Finite Element Approximations of Nonlinear Eigenvalue Problems in Density Functional Models

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Outline

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Density functional theory (DFT)

The ground state energy E_0 of a many-body system can be obtained by

$$E_0 = \mathscr{E}(\rho_0) = \min \left\{ \mathscr{E}(\rho) \ : \ \rho \geq 0, \sqrt{\rho} \in H^1(\mathbb{R}^3), \ \int_{\mathbb{R}^3} \rho = N \right\},$$

where ρ_0 is the density of the ground state and

$$\mathscr{E}(\rho) = T_s(\rho) + \mathscr{E}_{ext}(\rho) + \mathscr{E}_H(\rho) + \mathscr{E}_{xc}(\rho)$$

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with

$$\mathscr{E}_{ext}(\rho) = -\int_{\mathbb{R}^3} \sum_{i=1}^{M} \frac{Z_i}{|x - r_i|} \rho(x) dx$$

$$\mathscr{E}_H(\rho) = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x - y|} dxdy$$

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$T_s(\rho)$: Orbital-free DFT and Orbital-based DFT

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Orbital-free methods

Kinetic energy T_s can be approximated by

- Thomas-Fermi (TF) kinetic energy (1927):

$$T_{TF}(\rho) = C_{TF} \int_{\mathbb{R}^3} \rho^{\frac{5}{3}}.$$

- Thomas-Fermi von Weizsäcker (TFvW) kinetic energy (1935):

$$T_{TFW}(\rho) = T_{TF}(\rho) + \frac{\xi}{8} \int_{\mathbb{R}^3} \frac{|\nabla \rho|^2}{\rho}.$$

- Wang-Teter (WT) kinetic energy (1992):

$$T_{WT}^{\alpha,\beta}(\rho) = T_{TFW} + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K(|r - r'|)\rho^{\alpha}(r)\rho^{\beta}(r')drdr'.$$

- Wang-Govind-Carter (WGC) kinetic energy (1999):

$$T_{WGC}^{\alpha,\beta,\gamma}(\rho) = T_{TFW} + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} K\left(\zeta(\gamma, r, r'), |r - r'|\right) \rho^{\alpha}(r)\rho^{\beta}(r')drdr'.$$

Nonlinear eigenvalue problems

A model nonlinear eigenvalue problem:

$$\begin{cases} \left(-\alpha\Delta + V + \mathcal{N}(u^2)\right) u &= \lambda u \quad \text{in} \quad \Omega, \\ u &= 0, \\ \int_\Omega |u|^2 &= Z, \end{cases}$$

where $\Omega \subset \mathbb{R}^3$ is a bounded domain, $Z \in \mathbb{N}$, $\alpha \in (0, \infty)$, $V : \Omega \to \mathbb{R}$ is a given function, $\mathcal{N}$ maps a nonnegative function over Ω to some function defined on Ω.

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The associated energy functional can be formulated as

$$E(u) = \int_\Omega \left(\alpha|\nabla u(x)|^2 + V(x)u^2(x) + \mathcal{E}(u^2(x))\right) dx + \frac{1}{2q}\int_\Omega\int_\Omega u^{2q}(x)u^{2q}(y)K(x-y)dxdy.$$

Related works

Existing work on a priori error analysis:

- A. Zhou (Nonlinearity, 2004; MMAS, 2007)
  convex, convergence of eigenpair, upper bounds, +TFW model

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- H. Chen, L. He, and A. Zhou (preprint, 2010)
  local isomorphism condition, convergence rates, TFW type and Kohn-Sham models

Related works

Existing work on a posteriori error analysis:

- H. Chen, X. Gong, L. He, and A. Zhou (arXiv, 2010/AAMM, 2011)
  second-order optimality condition, Orbital-free model

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- H. Chen, X. Gong, L. He, and A. Zhou (arXiv, 2010/AAMM, 2011)
  second-order optimality condition, Orbital-free model
- W. Hackbusch, H.J. Flad, R. Schneider, and S. Schwinger (preprint, 2010)
  second-order optimality condition, Hartree-Fock model etc

Our progress

Obital-free DFT

A priori error analysis:

- Convergence of finite dimensional eigenpair approximations, nonconvex energy functional
- Convergence rate of finite dimensional eigenpair approximations, local isomorphism condition

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A posteriori error analysis:

- Convergence of adaptive finite element eigenpair approximations, nonconvex energy functional
- Convergence rate and complexity of adaptive finite element eigenpair approximations, local isomorphism condition + simple/nondegenerate eigenvalue

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Kohn-Sham DFT

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- Convergence rates of finite element eigenpair approximations, local isomorphism condition

A posteriori error analysis:

- Convergence of adaptive finite element eigenpair approximations, nonconvex energy functional
- Convergence rate and complexity of adaptive finite element eigenpair approximations, local isomorphism condition + ...

Outline

Ground state

The ground state solution u can be obtained by minimizing the associated energy in the admissible class

$$\mathcal{A} \equiv \left\{ \psi \in H_0^1(\Omega) \;:\; \|\psi\|_{0,\Omega}^2 = Z,\; \psi \geq 0 \right\}.$$

Namely,

$$u \in \arg\min \left\{ E(\psi) : \psi \in \mathcal{A} \right\}.$$

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Namely,

$$u \in \arg\min \{ E(\psi) : \psi \in \mathcal{A} \}.$$

Introduce the set of the ground state solutions

$$\mathcal{U} = \left\{ u \in \mathcal{A} : \ E(u) = \min_{\psi \in \mathcal{A}} E(\psi) \right\}$$

and the set of ground state eigenvalues

$$\Lambda = \{ \lambda \in \mathbb{R} : (\lambda, u) \text{ is an exact eigenpair and } u \in \mathcal{U} \}.$$

Approximation

We study approximations in class of finite dimensional subspaces $X_n \subset H_0^1(\Omega)(n = 1, 2, \cdots)$:

$$u_n \in \arg\min\{E(\psi) : \psi \in X_n \cap \mathcal{A}\}$$

and introduce $\mathcal{U}_n$:

$$\mathcal{U}_n = \{u_n \in X_n \cap \mathcal{A} : \ E(\phi_n) = \min_{\psi \in X_n \cap \mathcal{A}} E(\psi)\}$$

and Λ_n:

$$\Lambda_n = \{\lambda_n \in \mathbb{R} : (\lambda_n, u_n) \text{ is a discretize eigenpair and } u_n \in \mathcal{U}_n\}.$$

Convergence

Theorem (Chen, Gong, and Zhou (MMAS,2010))

Under some reasonable assumptions, there hold

$$\lim_{n\to\infty} \mathcal{D}_{H^1}(\mathcal{U}_n, \mathcal{U}) = 0,$$

$$\lim_{n\to\infty} E_n = \min_{\psi\in\mathcal{A}} E(\psi),$$

where $E_n = E(\phi_n)$ $(\forall \phi_n \in \mathcal{U}_n)$. Moreover,

$$\lim_{n\to\infty} \mathcal{D}(\Lambda_n, \Lambda) = 0.$$

Here for $\mathcal{W}, \mathcal{V} \subset H_0^1(\Omega)$,

$$\mathcal{D}_{H^1}(\mathcal{W}, \mathcal{V}) = \sup_{\phi\in\mathcal{W}} \inf_{\psi\in\mathcal{V}} \|\phi - \psi\|_{1,\Omega};$$

and for $A, B \subset \mathbb{R}$,

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All the limit points of finite dimensional eigenfunction/eigenvalue approximations are ground state solutions/eigenvalues.

Upper bounds

Theorem (Chen, Gong, and Zhou (MMAS,2010))

Under some reasonable assumptions, there hold

$$\mathcal{D}_{H^1}(\mathcal{U}_n,\mathcal{U}) \le C\left(\mathcal{D}_{L^\sigma}(\mathcal{U}_n,\mathcal{U}) + \mathcal{D}_{H^1}(\mathcal{U},X_n)\right),$$

$$| E_n - E | \le C\left(\mathcal{D}_{L^\sigma}(\mathcal{U}_n,\mathcal{U}) + \mathcal{D}^2_{H^1}(\mathcal{U},X_n)\right),$$

where $\sigma = 6/(3-2p_2)$, $E = E(\phi)$ $(\phi \in \mathcal{U})$, and $E_n = E(\phi_n)$ $(\phi_n \in \mathcal{U}_n)$. Moreover,

$$\mathcal{D}(\Lambda_n,\Lambda) \le C\left(\mathcal{D}_{L^\sigma}(\mathcal{U}_n,\mathcal{U}) + \mathcal{D}^2_{H^1}(\mathcal{U},X_n)\right).$$

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Assumptions for convergence rates

A.I. $V \in L^2(\Omega)$.

A.II. $\mathcal{E} \in C^1([0,\infty),\mathbb{R}) \cap C^2((0,\infty),\mathbb{R})$ and $\mathcal{E} \in \mathscr{P}(p,(c_1,c_2))$ satisfying one of the following conditions:

1. $c_1 \in (0,\infty)$;
2. $p \in [0,4/3]$;
3. $c_1 \in (-\infty,0)$, $p \in (4/3,\infty)$ and

$$\frac{|c_1|}{\varkappa} Z^{p-1} < \inf_{u \in H_0^1(\Omega), \|u\|_{0,\Omega}=1} \left(\int_\Omega |\nabla u|^2 / \int_\Omega |u|^{2p} \right).$$

A.III. $\mathcal{N}_1(t) \in \mathscr{P}(p_1,(c_1,c_2))$ for some $p_1 \in [0,1]$, and there exist $q \in (1,2]$, $s \in [0,5-q]$ such that for all $t_1, t_2 \in [0,\infty)$, there holds

$$\begin{aligned} & |\mathcal{N}_1(t_1^2)t_1 - \mathcal{N}_1(t_2^2)t_1 - 2\mathcal{N}_1'(t_2^2)t_2^2(t_1 - t_2)| \\ \leq \quad & C(1+\max\{t_1^s, t_2^s\})|t_1 - t_2|^q. \end{aligned}$$

A.IV. $\mathcal{N}_1'(t)t^{1/2} \in \mathscr{P}(p_2,(c_1,c_2))$ for some $p_2 \in [0,1/2]$.

Here $\mathcal{E}(s) = \int_0^s \mathcal{N}_1(t)dt$ and

$$\mathscr{P}(p,(c_1,c_2)) = \{f : \exists\, a_1, a_2 \in \mathbb{R} \text{ such that } c_1 t^p + a_1 \leq f(t) \leq c_2 t^p + a_2 \ \forall\, t \geq 0\}.$$

Assumptions

A.V. For the ground state solution (λ, u), $\mathcal{F}'_u(\lambda, u)$ is an isomorphism from $H_0^1(\Omega)$ to $H^{-1}(\Omega)$, namely, there exists a constant $\beta_0 > 0$ such that

$$\inf_{v \in H_0^1(\Omega)} \sup_{w \in H_0^1(\Omega)} \frac{\langle \mathcal{F}'_u(\lambda, u) w, v \rangle}{\|w\|_{1,\Omega} \|v\|_{1,\Omega}} \geq \beta_0; \tag{1}$$

$\mathcal{F}'_u(\lambda, u)$ is invertible on $u^\perp \equiv \{v \in H_0^1(\Omega) : \ (u, v) = 0\}$, namely, there exists a constant $\beta_1 > 0$ such that

$$\inf_{v \in u^\perp} \sup_{w \in u^\perp} \frac{\langle \mathcal{F}'_u(\lambda, u) w, v \rangle}{\|w\|_{1,\Omega} \|v\|_{1,\Omega}} \geq \beta_1. \tag{2}$$

As a result of Assumption A.V., u is an isolated solution.

- A sufficient condition of Assumption A.V. being true is that

$$\langle \mathcal{F}'_u(\lambda, u) v, v \rangle \geq C^{-1} \|\nabla v\|_{0,\Omega}^2 \quad \forall\, v \in H_0^1(\Omega) \tag{3}$$

  holds for some constant $C > 0$, which has been proved to be satisfied by some TFW models that are of convex functional (see Cances, Chakir, and Maday (preprint, 2009/JSC, 2010)).

- Indeed, a priori error estimate in H^1-norm can be obtained under assumption (2) instead of Assumption A.V..

Definition of $\mathcal{F}'$

For any $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$, define $\mathcal{F} : \mathbb{R} \times H_0^1(\Omega) \to H^{-1}(\Omega)$ by

$$\langle \mathcal{F}(\lambda, u), v \rangle = \alpha(\nabla u, \nabla v) + (Vu + \mathcal{N}(u^2)u - \lambda u, v) \quad \forall\, v \in H_0^1(\Omega).$$

The Fréchet derivative of $\mathcal{F}$ with respect to u at (λ, u) is denoted by $\mathcal{F}'_u(\lambda, u) : H_0^1(\Omega) \to H^{-1}(\Omega)$, where

$$\begin{aligned} \langle \mathcal{F}'_u(\lambda, u)v, w \rangle &= \alpha(\nabla v, \nabla w) + ((V + \mathcal{N}(u^2) - \lambda)v, w) \\ &\quad + 2(\mathcal{N}'_1(u^2)u^2 v, w) + 2D(uv, uw) \quad \forall\, w \in H_0^1(\Omega). \end{aligned}$$

Energy functional

The associated energy functional is

$$E(u) = \int_{\Omega} \left(\alpha |\nabla u(x)|^2 + V(x)u^2(x) + \mathcal{E}(u^2(x)) \right) dx + \frac{1}{2} D(u^2, u^2),$$

where $\mathcal{E} : [0, \infty) \to \mathbb{R}$ is defined by

$$\mathcal{E}(s) = \int_0^s \mathcal{N}_1(t) dt$$

and $D(\cdot, \cdot)$ is a bilinear form as follows

$$D(f, g) = \int_{\Omega} f(x)(r^{-1} * g)(x) dx.$$

Convergence theorem

Theorem (Chen, He, and Zhou (2010))

If $h_0 \ll 1$ and Assumptions A.I.–A.V. hold, then

$$\|u - u_h\|_{1,\Omega} \leq C \inf_{v \in S_0^h(\Omega)} \|u - v\|_{1,\Omega}, \tag{4}$$

$$\|u - u_h\|_{0,\Omega} \leq Cr(h)\|u - u_h\|_{1,\Omega}, \tag{5}$$

and

$$|\lambda - \lambda_h| \leq Cr(h)\|u - u_h\|_{1,\Omega}, \tag{6}$$

where $r(h) = h + \|u - u_h\|_{1,\Omega}^{q-1}$ with $q \in (1, 2]$ and $r(h) \to 0$ as $h \to 0$.

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Some ground state solutions can be approximated well by finite dimensional approximations.

Outline of proof

Proof. Three steps

- An identity (c.f. Babuska and Osborn (1989), Zhou (2004, 2007)) leads to
$$|\lambda - \lambda_h| \leq C \left(\|u - u_h\|_{1,\Omega}^2 + \|u - u_h\|_{0,\Omega} \right).$$
- The dual argument (c.f. Babuska and Osborn (1989), Cances, Chakir, and Maday (2009/2010)) yields
$$\|u - u_h\|_{0,\Omega} \leq Cr(h)\|u - u_h\|_{1,\Omega}.$$
- Linearization approach (c.f. Cances, Chakir, and Maday (2009/2010), Xu and Zhou (2001)) produces
$$\|u - u_h\|_{1,\Omega} \leq C \left(\inf_{v \in S_0^h(\Omega)} \|u - v\|_{1,\Omega} + \|u - u_h\|_{0,\Omega} + \|u - u_h\|_{1,\Omega}^q \right).$$

An identity

Associated with eigenpair (λ, u) , we have a useful identity

$$
\begin{aligned}
& \frac{\alpha(\nabla v, \nabla v) + ((V + \mathcal{N}(v^2))v, v)}{(v, v)} - \lambda \\
= \quad & \frac{\alpha(\nabla(v-u), \nabla(v-u)) + ((V + \mathcal{N}(u^2))(v-u), v-u)}{(v, v)} \\
& + \frac{((\mathcal{N}(v^2) - \mathcal{N}(u^2))v, v)}{(v, v)} - \lambda \frac{(v-u, v-u)}{(v, v)} \qquad \forall\, v \in H_0^1(\Omega).
\end{aligned}
$$

Outline

Existing work for linear boundary value problems

A posteriori error analysis and adaptive finite element methods:

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Adaptive finite element algorithm

Solve $\longrightarrow$ **Estimate** $\longrightarrow$ **Mark** $\longrightarrow$ **Refine**

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Algorithm

Choose parameter $0 < \theta < 1$.

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7. Let $k = k + 1$ and go to Step 2.

Estimator

Let $\mathcal{T}_h$ be a finite element mesh and u_h be a finite element solution. Define

$$\mathcal{R}_T(u_h) := \lambda_h u_h + \alpha \Delta u_h - V u_h - \mathcal{N}(u_h^2) u_h \quad \text{in } T \in \mathcal{T}_h,$$

$$J_e(u_h) := \alpha \nabla u_h|_{T_1} \cdot \overrightarrow{n_1} + \alpha \nabla u_h|_{T_2} \cdot \overrightarrow{n_2} = [[\alpha \nabla u_h]]_e \cdot \overrightarrow{n_1} \quad \text{on } e \in \mathcal{E}_h.$$

where T_1 and T_2 are elements in $\mathcal{T}_h$ which share e and $\overrightarrow{n_i}$ is the outward normal vector of T_i on E for $i = 1, 2$.

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where T_1 and T_2 are elements in $\mathcal{T}_h$ which share e and $\overrightarrow{n_i}$ is the outward normal vector of T_i on E for $i = 1, 2$.
Define a local error indicator $\eta_h(u_h, T)$ by

$$\eta_h^2(u_h, T) := h_T^2\|\mathcal{R}_T(u_h)\|_{0,T}^2 + \sum_{e\in\mathcal{E}_h, e\subset\partial T} h_e\|J_e(u_h)\|_{0,e}^2 \qquad (7)$$

and a global error estimator $\eta_h(u_h, \Omega)$ by

$$\eta_h^2(u_h, \Omega) := \sum_{T\in\mathcal{T}_h, T\subset\Omega} \eta_h^2(u_h, T).$$

Marking Strategy

Given a parameter $0 < \theta < 1$:

1. Construct a minimal subset $\hat{\mathcal{T}}_H$ of $\mathcal{T}_H$ by selecting some elements in $\mathcal{T}_H$ such that

$$\sum_{T \in \hat{\mathcal{T}}_H} \eta_H^2(u_H, T) \geq \theta \eta_H^2(u_H, \Omega).$$

2. Mark all the elements in $\hat{\mathcal{T}}_H$.

Convergence

Theorem (Chen, Gong, He, and Zhou (arXiv, 2010/AAMM, 2011))

Given a sufficiently fine initial mesh $\mathcal{T}_0$. If $\{\mathcal{U}_k\}_{k\in\mathbb{N}}$ is the sequence of adaptive finite element approximations, then

$$\lim_{k\to\infty} E_k = \min_{v\in\mathcal{A}} E(v),$$

$$\lim_{k\to\infty} \mathcal{D}_{H^1}(\mathcal{U}_k, \mathcal{U}) = 0,$$

and

$$\lim_{k\to\infty} \mathcal{D}(\Lambda_k, \Lambda) = 0.$$

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If the nonnegative ground states are unique, then

$$\lim_{k\to\infty} \|\phi_k - \phi\|_{1,\Omega} = 0,$$

$$\lim_{k\to\infty} |\lambda_k - \lambda| = 0.$$

Convergence rate

Assume that Assumptions A.I.–A.V. hold (for instance, the energy functional is convex with respect to the density). Let $(\lambda, u) \in \mathbb{R} \times \mathcal{A}$ be the ground state solution.

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Theorem (Chen, He, and Zhou (2010))

Given a sufficiently fine initial mesh $\mathcal{T}_0$ and $\theta \in (0, 1)$. If $\{u_k\}_{k\in\mathbb{N}}$ is the sequence of adaptive finite element approximations, then there exist constants $\gamma > 0$ and $\xi \in (0, 1)$ depending only on the shape regularity constant and the marking parameter θ such that

$$\begin{aligned} & \|u - u_{k+1}\|^2_{a,\Omega} + \gamma\eta^2_{k+1}(u_{k+1}, \Omega) \\ \leq \quad & \xi^2(\|u - u_k\|^2_{a,\Omega} + \gamma\eta^2_k(u_k, \Omega)). \end{aligned} \tag{8}$$

Consequently

$$\lim_{k\to\infty} (\|u_k - u\| + \|\lambda_k - \lambda\|) = 0.$$

Notation

Define

$$\mathcal{A}^s := \{v \in H_0^1(\Omega) : |v|_{s,*} < \infty\},$$

where $\gamma > 0$ is some constant,

$$|v|_{s,*} = \sup_{\varepsilon>0} \varepsilon \inf_{\{\mathcal{T}\subset\mathcal{T}_0 : \inf(\|v-v'\|^2_{a,\Omega}+2osc^2_{\mathcal{T}}(v',\mathcal{T}))^{1/2}\leq\varepsilon\}} (\#\mathcal{T} - \#\mathcal{T}_0)^s.$$

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$$H_0^1(\Omega) \cap H^2(\Omega) \subsetneq \mathcal{A}^{1/3}$$

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$$H_0^1(\Omega) \cap H^2(\Omega) \subsetneq \mathcal{A}^{1/3}$$

Define element oscillation $osc_h(u_h, \tau)$ by

$$osc_h^2(u_h, \tau) := h_\tau^2 \|\mathcal{R}_\tau(u_h) - \overline{\mathcal{R}_\tau(u_h)}\|^2_{0,\tau}$$

and patch oscillation $osc_h(u_h, \omega)$ by

$$osc_h^2(u_h, \omega) := \sum_{\tau\in\mathcal{T}_h, \tau\subset\omega} osc_h^2(u_h, \tau),$$

where $\omega \subset \Omega$.

Complexity

Assume that Assumptions A.I.–A.V. hold (for instance, the energy functional is convex with respect to the density). Let$(\lambda, u) \in \mathbb{R} \times \mathcal{A}$ be the ground state solution.

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Given a sufficiently fine initial mesh $\mathcal{T}_0$, and $u \in \mathcal{A}^s$. If $\{u_k\}_{k\in\mathbb{N}}$ is the sequence of adaptive finite element approximations, then there exist constants $\gamma > 0$ and $\xi \in (0,1)$ depending only on the shape regularity constant and the marking parameter θ such that

$$\|u - u_k\|_{a,\Omega}^2 + \gamma osc_k^2(u_k, \mathcal{T}_k) \leq C(\#\mathcal{T}_k - \#\mathcal{T}_0)^{-2s}|u|_{s,*}^2.$$

Consequently,

$$|\lambda - \lambda_k| \leq C\,(\#\mathcal{T}_k - \#\mathcal{T}_0)^{-2s}|u|_{s,*}^2.$$

Outline

TFW model for helium atoms

Find $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ such that $\|u\|_{0,\Omega}^2 = 2$ and

$$\begin{cases} -\frac{1}{10}\Delta u - \frac{2}{|x|}u + u\int_\Omega \frac{|u(y)|^2 dy}{|x-y|} + \frac{5}{3}C_{TF}u^{7/3} + v_{xc}(u^2)u & = & \lambda u & \text{in } \Omega, \\ u & = & 0 & \text{on } \partial\Omega, \end{cases}$$

where $\Omega = (-5.0, 5.0)^3$.

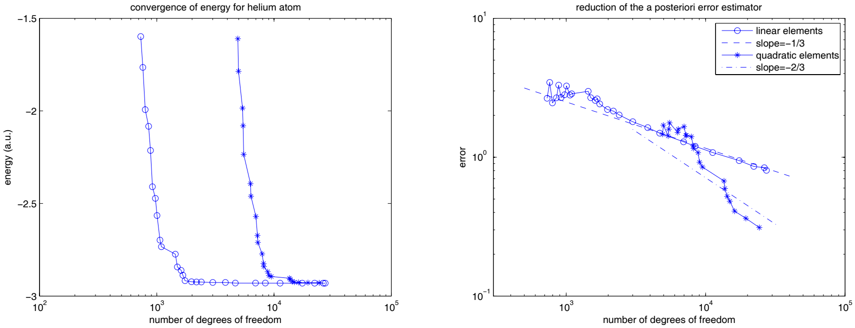


Figure: Left: Convergence curves of energy for the helium atom. Right: Reduction of the a posteriori error estimators.

TFW-GHN model for an aluminum cluster

Find $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega)$ such that $\|u\|_{0,\Omega}^2 = 172$ and

$$\begin{cases} -\frac{1}{10}\Delta u + V_{pseu}^{GHN} u + u\int_\Omega \frac{|u(y)|^2 dy}{|x-y|} + \frac{5}{3} C_{TF} u^{7/3} + v_{xc}(u^2)u & = & \lambda u & \text{in } \Omega, \\ u & = & 0 & \text{on } \partial\Omega, \end{cases}$$

where $\Omega = (-25.0, 25.0)^3$.

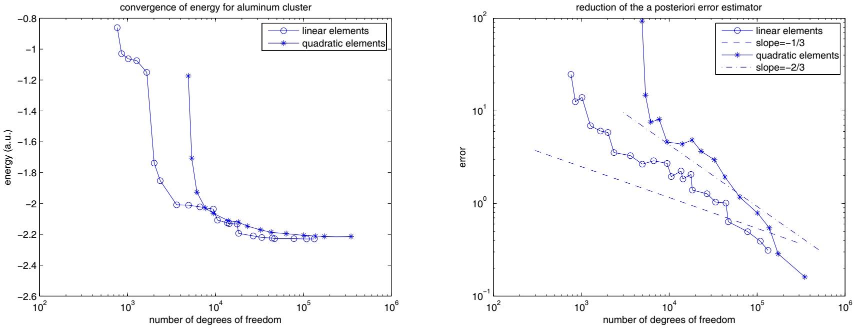
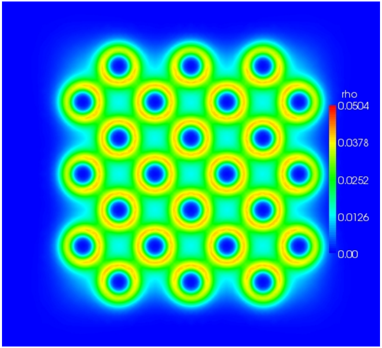
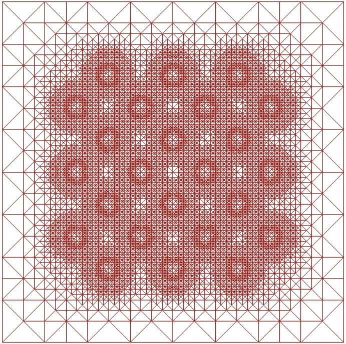


Figure: Left: Convergence curves of energy for the aluminium cluster in FCC lattice. Right: Reduction of the a posteriori error estimators.

Aluminium clusters in face-center-cubic (FCC) lattice

TFW model for simulating 172 atoms in FCC lattice.





Left: A contour plot of electron density on interior slice $z = 0$.

Right: The corresponding adaptive mesh.

Thank You!