Functional a posteriori error estimate for the PBE

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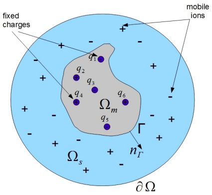
Outline

Derivation

- Poisson equation

$$-\nabla \cdot (\epsilon \nabla \phi) = \frac{4\pi}{\epsilon_0} \rho$$

$\rho(x)$-charge distribution,
$\epsilon(x)$-relative dielectric permittivity
ϵ_0-dielectric permittivity constant of vacuum



- 1) molecular region Ω_m

$$\rho_f = \sum_{i=1}^{N} q_i \delta_{x_i}(x), \quad x_i \in \Omega_m \Rightarrow -\nabla \cdot (\epsilon_m \nabla \phi) = \frac{4\pi}{\epsilon_0} \rho_f$$

- 2) solvent region Ω_s

$$\rho_s = cqe^{\frac{q\phi}{kT}} - cqe^{\frac{-q\phi}{kT}} = 2cq \sinh \frac{q\phi}{kT} \Rightarrow -\nabla \cdot (\epsilon_s \nabla \phi) = \frac{4\pi}{\epsilon_0} \rho_s$$

- Interface conditions $[\phi]_\Gamma = 0$, $\left[\epsilon \frac{\partial \phi}{\partial n}\right]_\Gamma = 0$

- Combining 1) and 2) with generalized coefficients $\epsilon(x)$ and $c(x)$

$$\begin{aligned} -\nabla \cdot (\epsilon \nabla \phi) &= \frac{4\pi}{\epsilon_0} (\rho_f + \rho_s) \\ \phi(\infty) &= 0 \\ [\phi]_\Gamma &= 0 \\ \left[\epsilon \frac{\partial \phi}{\partial n}\right]_\Gamma &= 0 \end{aligned}$$

The equation for the dimensionless potential $\tilde{u}$ is:

$$-\nabla \cdot (\epsilon(x)\nabla\tilde{u}) + k^2 sinh\,(\tilde{u}) = \sum_{i=1}^{N} z_i \delta_{x_i}(x)$$

3-term regularization: $\tilde{u} = G + u^h + u \Rightarrow$

$$\left|\begin{array}{l} -\nabla \cdot (\epsilon\nabla u) + k^2 \sinh(u) = 0 \\ [u]_\Gamma = 0, \quad \left[\epsilon \frac{\partial u}{\partial n}\right]_\Gamma = g_\Gamma \\ u = g, \qquad \text{on} \quad \partial\Omega \end{array}\right. \tag{1}$$

The weak formulation:

Find $u \in H_g^1(\Omega) := \{v \in H^1(\Omega) : v = g \text{ on } \partial\Omega\}$ such that

$$\int_\Omega \epsilon\nabla u \cdot \nabla v dx + \int_\Omega k^2 \sinh(u) v dx = \int_\Gamma g_\Gamma v ds, \quad \forall v \in H_0^1(\Omega) \tag{2}$$

This formulation has a unique weak solution $u \in H_g^1(\Omega) \cap L^\infty(\Omega)$

Another splitting: $u = u^l + u^n$

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

$$a(u^l, v) = \langle g_\Gamma, v \rangle, \ \forall v \in H^1_0(\Omega) \tag{3}$$

Find $u^n \in H^1_0(\Omega)$ such that

$$a(u^n, v) + \int_\Omega b(x, u^n + u^l) v dx = 0, \ \forall v \in H^1_0(\Omega) \tag{4}$$

$$a(u, v) = \int_\Omega \epsilon \nabla u \cdot \nabla v dx, \qquad \begin{array}{l} b(x,s) : \Omega \times \mathbb{R} \to \mathbb{R} \\ b(x,s) = k^2(x) \sinh(s) \end{array}$$

(3) has a unique solution $u^l \in H^1_0(\Omega) \cap L^\infty(\Omega) \Rightarrow$ (4) also has a unique weak solution $u^n \in H^1_0(\Omega) \cap L^\infty(\Omega)$ which is the unique minimizer of

$$J(v) = \int_\Omega \frac{\epsilon}{2} |\nabla v|^2 dx + \int_\Omega B(x, v + u^l) dx$$

$$B(x,s) : \Omega \times \mathbb{R} \to \mathbb{R}, \quad B(x,s) = k^2(x) \cosh(s)$$

Functional a posteriori error estimate for u^n

Notation:

$V := H_0^1(\Omega), \quad Y := (L_2(\Omega))^3$

$\Lambda = \nabla : V \to Y$ is bounded from above and below

$\Rightarrow \exists \Lambda^* : Y^* \to V^*$

$$g(x,\xi) = \frac{\epsilon(x)}{2}\xi \cdot \xi : \Omega \times \mathbb{R}^3 \to \mathbb{R}$$

$$B(x,s) = k^2(x)\cosh(s) : \Omega \times \mathbb{R} \to \mathbb{R}$$

$$G : Y \to \mathbb{R}, \quad G(y) = \int_\Omega \frac{\epsilon}{2}|y|^2 dx$$

$$\left.\begin{aligned} G(\Lambda v) &= \int_\Omega g(x,\nabla v)dx = \int_\Omega \tfrac{\epsilon(x)}{2}\,|\nabla v|^2\,dx \\ F(v) &= \int_\Omega B(x, v+u^l)dx = \int_\Omega k^2(x)\cosh(v+u^l)dx \end{aligned}\right\} \Rightarrow J(v) = G(\Lambda v) + F(v)$$

Definition ([1])

A convex functional $J : V \to \mathbb{R}$ is called uniformly convex if there exists a nonnegative proper and l.s.c functional $\Upsilon : V \to \mathbb{R} : \Upsilon(v) = 0 \Leftrightarrow v = 0$ such that for all $v_1, v_2 \in V$ the following inequality holds:

$$J\left(\frac{v_1 + v_2}{2}\right) + \Upsilon(v_1 - v_2) \leq \frac{1}{2}\left(J(v_1) + J(v_2)\right)$$

Definition (Dual functional/ Fenchel conjugate/ convex conjugate)

Let $J : V \to \mathbb{R}$. The functional $J^* : V^* \to \mathbb{R}$ defined by

$$J^*(v^*) := \sup_{v \in V} \{\langle v^*, v\rangle - J(v)\}$$

is called the dual functional / Fenchel conjugate functional of J

Definition (Second conjugate)

Let $J : V \to \mathbb{R}$. The functional $J^{**} : V \to \mathbb{R}$ defined by

$$J^{**}(v) := \sup_{v^* \in V^*} \{\langle v^*, v\rangle - J^*(v^*)\}$$

is called the second conjugate functional J

Theorem (Fenchel-Moreau)

If J is a convex, proper ($J : V \to (-\infty, +\infty]$ and $J \not\equiv +\infty$), l.s.c functional, then $J = J^{**}$

$$J(v) = G(\Lambda v) + F(v) = \sup_{y^* \in Y^*} \{\langle y^*, \Lambda v\rangle - G^*(y^*) + F(v)\},$$

$G^* : Y^* \to \mathbb{R}$ is the Fenchel conjugate of G

$L : V \times Y^* \to \mathbb{R}$ the Lagrangian for J, $L(v, y^*) := \langle y^*, \Lambda v\rangle - G^*(y^*) + F(v),$

$$\inf_{v \in V} J(v) = \inf_{v \in V} \sup_{y^* \in Y^*} L(v, y^*)$$

$$I^*(y^*) := \inf_{v \in V} L(v, y^*) = -G^*(y^*) + \inf_{v \in V} \{\langle y^*, \Lambda v\rangle + F(v)\}$$

$$= -G^*(y^*) - \sup \{\langle -\Lambda^* y^*, v\rangle - F(v)\} = -G^*(y^*) - F^*(-\Lambda^* y^*)$$

Strong duality

Under certain conditions like lower/upper semicontinuity and convexity/concavity on $L(v, y^*)$ with respect to v and y^* respectively, and lower semicontinuity for J and $-I^*$, some coercivity conditions on L, there are $u \in V$ and $p^* \in Y^*$ such that

$$J(u) = \inf_{v \in V} J(v) = \inf_{v \in V} \sup_{y^* \in Y^*} L(v, y^*)$$

$$I^*(p^*) = \sup_{y^* \in Y^*} I^*(y^*) = \sup_{y^* \in Y^*} \inf_{v \in V} L(v, y^*)$$

$$J(u) = I^*(p^*) \text{ (strong duality holds)}$$

J is uniformly convex

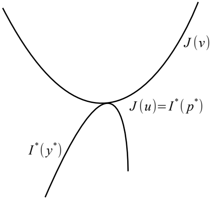
$$
\begin{aligned}
&\frac{1}{2}G(\Lambda v_1) + \frac{1}{2}G(\Lambda v_2) - G\left(\frac{\Lambda(v_1+v_2)}{2}\right) \\
&= \frac{1}{4}\int_\Omega \left(\epsilon|\nabla v_1|^2 + \epsilon|\nabla v_2|^2 - \frac{\epsilon}{2}|\nabla v_1 + \nabla v_2|^2\right) dx \\
&= \frac{1}{8}\int_\Omega \epsilon|\nabla(v_1 - v_2)|^2 dx
\end{aligned}
$$

$\Rightarrow$ G is uniformly convex with $\Upsilon_G(v-u) = \frac{1}{8}\int_\Omega \epsilon\,|\nabla\,(v-u)|^2\,dx$. Therefore J is also uniformly convex with the same forcing functional.

If u is the minimizer of J, by the definition of uniformly convex functional, applied to J and its forcing functional Υ_G [1] $\Rightarrow$

$$\Upsilon_G(v-u) \leq \frac{1}{2}(J(v)+J(u)) - J\left(\frac{v+u}{2}\right) \leq \frac{1}{2}(J(v)-J(u))$$

$$\leq \frac{1}{2}(J(v)-I^*(y^*)) = \frac{1}{2}(G(\Lambda v)+F(v)+G^*(y^*)+F^*(-\Lambda^* y^*))$$



So we get

$$\|u-v\|_{H^1(\Omega)} \sim \Upsilon_G(v-u)$$

$$\leq \frac{1}{2}(G(\Lambda v)+F(v)+G^*(y^*)+F^*(-\Lambda^* y^*)) =: M_{\oplus}(v,y^*)$$

with "=" iff $v=u$ and $y^*=p^*=\epsilon\nabla u$.

Computing $G^*(y^*)$

$$G^*(y^*) = \sup_{y \in Y} \left(\langle y^*, y \rangle - G(y) \right)$$

$$= \sup_{y \in Y} \int_\Omega \left[y^*(x) \cdot y(x) - \frac{\epsilon(x)}{2} y(x) \cdot y(x) \right] dx$$

$$\leq \int_\Omega \sup_{\xi \in \mathbb{R}^3} \{ y^*(x) \cdot \xi - \frac{\epsilon(x)}{2} \xi \cdot \xi \} dx$$

$$\overset{\xi(x) = \frac{1}{\epsilon(x)} y^*(x)}{=} \int_\Omega \frac{1}{2\epsilon(x)} |y^*(x)|^2 dx$$

Computing $F^*(-\Lambda^* y^*)$

$$F^*(-\Lambda^* y^*) = \sup_{w \in H_0^1(\Omega)} [\langle -\Lambda^* y^*, w\rangle - F(w)] = \sup_{w \in H_0^1(\Omega)} [\langle -y^*, \Lambda w\rangle - F(w)]$$

$$= \sup_{w \in H_0^1(\Omega)} \int_\Omega \left[-y^* \cdot \nabla w - B(x, w + u^l) \right] dx = \quad (\text{if } y^* \in H(\mathrm{div};\Omega))$$

$$= \sup_{w \in H_0^1(\Omega)} \int_\Omega \left[\mathrm{div}\, y^* w - B(x, w + u^l) \right] dx$$

$$= \underbrace{\sup_{w \in H_0^1(\Omega)} \int_\Omega \left[\mathrm{div}\, y^* (w + u^l) - B(x, w + u^l) \right] dx}_{:= I(w)} - \int_\Omega \mathrm{div}\, y^* u^l dx$$

$$\leq \int_\Omega \sup_{\xi \in \mathbb{R}} \left[\mathrm{div}\, y^*(x) \left(\xi + u^l(x) \right) - B\left(x, \xi + u^l(x) \right) \right] dx - \int_\Omega \mathrm{div}\, y^*(x) u^l(x) dx$$

$$= \int_\Omega \left[\mathrm{div}\, y^*(x) \left(\xi_0(x) + u^l(x) \right) - B\left(x, \xi_0(x) + u^l(x) \right) \right] dx - \int_\Omega \mathrm{div}\, y^*(x) u^l(x) dx$$

$$= I(\xi_0) - \int_\Omega \operatorname{div} y^* u^l \, dx$$

where $\xi_0 : \Omega \to \mathbb{R}$ is computed from the necessary (and sufficient) condition for maximum:

$$\frac{d}{d\xi}\left(\operatorname{div} y^*(x)\left(\xi + u^l(x)\right) - B\left(x, \xi + u^l(x)\right)\right) = 0$$

$$\xi_0(x) = \operatorname{arcsinh}\left(\frac{\operatorname{div} y^*(x)}{k^2(x)}\right) - u^l(x)$$

$$= \underbrace{\ln\left(\frac{\operatorname{div} y^*(x)}{k^2(x)} + \sqrt{\left(\frac{\operatorname{div} y^*(x)}{k^2(x)}\right)^2 + 1}\right)}_{\in L^2(\Omega)\ \forall y^* \in H(\operatorname{div};\Omega),\ \text{because}\ \left|\ln\left(y + \sqrt{y^2+1}\right)\right| \le |y|,\ \forall y \in \mathbb{R}} - u^l(x)$$

Is it really true $\sup_{w \in H_0^1(\Omega)} I(w) = I(\xi_0)$? $\rightarrow$ Note that $\xi_0 \notin H_0^1(\Omega)$

Theorem

For any $y^* \in H(\mathrm{div};\Omega)$ *it is true that* $\sup_{w \in H_0^1(\Omega)} I(w) = I(\xi_0)$.

Idea of the proof:

- find a suitable sequence $w_n \in H_0^1(\Omega)$ s.t $I(w_n) \rightarrow I(\xi_0)$
- For this, find $\{f_n\} \subset C_0^\infty(\Omega) : f_n(x) \rightarrow f(x) := \frac{\mathrm{div}\, y^*}{k^2}$ $a.e$ and $\{u_n^l\} \subset C_0^\infty(\Omega) : u_n^l(x) \rightarrow u^l(x)$, $a.e$, s.t $|f_n(x)| \leq h(x) \in L^2(\Omega)$ and $|u_n^l(x)| \leq \|u^l\|_{L^\infty(\Omega)} + 2$.
- Then $w_n(x) := \ln\left(f_n(x) + \sqrt{f_n^2(x) + 1}\right) - u_n^l(x) \rightarrow \xi_0(x)$, $a.e$ in Ω and $w_n \in C_0^\infty(\Omega) \subset H_0^1(\Omega)$
- $\mathrm{div}\, y^*(x)\left(w_n(x) + u^l(x)\right) - B\left(x, w_n(x) + u^l(x)\right) \rightarrow$ $\mathrm{div}\, y^*(x)(\xi_0(x) + u^l(x)) - B(x, \xi_0(x) + u^l(x))$
- (*) Find a dominating summable function for $\mathrm{div}\, y^*(x)\left(w_n(x) + u^l(x)\right) - \cosh\left(x, w_n(x) + u^l(x)\right)$ and apply Lebesgue DCT

Thank you for listening!

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Elsevier, 2004.