{kl} = |k|^2 \delta_{kl} + \widehat{V}_{k-l}^{\mathrm{FFT},N_g} + \widehat{|v_N|^2}_{k-l}^{\mathrm{FFT},N_g}$$

Pseudospectral error

If $|\widehat{V}_k| \leq C|k|^{-s}$ with $s > d$, then $V \in H_\#^{s-d/2-\varepsilon}(\Omega)$ and

$$\|u_{N,N_g} - u_N\|_{H^1_\#} \leq CN^{d/2}N_g^{-s} \qquad \|u_N - u\|_{H^1_\#} \leq CN^{-(s-d/2+1-\varepsilon)}$$

$$\|u_{N,N_g} - u_N\|_{L^2_\#} \leq CN^{d/2}N_g^{-s} \qquad \|u_N - u\|_{L^2_\#} \leq CN^{-(s-d/2+2-\varepsilon)}$$

$$|\lambda_{N,N_g} - \lambda_N| \leq CN^{d/2}N_g^{-s} \qquad |\lambda_N - \lambda| \leq CN^{-2(s-d/2+1-\varepsilon)}$$

The optimal choice for N_g therefore is

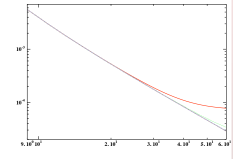
$N_g \sim N^{1+1/s-\varepsilon}$ if the criterion is the H^1 norm (or the energy)

$N_g \sim N^{1+2/s-\varepsilon}$ if the criterion is the L^2 norm

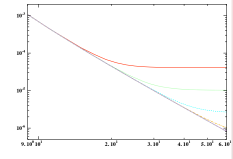
$N_g \sim N^{2-d/(2s)+2/s-\varepsilon}$ if the criterion is the eigenvalue

Numerical simulations

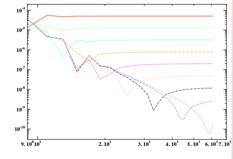
$d = 1$, $V(x) = \sin(|x - \pi|/2)$ ($s = 2$ and $V \in H^{3/2-\varepsilon}_{\#}(0, 2\pi)$)



$N_g \sim N^{3/2-\varepsilon}$



$N_g \sim N^{2-\varepsilon}$

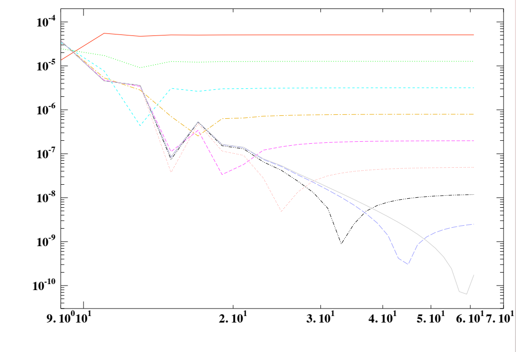


$N_g \sim N^{11/4-\varepsilon}$

Numerical errors $\|u_{N,N_g} - u\|_{H^1_{\#}}$ (left), $\|u_{N,N_g} - u\|_{L^2_{\#}}$ (middle) and $|\lambda_{N,N_g} - \lambda|$ (right), as functions of $2N + 1$ (the dimension of V_N), for $N_g = 128$ (red), $N_g = 256$ (green), $N_g = 512$ (cyan), $N_g = 1024$ (gold), $N_g = 2048$ (magenta), $N_g = 4096$ (pink), $N_g = 8192$ (black), $N_g = 16384$ (blue), $N_g = 32768$ (light blue)

Numerical simulations

$$d = 1,\ V(x) = \sin(|x-\pi|/2)\ (s = 2 \text{ and } V \in H_\#^{3/2-\varepsilon}(0, 2\pi))$$



Two grids method – Numerical simulations fine mesh $= N = 100$

$$\|u - u_N\|_{H^1} = 1.310^{-6}$$

$$\|u - u_N\|_{L^2} = 1.110^{-8}$$

$$|\lambda - \lambda_N| = 8.10^{-12}$$

Ng	$\|u - u_{N_f}^{N_g}\|_{H^1(\Omega_1)}$	$\|u - u_{N_f}^{N_g}\|_{L^2(\Omega_1)}$	$\lvert\lambda - \lambda_{N_f}^{N_g}\rvert$
5	5.608×10^{-4}	9.032×10^{-6}	4.932×10^{-7}
10	1.673×10^{-5}	2.530×10^{-7}	9.006×10^{-9}
20	1.429×10^{-6}	1.280×10^{-8}	2.598×10^{-10}
30	1.337×10^{-6}	1.085×10^{-8}	3.897×10^{-11}
40	1.336×10^{-6}	1.083×10^{-8}	2.140×10^{-11}
50	1.336×10^{-6}	1.083×10^{-8}	1.143×10^{-11}
60	1.336×10^{-6}	1.083×10^{-8}	9.342×10^{-12}
70	1.336×10^{-6}	1.083×10^{-8}	1.043×10^{-11}
80	1.336×10^{-6}	1.083×10^{-8}	1.083×10^{-11}
90	1.336×10^{-6}	1.083×10^{-8}	3.40×10^{-12}

3 - Planewave discretization of the periodic TFW model

The periodic Thomas-Fermi-von Weizsäcker (TFW) model

$$I^{\mathrm{TFW}} = \inf \left\{ \mathcal{E}^{\mathrm{TFW}}(\rho), \ \rho \in \mathfrak{R}_{\mathcal{N}} \right\}, \tag{6}$$

Set of admissible densities

$$\mathfrak{R}_{\mathcal{N}} = \left\{ \rho \geq 0 \mid \sqrt{\rho} \in H^1_{\#}((0,L)^3), \ \int_{(0,L)^3} \rho = \mathcal{N} \right\}$$

TFW energy functional

$$\mathcal{E}^{\mathrm{TFW}}(\rho) = \frac{C_{\mathrm{W}}}{2} \int_{(0,L)^3} |\nabla \sqrt{\rho}|^2 + C_{\mathrm{TF}} \int_{(0,L)^3} \rho^{5/3} + \int_{(0,L)^3} \rho V^{\mathrm{ion}} + \frac{1}{2} D_L(\rho, \rho)$$

where

$$D_L(\rho, \rho') := 4\pi \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3 \setminus \{0\}} \frac{\widehat{\rho}_k^* \, \widehat{\rho}'_k}{|k|^2}$$

Reformulation of TFW model in terms of $v = \sqrt{\rho}$

$$I^{\mathrm{TFW}} = \inf \left\{ E^{\mathrm{TFW}}(v),\ v \in H^1_\#((0,L)^3),\ \int_{(0,L)^3} |v|^2 = \mathcal{N} \right\} \qquad (7)$$

where

$$E^{\mathrm{TFW}}(v) = \frac{C_{\mathrm{W}}}{2} \int_{(0,L)^3} |\nabla v|^2 + C_{\mathrm{TF}} \int_{(0,L)^3} |v|^{10/3} + \int_{(0,L)^3} V^{\mathrm{ion}} |v|^2 + \frac{1}{2} D_L(|v|^2, |v|^2)$$

Mathematical properties of the periodic TFW model

Under the following assumption

$$\exists m > 3,\ C \geq 0 \text{ s.t. } \forall k \in \mathcal{R}^*,\ |\widehat{V}_k^{\rm ion}| \leq C|k|^{-m} \tag{8}$$

1. (6) has a unique minimizer ρ^0, and the minimizers of (7) are u and $-u$ where $u = \sqrt{\rho^0}$
2. u is positive everywhere in $(0, L)^3$ and satisfies the Euler equation
$$-\frac{C_{\rm W}}{2}\Delta u + \left(\frac{5}{3}C_{\rm TF}u^{4/3} + V^{\rm ion} + V_{u^2}^{\rm Coulomb}\right)u = \lambda u$$
for some $\lambda \in \mathbb{R}$
3. the function u is in $H_\#^{m+1/2-\varepsilon}((0, L)^3)$ (and therefore in $C_\#^2((0, L)^3)$)

The PW discretization of the TFW model is obtained by choosing

1. an energy cut-off $E_c > 0$ or, equivalently, a finite dimensional Fourier space V_{N_c}, the integer N_c being related to E_c through the relation $N_c := [\sqrt{2E_c}\, L/2\pi]$;
2. a cartesian grid $\mathcal{G}_{N_g}$ with step size L/N_g where $N_g \in \mathbb{N}^*$ is such that $N_g \geq 4N_c + 1$,

and by considering the finite dimensional minimization problem

$$I^{\rm TFW}_{N_c,N_g} = \inf \left\{ E^{\rm TFW}_{N_g}(v_{N_c}),\ v_{N_c} \in V_{N_c},\ \int_\Gamma |v_{N_c}|^2 = \mathcal{N} \right\}, \tag{9}$$

where

$$E^{\rm TFW}_{N_g}(v_{N_c}) = \frac{C_{\rm W}}{2} \int_\Gamma |\nabla v_{N_c}|^2 + C_{\rm TF} \int_\Gamma \mathcal{I}_{N_g}(|v_{N_c}|^{10/3}) + \int_\Gamma \mathcal{I}_{N_g}(V^{\rm ion})|v_{N_c}$$
$$+\frac{1}{2} D_\Gamma(|v_{N_c}|^2, |v_{N_c}|^2),$$

$\mathcal{I}_{N_g}$ denoting the Fourier interpolation operator

Spectral approximation of the TFW model

Theorem (Cancès, Chakir, Y.M. 2009) For $N_c \in \mathbb{N}$, we denote by u_{N_c} a minimizer to

$$I_{N_c}^{\mathrm{TFW}} = \inf \left\{ E^{\mathrm{TFW}}(v_{N_c}),\ v_{N_c} \in V_{N_c},\ \int_\Gamma |v_{N_c}|^2 = \mathcal{N} \right\}. \qquad (10)$$

such that $(u_{N_c}, u)_{L^2_\#} \geq 0$. Then for N_c large enough, u_{N_c} is unique, and for each $\varepsilon > 0$, the following estimates hold true

$$\begin{aligned} \|u_{N_c} - u\|_{H^s_\#} &\leq C_s N_c^{-(m-s+1/2-\varepsilon)} && (11) \\ |\lambda_{N_c} - \lambda| &\leq C N_c^{-(2m-1-\varepsilon)} && (12) \\ \gamma \|u_{N_c} - u\|^2_{H^1_\#} \leq I_{N_c}^{\mathrm{TFW}} - I^{\mathrm{TFW}} &\leq C \|u_{N_c} - u\|^2_{H^1_\#} && (13) \end{aligned}$$

for all $-m + 3/2 < s < m + 1/2$ and for some constants $\gamma > 0$, $C \geq 0$ and $C_s \geq 0$ independent of N_c

Pseudospectral approximation of the TFW model

Theorem (Cancès, Chakir, Y.M. 2009) For $N_c \in \mathbb{N}$ and $N_g \geq 4N_c + 1$, we denote by u_{N_c} a minimizer to

$$I_{N_c,N_g}^{\mathrm{TFW}} = \inf \left\{ E_{N_g}^{\mathrm{TFW}}(v_{N_c}),\ v_{N_c} \in V_{N_c},\ \int_\Gamma |v_{N_c}|^2 = \mathcal{N} \right\}, \tag{14}$$

such that $(u_{N_c,N_g}, u)_{L^2_\#} \geq 0$. Then for N_c large enough, u_{N_c,N_g} is unique, and the following estimates hold true

$$\|u_{N_c,N_g} - u_{N_c}\|_{H^s_\#} \leq C_s\, N_c^{3/2+(s-1)_+} N_g^{-m}, \tag{15}$$

$$|\lambda_{N_c,N_g} - \lambda_{N_c}| \leq C N_c^{3/2} N_g^{-m}, \tag{16}$$

$$|I_{N_c,N_g}^{\mathrm{TFW}} - I_{N_c}^{\mathrm{TFW}}| \leq C N_c^{3/2} N_g^{-m}, \tag{17}$$

for all $-m + 3/2 < s < m + 1/2$ and for some constants $\gamma > 0$, $C \geq 0$ and $C_s \geq 0$ independent of N_c and N_g

4 - Planewave discretization of the Kohn-Sham model

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Continuation of our program

The Kohn-Sham model LDA model

$$I^{\mathrm{KS}} = \inf\left\{E^{\mathrm{KS}}(\Phi),\ \Phi \in \mathcal{M}\right\} \tag{18}$$

where

$$\mathcal{M} = \left\{\Phi = (\phi_1, \cdots, \phi_{\mathcal{N}})^T \in (H^1_\#(\Gamma))^{\mathcal{N}} \mid \int_\Gamma \phi_i \phi_j = \delta_{ij}\right\},$$

$\mathcal{N}$ being the number of valence electron pairs in the simulation cell, and

$$E^{\mathrm{KS}}(\Phi) = \sum_{i=1}^{\mathcal{N}} \int_\Gamma |\nabla\phi_i|^2 + \int_\Gamma \rho_\Phi V_{\mathrm{local}} + 2\sum_{i=1}^{\mathcal{N}} \langle\phi_i|V_{\mathrm{nl}}|\phi_i\rangle + J(\rho_\Phi) + E^{\mathrm{LDA}}_{\mathrm{xc}}(\rho_\Phi). \tag{19}$$

The Kohn-Sham model LDA model

It is possible to prove that under appropriate assumptions, (18) has a minimizer $\Phi^0 = (\phi_1^0, \cdots, \phi_{\mathcal{N}}^0)^T$ with density $\rho^0 = \rho_{\Phi^0}$. Some regularity assumptions on $V_{\rm local}$, on $E_{\rm xc}^{\rm LDA}$ and on $V_{\rm nl}$ allow to state that the minimizer Φ^0 is in $[H^3_\#(\Gamma)]^{\mathcal{N}}$, and even in $[H_\#^{m+1/2-\varepsilon}(\Gamma)]^{\mathcal{N}}$ for any $\varepsilon > 0$, if at least one of the following conditions is satisfied : $E_{\rm xc}^{\rm LDA} \in C^{[m]}([0,+\infty))$ or $\rho_{\rm c} + \rho^0 > 0$ in $\mathbb{R}^3$.

The former condition is not satisfied for usual LDA exchange-correlation functionals. On the other hand, it is satisfied for the Hartree (also called reduced Hartree-Fock) model, for which $e_{\rm xc}^{\rm LDA} = 0$. The latter condition seems to be satisfied in practice, but we were not able to establish it rigourously.

Remember that the uniqueness is not at all proven... In fact, (18) has an infinity of minimizers since any unitary transform of the Kohn-Sham orbitals Φ^0 is also a minimizer of the Kohn-Sham energy.

The Kohn-Sham model LDA model

$\forall \Phi = (\phi_1, \cdots, \phi_{\mathcal{N}})^T \in \mathcal{M}$, we introduce the tangent space to $\mathcal{M}$ at Φ

$$T_\Phi \mathcal{M} = \left\{ (\psi_1, \cdots, \psi_{\mathcal{N}})^T \in (H^1_\#(\Gamma))^{\mathcal{N}} \mid \int_\Gamma \phi_i \psi_j + \psi_i \phi_j = 0 \right\}$$

Since the problem we are considering is a minimization problem, the second order condition further states

$$\forall W \in T_{\Phi^0}\mathcal{M}, \quad a_{\Phi^0}(W, W) \geq 0,$$

where

$$a_{\Phi^0}(\Psi, \Upsilon) \;=\; \frac{1}{4} E^{\mathrm{KS}''}(\Phi^0)(\Psi, \Upsilon) - \sum_{i=1}^{N} \varepsilon_i^0 \int_\Gamma \psi_i \upsilon_i \tag{20}$$

It follows from the invariance property through unitary transform that

$$a_{\Phi^0}(\Psi, \Psi) = 0 \quad \text{for all } \Psi \in \mathcal{A}\Phi^0.$$

where $\mathcal{A} = \left\{ A \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}} \mid A^T = -A \right\}$ is the space of the $\mathcal{N} \times \mathcal{N}$ antisymmetric real matrices.

The Kohn-Sham model LDA model

$\forall \Phi = (\phi_1, \cdots, \phi_{\mathcal{N}})^T \in \mathcal{M}$, we denote by

$$\Phi^{\perp\!\!\!\perp} = \left\{ \Psi = (\psi_1, \cdots, \psi_{\mathcal{N}})^T \in (H^1_\#(\Gamma))^{\mathcal{N}} \;\middle|\; \int_\Gamma \phi_i \psi_j = 0 \right\}.$$

Let us indicate that

$$T_\Phi \mathcal{M} = \mathcal{A}\Phi \oplus \Phi^{\perp\!\!\!\perp},$$

We are lead to make the assumption (see M. Turinici Numer. Math., 2003) that a_{Φ^0} is positive definite on $\Phi^{0,\perp\!\!\!\perp}$, in which case there exists a positive constant c_{Φ^0} such that

$$\forall \Psi \in \Phi^{0,\perp\!\!\!\perp}, \quad a_{\Phi^0}(\Psi, \Psi) \geq c_{\Phi^0} \|\Psi\|^2_{H^1_\#}. \tag{21}$$

In the linear framework ($J = 0$ and $E_{\mathrm{xc}}^{\mathrm{LDA}} = 0$ in (19)), this condition amounts to assuming that there is a gap between the lowest $\mathcal{N}^{\mathrm{th}}$ and $(\mathcal{N}+1)^{\mathrm{st}}$ eigenvalues of the linear self-adjoint operator $h = -\frac{1}{2}\Delta + V_{\mathrm{local}} + V_{\mathrm{nl}}$.

Variational approximation

Let us focus on the variational approximation

$$I_{N_c}^{\mathrm{KS}} = \inf \left\{ E^{\mathrm{KS}}(\Phi_{N_c}),\ \Phi_{N_c} \in V_{N_c}^{\mathcal{N}} \cap \mathcal{M} \right\} \tag{22}$$

One way to take the unitary invariance of the Kohn-Sham model into account is to work with density matrices. An alternative is to define for each $\Phi \in \mathcal{M}$ the set

$$\mathcal{M}^{\Phi} := \left\{ \Psi \in \mathcal{M} \mid \|\Psi - \Phi\|_{L^2_\#} = \min_{U \in \mathcal{U}(\mathcal{N})} \|U\Psi - \Phi\|_{L^2_\#} \right\},$$

and to use the fact that all the local minimizers of (22) are obtained by unitary transforms from the local minimizers of

$$I_{N_c}^{\mathrm{KS}} = \inf \left\{ E^{\mathrm{KS}}(\Phi_{N_c}),\ \Phi_{N_c} \in V_{N_c}^{\mathcal{N}} \cap \mathcal{M}^{\Phi^0} \right\}. \tag{23}$$

A priori estimates

The main result is the following.

Theorem

Let Φ^0 be a local minimizer of (18) satisfying (21). Then there exists $r^0 > 0$ and N_c^0 such that for $N_c \geq N_c^0$, (23) has a unique local minimizer $\Phi_{N_c}^0$ in the set

$$\left\{ \Phi_{N_c} \in V_{N_c}^{\mathcal{N}} \cap \mathcal{M}^{\Phi^0} \mid \|\Phi_{N_c} - \Phi^0\|_{H^1_\#} \leq r^0 \right\}.$$

If we assume either that $e_{\mathrm{xc}}^{\mathrm{LDA}} \in C^{[m]}([0, +\infty))$ or that $\rho_{\mathrm{c}} + \rho^0 > 0$ on Γ, then we have the following estimates :

$$\begin{aligned}
\|\Phi_{N_c}^0 - \Phi^0\|_{H^s_\#} &\leq C_{s,\varepsilon} N_c^{-(m-s+1/2-\varepsilon)}, && (24)\\
|\varepsilon_{i,N_c}^0 - \varepsilon_i^0| &\leq C_\varepsilon N_c^{-(2m-1-\varepsilon)}, && (25)\\
\gamma\|\Phi_{N_c}^0 - \Phi^0\|_{H^1_\#}^2 \leq I_{N_c}^{\mathrm{KS}} - I^{\mathrm{KS}} &\leq C\|\Phi_{N_c}^0 - \Phi^0\|_{H^1_\#}^2, && (26)
\end{aligned}$$

Numerical simulations

We have run simulation tests with the Hartree functional (i.e. with $e_{\rm xc}^{\rm LDA} = 0$), for which there is no numerical integration error. In this particular case, the problems solved numerically by Abinit and (22) (analyzed in Theorem 1) are identical.
For Troullier-Martins pseudopotentials, the parameter m in Theorem 1 is equal to 5. Therefore, we expect the following error bounds (as functions of the cut-off energy $E_{\rm c} = \frac{1}{2}\left(\frac{2\pi N_c}{L}\right)^2$)

$$\begin{aligned} \|\Phi^0_{N_c} - \Phi^0\|_{H^1_\#} &\leq C_{1,\varepsilon} E_{\rm c}^{-2.25+\varepsilon}, && (27)\\ \|\Phi^0_{N_c} - \Phi^0\|_{L^2_\#} &\leq C_{2,\varepsilon} E_{\rm c}^{-2.75+\varepsilon}, && (28)\\ |\varepsilon^0_{i,N_c} - \varepsilon^0_i| &\leq C_{3,\varepsilon} E_{\rm c}^{-4.5+\varepsilon}, && (29)\\ 0 \leq I^{\rm KS}_{N_c} - I^{\rm KS} &\leq C_{4,\varepsilon} E_{\rm c}^{-4.5+\varepsilon}. && (30) \end{aligned}$$

Numerical simulations

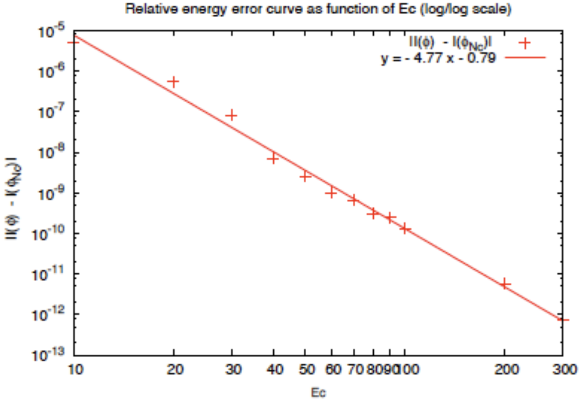

Figure 1: Error on the energy as a function of E_c for H_2

Numerical simulations

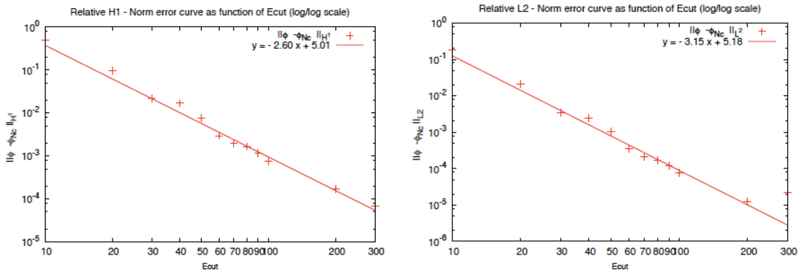

Figure 3: Errors on $\|\Phi^0_{N_c} - \Phi^0\|_{H^1_\#}$ (left) and $\|\Phi^0_{N_c} - \Phi^0\|_{L^2_\#}$ (right) as functions of E_c for N_2

Two grids method – Numerical simulations – hydrogen atom

fine mesh $= E = 300$

$$\|u - u_E\|_{H^1} = 3.10^{-5}$$

$$\|u - u_E\|_{L^2} = 7.10^{-7}$$

$$|\lambda - \lambda_E| = 7.10^{-10}$$

Ecg	$\|u - u_{Ec_f}^{Ec_g}\|_{H^1(\Omega_1)}$	$\|u - u_{Ec_f}^{Ec_g}\|_{L^2(\Omega_1)}$	$\lvert\lambda - \lambda_{Ec_f}^{Ec_g}\rvert$
70	3.0108×10^{-5}	7.5493×10^{-7}	7.830×10^{-7}
80	3.0106×10^{-5}	7.2487×10^{-7}	3.807×10^{-7}
90	3.0105×10^{-5}	7.2042×10^{-7}	2.856×10^{-7}
100	3.0105×10^{-5}	7.1678×10^{-7}	1.615×10^{-7}
110	3.0105×10^{-5}	7.1542×10^{-7}	7.772×10^{-8}
120	3.0105×10^{-5}	7.1516×10^{-7}	6.345×10^{-8}
130	3.0105×10^{-5}	7.1507×10^{-7}	4.690×10^{-8}
140	3.0105×10^{-5}	7.1505×10^{-7}	2.779×10^{-8}
150	3.0105×10^{-5}	7.1502×10^{-7}	2.109×10^{-9}
200	3.0105×10^{-5}	7.1502×10^{-7}	4.897×10^{-10}

Conclusions and perspectives

1. *A priori* error estimates for the finite element, and for the Fourier spectral and pseudospectral approximations of nonlinear eigenvalue problems of the form

$$-\Delta u + Vu + u^3 = \lambda u$$

have been derived pay attention to the numerical integration

2. The optimality of these error estimates is confirmed by numerical simulations

3. Similar results can be obtained for orbital-free and Kohn-Sham models (numerical simulations with numerical integration are work in progress)

4. The two grid method can be implemented leading to large speed-up numerical analysis has to be completed

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