Minimization Protocols for Solving Mortar Finite Element Equations of Nonlinear Poisson-Boltzmann Equation

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OUTLINE

1. Poisson-Boltzmann equation (PBE) in protein simulations
2. Three Difficulties in Solving PBE
3. Mortar Finite Element Approximation of PBE
4. Two PBE Related Minimization Problems
5. Formulation of Nonlinear Algebraic Equations
6. Truncated Newton Minimization Method for PBE
7. Future Work

1. PBE in Protein Simulations

Partition of 3D domain Ω: $\Omega = \Omega_1 \cup \Omega_2, \quad \Omega_1 \cap \Omega_2 = \emptyset$, and Ω_1 is surrounded by Ω_2. Further, set $\Omega_3 \subset \Omega_2$.

We consider PBE as below:

$$-\nabla \cdot (\epsilon(x)\nabla u) + \kappa(x) \sinh u = f(x) \text{ in } \Omega, \quad u = g \text{ on } \partial\Omega,$$

$$\epsilon(x) = \begin{cases} \epsilon_1 & \text{for } x \in \Omega_1, \\ \epsilon_2 & \text{for } x \in \Omega_2, \end{cases} \quad \kappa(x) = \begin{cases} 0 & \text{for } x \in \Omega_1 \cup (\Omega_2 - \Omega_3), \\ \bar{\kappa} & \text{for } x \in \Omega_3, \end{cases}$$

- $\Omega 1$: protein region. Ω_2: solvent region. Ω_3: ionic region. $\Omega_2 - \Omega_3$: ion exclusive region.
- u: the electrostatic potential. $\epsilon(x)$: the permittivity. $\epsilon(x) > 0$.
- $\kappa(x)$: the ion concentration. $\bar{\kappa} > 0$. $f(x)$: the charge distribution. q_i: the charge at position x^i of atom i. $\bar{c}$: given constant.

$$f(x) = \begin{cases} \bar{c} \sum_{i=1}^n q_i \delta(x - x^i) & \text{for } x \in \Omega_1, \\ 0 & \text{for } x \in \Omega_2. \end{cases}$$

2. Three Difficulties in Solving PBE

1. Singularity of the source term f (a sum of δ-functions). It causes difficulties in finite element analysis due to $u \notin H^1(\Omega)$.

2. Exponential nonlinear term ($\sinh(u) = (e^u - e^{-u})/2$). It leads to a system with strong nonlinear properties.

3. Discontinuous coefficients $\epsilon(x)$ and $\kappa(x)$. They lead to difficulties in theory and computing.

Note: Original PBE has $\Omega = R^3$. In numerical PBE, Ω is often selected as a cube or another regular bounded domain. The corresponding boundary function g can be well defined by several well developed numerical techniques.

On Difficulty 1: $u \notin H^1(\Omega)$ caused by singular source term f

If a fundamental solution of PBE is given as $G(x)$, then the singular part of $u(x)$ can be expressed in the form

$$\mathcal{G}(x) = \bar{c} \sum_{i=1}^{n} q_i G(x - x^i).$$

Thus, we can define $w(x) = u(x) - \mathcal{G}$ such that $w \in H^1(\Omega)$.

In this way, we can consider $w(x)$ instead of $u(x)$ for the convergence analysis of the finite element equation of PBE.

References:

- *Chen, Shen and Xia, Applied Mathematics and Computation, 164 (2005) 11-23 (for linearized PBE only).*
- *M. Holst and J. Xu, "The Poisson-Boltzmann equation: Approximation theory, regularization by singular functions, and adaptive techniques". In preparation.*

On Difficulty 2: Large scale nonlinear systems

Note that the derivative of the nonlinear discrete algebraic equations can be found easily. Hence, Newton method is a good choice. Due to the large scale of the systems, the challenge is how to develop a high efficient nonlinear solver for PBE.

Prof. Holst and his group developed an inexact Newton method for solving PBE, in which a linear multigrid algorithm is applied to solve the Newton equations approximately, together with adaptive techniques. The inexact Newton method has been a core part of a program package called APBS (Adaptive Poisson-Boltzmann Solver at http://apbs.sourceforge.net).

References:

- *M. Holst and F. Saied, J. Comput. Chem., 16 (1995) 337-364.*
- *M. Holst, N. Baker, and F. Wang, J. Comput. Chem., 21 (2000) 1249-1352.*

On Difficulty 3: Large jump discontinuity coefficients

Due to the discontinuous coefficients, the solution $u \notin H^2(\Omega)$ even assuming the source term f does not contain any singularities. Hence, from the classic finite element method it cannot follow that

$$\|u - u_h\|_{H^1} \leq Ch\|u\|_{H^2},$$

where u_h is the finite element solution.

In order to raise the accuracy of solution, mesh refinement techniques and interface continuity conditions should be used in computing of a solution of PBE. Further, to reduce the size of the nonlinear system, unstructured meshes and adaptive techniques are needed in solving PBE.

3. Mortar Finite Element Approximation of PBE

Mortar finite element methods:

- A nonconfirming domain decomposition technique.
- Allow different discretization schemes and non-matching triangulations on different subdomains.
- Good for problems with discontinuous coefficients, singular sources, or corner singularities.
- Two different formulations of mortar methods:
  - A nonconforming finite element setting based on a constrained functional space. Lead to a positive definite system.
  - A mixed finite element setting based on a unconstrained functional space. Lead to an indefinite system.

Clearly, mortar finite element methods are particularly effective to PBE. Here it is natural to have two disjoint subdomains, Ω_1 and Ω_2. Thus, two independent triangulations, $\mathcal{T}_{1,h}$ and $\mathcal{T}_{2,h}$, and the two related finite element function spaces, V_{Ω_1} and V_{Ω_2}, are defined, independently.

Mortar Condition

- The interface Γ of PBE: $\Gamma = \partial\Omega_1$.
- Notation $v|_S$: Restruction of v onto region S.
- Conventional interface continuity condition:

$$u|_{\Omega_1} = u|_{\Omega_2} \text{ on } \Gamma \quad \text{and} \quad \epsilon_1 \frac{\partial u|_{\Omega_1}}{\partial \nu} = \epsilon_2 \frac{\partial u|_{\Omega_2}}{\partial \nu} \quad \text{on } \Gamma.$$

- Mortar condition:

$$b(u, w) = 0 \quad \forall w \in \Lambda_h,$$

where $b(u, w) = \int_\Gamma (u|_{\Omega_1} - u|_{\Omega_2}) w ds$, and Λ_h is a finite element space based on the grid mesh Γ_h that inherits from $\mathcal{T}_{1,h}$.

Mortar finite element equation of PBE

Define product function space V_h:

$$V_h = \{v \in L^2(\Omega) \mid v|_{\Omega_1} \in V_{\Omega_1}, \text{ and } v|_{\Omega_2} \in V_{\Omega_2}\}.$$

Define a subspace $\tilde{V}_h$ of V_h by

$$\tilde{V}_h = \{v \in V_h \mid b(v, w) = 0 \quad \text{for all } w \in \Lambda_h\}.$$

Mortar finite element equation of PBE: Find $u \in \tilde{V}_h$ such that

$$a(u, v) + \int_\Omega v\kappa(x) \sinh u dx = \int_\Omega f v dx, \quad \forall v \in \tilde{V}_h, \tag{1}$$

where $a(u, v)$ is a symmetric bilinear functional defined by

$$a(u, v) = \int_{\Omega_1} \epsilon_1 \nabla u \cdot \nabla v dx + \int_{\Omega_2} \epsilon_2 \nabla u \cdot \nabla v dx.$$

4. Two PBE Related Minimization Problems

Define a functional, $\mathcal{J}$, as below:

$$\mathcal{J}(v) = \frac{1}{2}a(v,v) + \int_\Omega \kappa(x)\cosh v dx - \int_\Omega f v dx, \qquad \text{for } v \in V_h.$$

Let $\mathcal{J}'$ and $\mathcal{J}''$ be the first and second G-derivatives of $\mathcal{J}$. Then,

$$(\mathcal{J}'(u), v) = a(u,v) + \int_\Omega v\kappa(x)\sinh u dx - \int_\Omega f v dx, \quad \forall v \in V_h,$$

$$(\mathcal{J}''(u)v, v) = a(v,v) + \int_\Omega v^2\kappa(x)\cosh u dx, \quad \forall v \in V_h.$$

(1) A unconstrained minimization problem: Find $u \in \tilde{V}_h$ such that

$$\mathcal{J}(u) = \min\{\mathcal{J}(v) \mid v \in \tilde{V}_h\},$$

where $\tilde{V}_h = \{v \in V_h \mid b(v,w) = 0 \quad \text{for all } w \in \Lambda_h\}$.

(2) A constrained minimization problem: Find $u \in V_h$ such that

$$\mathcal{J}(u) = \min\{\mathcal{J}(v) \mid v \in V_h\} \qquad \text{subject to } b(u,w) = 0 \text{ for all } w \in \Lambda_h.$$

Theorem 1: *The PBE mortar finite element problem and the above two minimization problems are equivalent.*

Uniqueness of Solution of Mortar Finite Element Equation

Remark: $a(v, v)$ may be zero in V_h since Ω_1 is surrounded by Ω_2.

For example, set $v^0 = 1$ in the closure of Ω_1 and $v^0 = 0$ others. Then, $v^0 \in V_h$, and $a(v^0, v^0) = 0$. But, for the mortar finite element approximation of PBE, we have that

Theorem 2: $\exists \alpha > 0$ *such that* $a(v, v) > \alpha \|v\|^2$ *for all* $v \in \tilde{V}_h$.

Consequently, $(\mathcal{J}''(u)v, v) > 0$ for all nonzero $v \in \tilde{V}_h$, implying that $\mathcal{J}(v)$ is a strictly convex functional in $\tilde{V}_h$.

We then proved that

Theorem 3: *The unconstrained minimization problem has a unique solution in* $\tilde{V}_h$.

Corollary: *The mortar finite element equation and the constrained minimization problem have a unique solution, respectively.*

5. Formulation of Nonlinear Algebraic Equations

With a set of basis functions of V_h, φ_j for $j = 1, 2, \ldots, N$, we have that for u in V_h, $u = \sum_{j=1}^{N} u_j \varphi_j$, and the PBE mortar finite element equation in V_h is equivalent to the nonlinear system: For $j = 1, 2, \ldots, N$,

$$\sum_{i=1}^{N} a(\varphi_i, \varphi_j) u_i + \int_\Omega \varphi_j \kappa(x) \sinh(\sum_{i=1}^{N} u_i \varphi_i) dx = \int_\Omega f \varphi_j dx.$$

In matrix form, the nonlinear system becomes

$$AU + S(U) = F,$$

where $A = (a(\varphi_i, \varphi_j))$ is a $N \times N$ matrix, U, $S(U)$ and F are column vectors with the jth entry u_j, $s_j = \int_\Omega \varphi_j \kappa(x) \sinh(\sum_{i=1}^{N} u_i \varphi_i) dx$, and $f_j = \int_\Omega f \varphi_j dx$.

By the definition of δ-function, $\int_\Omega \delta(x - x^i) \varphi_j(x) dx = \varphi_j(x^i)$, f_j is evaluated by

$$f_j = \int_\Omega f \varphi_j dx = \bar{c} \sum_{i=1}^{n} q_i \varphi_j(x^i), \quad j = 1, 2, \ldots, N.$$

By a simple quadrature, s_j can be evaluated as below:

$$s_j = \int_{\tau^j} \varphi_j \kappa(x) \sinh(\sum_{i=1}^{N} u_i \varphi_i) dx \approx \kappa(x^j) |\tau^j| \sinh(u_j),$$

where τ^j denotes the support set of φ_j, and $|\tau^j|$ denotes the size of τ^j.

Algebraic Form of Mortar Condition

Define four subspaces of V_h as below:

$$\mathcal{V}_{\Omega_1} = Span\{\varphi_j | x^j \in \Omega_{1,h}\}, \quad \mathcal{V}_{\Omega_2} = Span\{\varphi_j | x^j \in \Omega_{2,h}\},$$
$$\mathcal{V}_{\Gamma_{\Omega_1}} = Span\{\varphi_j | x^j \in \Gamma_{\Omega_1,h}\}, \quad \text{and} \quad \mathcal{V}_{\Gamma_{\Omega_2}} = Span\{\varphi_j | x^j \in \Gamma_{\Omega_2,h}\},$$

For convenience, we assign local ordering numbers to the basis functions, and denote these local basis functions as $\{\varphi_j\}_{j=1}^{n_1}$, $\{\tilde{\varphi}_j\}_{j=1}^{n_2}$, $\{\hat{\varphi}_j\}_{j=1}^{l}$, and $\{\bar{\varphi}_j\}_{j=1}^{m}$. Then, for $v \in V_h$, we have

$$v|_{\Omega_1} = \sum_{j=1}^{n_1} v_j \varphi_j, v|_{\Omega_2} = \sum_{j=1}^{n_2} \tilde{v}_j \tilde{\varphi}_j, v|_{\Gamma_{\Omega_1}} = \sum_{j=1}^{l} \hat{v}_j \hat{\varphi}_j, \text{ and } v|_{\Gamma_{\Omega_2}} = \sum_{j=m}^{m} \bar{v}_j \bar{\varphi}_j.$$

We then label the unknowns in a global ordering: first on the nodes of $\Omega_{1,h}$, then $\Gamma_{\Omega_1,h}$, next $\Omega_{2,h}$, and finally $\Gamma_{\Omega_2,h}$. In this global ordering, V has the 4-block form $V = (V_{\Omega_1}, V_{\Gamma_{\Omega_1}}, V_{\Omega_2}, V_{\Gamma_{\Omega_2}})^T$, where

$$V_{\Omega_1} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n_1} \end{pmatrix}, V_{\Gamma_{\Omega_1}} = \begin{pmatrix} \hat{v}_1 \\ \hat{v}_2 \\ \vdots \\ \hat{v}_l \end{pmatrix}, V_{\Omega_2} = \begin{pmatrix} \tilde{v}_1 \\ \tilde{v}_2 \\ \vdots \\ \tilde{v}_{n_2} \end{pmatrix}, \text{ and } V_{\Gamma_{\Omega_2}} = \begin{pmatrix} \bar{v}_1 \\ \bar{v}_2 \\ \vdots \\ \bar{v}_m \end{pmatrix}.$$

We obtained the following theorem.

Theorem 4: *Let ψ_j for $j = 1, 2, \ldots, l$ be a set of basis functions of the finite element space Λ_h. Then the algebraic expression of the mortar condition $b(u, w) = 0$ can be formulated in the matrix form*

$$MV_{\Gamma_{\Omega_1}} - WV_{\Gamma_{\Omega_2}} = 0,$$

where M and W are two matrices of $l \times l$ and $l \times m$, respectively, with entries $m_{ji} = \int_\Gamma \hat{\varphi}_i \psi_j ds \quad$ and $\quad w_{jk} = \int_\Gamma \bar{\varphi}_k \psi_j ds$ for $i, j = 1, 2, \ldots, l, k = 1, 2, \ldots, m$. Moreover, M is nonsingular.

Thus, the mortar finite element equation in the restricted finite element space $\tilde{V}_h$ has the following algebraic form:

$$\begin{cases} AU + S(U) = F \\ MU_{\Gamma_{\Omega_1}} - WU_{\Gamma_{\Omega_2}} = 0, \end{cases}$$

Note that the mortar algebraic condition can be written as

$$U_{\Gamma_{\Omega_1}} = TU_{\Gamma_{\Omega_2}} \quad \text{with} \quad T = M^{-1}W.$$

Hence, the sub-unknown vector $U_{\Gamma_{\Omega_1}}$ can be eliminated so that the above two equations are combined as one equation.

Algebraic Formulation of Minimization Problem of PBE

Set $\tilde{U} = \begin{pmatrix} U_{\Omega_1} \\ U_{\Omega_2} \\ U_{\Gamma_{\Omega_2}} \end{pmatrix}$, and $\bar{B} = \begin{pmatrix} I & 0 & 0 \\ 0 & 0 & T \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix}$. Then $U = \bar{B}\tilde{U}$ and the mortar finite element equation is expressed as $\tilde{A}\tilde{U} + \tilde{S}(\tilde{U}) = \tilde{F}$, where $\tilde{A} = \bar{B}^T A \bar{B}$, $\tilde{S}(\tilde{U}) = \bar{B}^T S(\bar{B}\tilde{U})$, and $\tilde{F} = \bar{B}^T F$.

If the jth component of $S(U)$ is approximated by $s_j = \kappa(x^i)|\tau^i|\sinh(u_j)$, the equivalent minimization problem becomes

$$\tilde{J}(\tilde{U}) = \min\{\tilde{J}(\tilde{V}) \mid \tilde{V} \in R^{N-l}\},$$

where $\tilde{J}(\tilde{V}) = \frac{1}{2}\tilde{V}^T\tilde{A}\tilde{V} + \tilde{C}(\tilde{V}) - \tilde{F}^T\tilde{V}$, $\tilde{C}(\tilde{V}) = \sum_{i=1}^N \kappa(x^i)|\tau^i|\cosh(B_i\tilde{V})$, and B_i denotes the ith row of the matrix $\bar{B}$.

Theorem 5: *The Hessian matrix $\nabla^2\tilde{J}(\tilde{V})$ is symmetric, positive definite in R^{N-l}. Thus, the minimization problem has a unique solution.*

In fact, $\nabla^2\tilde{J}(\tilde{V}) = \tilde{A} + \sum_{i=1}^N \kappa(x^i)|\tau^i|\cosh(B_i\tilde{V})B_i^T B_i$.

6. Truncated Newton Minimization Method for PBE

A sequence of TN iterates, $\{\tilde{U}^k\}$, is defined in the form

$$\tilde{U}^{k+1} = \tilde{U}^k + \lambda_k P^k,$$

where λ_k is a step length determined by the line search algorithm, and P^k is a search direction generated by the preconditioned conjugate gradient method for solving the classic Newton equation at step k,

$$H(\tilde{U}^k)P = -g(\tilde{U}^k). \tag{2}$$

Here $H(\tilde{U}^k) = \nabla^2 \tilde{J}(\tilde{U}^k)$, and $g(\tilde{U}^k) = \nabla \tilde{J}(\tilde{U}^k) = \tilde{A}\tilde{U}^k + \tilde{S}(\tilde{U}^k) - \tilde{F}$.

Since H is sparse and symmetric positive definite, a multigrid preconditioner can be defined by applying one iteration of a multigrid method for solving (2).

Truncation test: If $\|r_{j+1}\| \le \min\{c_r/k, \ \|g_k\|\}\|g_k\|$, exit PCG loop with $P^k = p_{j+1}$. By default, $c_r = 0.5$. Here p_j represent the jth PCG iterate, and r_j the residual vector of (2).

- *All the PCG iterates are descent search directions.*
- *The TN iterates converges for any initial guess $\tilde{U}^0$.*

Future Work

- Make numerical experiments and compare with other methods (e.g., the inexact Newton method by M. Holst).
- Develop a parallel version of TN for solving PBE.
- Extend the approach and schemes to other application problems.

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