Accurate Gradient Approximation for Complex Interface Problems in 3D by an Improved Coupling Interface Method

Yu-Chen Shu¹, I-Liang Chern², and Chien-Cheng Chang³

¹Department of Mathematics, National Cheng Kung University, Tainan, Taiwan
²Department of Mathematics, National Chiao Tung University, Hsinchu, Taiwan
³Institute of Applied Mechanics, National Taiwan University, Taipei, Taiwan
Outline

- Interface Problems
  - What is the problem caused by complex interfaces?
- Numerical Results
- Concluding Remarks
Interface Problems

Interface problems appears in many fields such as fluid dynamics, solid mechanics, electrodynamics, material sciences, biochemistry, and etc..
Application: Drug Design

Quoted from http://www.proxychem.com/sbdd.html
An important key: Electric potential

Molecular electrostatic potentials are key for drug design
Molecules in ionic solution

- A continuum model for computing the electro-static potential in an ionic solution.

- Based on Gauss’ law and Boltzmann distribution law.
Poisson-Boltzmann Equation

\[ \nabla \cdot (\varepsilon(r) \nabla u(r)) = -\sum_i c_i z_i q \lambda(r) \exp\left(\frac{-z_i q u(r)}{k_B T}\right) - \sum_j z_j q \delta(r - r_j) \]

- \( r \): location
- \( \varepsilon \): dielectric coefficient
- \( u \): electrostatic potential (unknown)
- \( c_i \): concentration of the \( i \)-th ion at a distance of infinity
- \( z_i, z_j \): the number of charges of the \( i \)-th ion, \( j \)-th point charge
- \( q \): charge of a proton
- \( k_B \): Boltzmann constant
- \( T \): temperature
- \( \lambda \): accessibility to the ions in the solution. 1 in the solution.
- \( \delta \): delta function
Model problem

- Governing equation:
  
  \[-\nabla \cdot (\varepsilon(r) \nabla u(r)) + \kappa^2 (r) u(r) = f\]

- Dielectric coefficient:
  
  \[\varepsilon(r) = \begin{cases} 
  \varepsilon^-, & r \in \Omega^- \\
  \varepsilon^+, & r \in \Omega^+ 
  \end{cases}\]

- Interface conditions:
  
  \([u]_\Gamma = 0, [\varepsilon \nabla u \cdot n]_\Gamma = 0\]

- No ion-exclusion layer
Some approaches

Body-fitting approaches
- W. Wang, A jump condition capturing finite difference scheme for elliptic interface problems

Finite element approaches
- Z. Li, T. Lin, X. Wu, New Cartesian grid methods for interface problems using the finite element formulation
- J. Huang, J. Zou, A mortar element method for elliptic problems with discontinuous coefficients

Finite difference approaches
- A. Tornberg, B. Engquist, Regularization techniques for numerical approximation of PDEs with singularities
- C. Peskin, The immersed boundary method
- R. Leveque, Z. Li, The immersed interface method for elliptic equations with discontinuous coefficients and singular sources
- Y. Zhou, S. Zhao, M. Feig, G. Wei, High order matched interface and boundary method for elliptic equations with discontinuous coefficients and singular sources
Our approach: coupling interface method

Finite difference approach on Cartesian grid.

Dimension-by-dimension approach.

The information of each dimension is coupled by the interface conditions.
Advantages of coupling interface method

- **Accuracy:** second-order for the solution in maximum norm.

- **Simplicity:** smaller size of stencil among second order method.

- **Robustness:** capable to handle complex interfaces with hybrid order method.

- **Speed:** linear computational complexity
However, I don’t have enough time

Today, Due to the time limit, I don’t have time to introduce the coupling interface method.

Instead, I will show you the problems of complex interface. It is a common problem for finite difference approaches.
Outline

- Interface Problems
  What is the problem caused by complex interfaces?
- Numerical Results
- Concluding Remarks
What is the problem of complex interfaces?

Case 1: At a grid point, if we have two adjacent points in one coordinate directions, we can approximated the second order derivative easily by central finite difference.

Case 2: If we have one adjacent point at each side of the interface, the second order derivatives can be approximated by the coupling interface method.

Case 3: If you have no adjacent point, that would be a trouble.
Case 1: two adjacent points

\[ u''(x_i) = \frac{1}{h^2}(u_{i-1} - 2u_i + u_{i+1}) + O(h^2) \]
Case 2: one adjacent point

Quadratic approximations on both side of the interface: (second order version of coupling interface method)

\[
u(x) = \begin{cases} 
  u_j + \frac{u_j - u_{j-1}}{h}(x - x_j) + \frac{1}{2}u_j''(x - x_j)(x - x_{j-1}) + O(h^3), & x < \hat{x} \\
  u_{j+1} + \frac{(u_{j+2} - u_{j+1})}{h}(x - x_{j+1}) + \frac{1}{2}u_{j+1}''(x - x_{j+1})(x - x_{j+2}) + O(h^3), & x > \hat{x}
\end{cases}
\]
The second order derivatives can be approximated by the linear combination of four grid values and two interface conditions.

\[
\begin{align*}
\left(\frac{1}{2} (\alpha + \alpha^2) u_j - \frac{1}{2} (\beta + \beta^2) u_{j+1}\right) &= \frac{1}{h^2} \left( \alpha u_{j-1} - (1 + \alpha) u_j + (1 + \beta) u_{j+1} - \beta u_{j+2} - [u]_i \right) + O(h) \\
\left(\frac{1}{2} + \alpha \right) \epsilon^- u_j + \left(\frac{1}{2} + \beta \right) \epsilon^+ u_{j+1} &= \frac{1}{h^2} \left( \epsilon^- u_{j-1} - \epsilon^- u_j - \epsilon^+ u_{j+1} + \epsilon^+ u_{j+2} - h [\omega']_i \right) + O(h)
\end{align*}
\]

The determinant is positive and bounded when \( \epsilon \) is positive.

\[
\begin{align*}
u_j^* &= \frac{1}{h^2} \left( c_{j-1} u_{j-1} + c_{j,0} u_j + c_{j,1} u_{j+1} + c_{j,2} u_{j+2} + \tau_j [u]_i + \sigma_j h [\omega']_i \right) + O(h) \\
&= \frac{1}{h^2} \left( \mathcal{L}_j (u_{j-1}, u_j, u_{j+1}, u_{j+2}) + \tau_j [u]_i + \sigma_j h [\omega']_i \right) + O(h) \\
u_{j+1}^* &= \frac{1}{h^2} \left( c_{j+1,-1} u_{j-1} + c_{j+1,0} u_j + c_{j+1,1} u_{j+1} + c_{j+1,2} u_{j+2} + \tau_{j+1} [u]_i + \sigma_{j+1} h [\omega']_i \right) + O(h) \\
&= \frac{1}{h^2} \left( \mathcal{L}_{j+1} (u_{j-1}, u_j, u_{j+1}, u_{j+2}) + \tau_{j+1} [u]_i + \sigma_{j+1} h [\omega']_i \right) + O(h)
\end{align*}
\]
Case 3: no adjacent point

First order approximation (CIM1) is Okay. But, do we have high order approximation? What happen if the yellow region is very small? What is the situation in high dimensions?
Why we need an improvement?

When the interface is very complicated, we can only get a first-order approximation for the gradient at some grid by CIM.

In some application, we need an accurate gradient for the later application. For example, below is the velocity of the interface in some moving interface problems:

$$v_n = -\delta F[\Gamma] = \gamma_0 H + \frac{\epsilon_+}{2} |\nabla u_+|^2 - \frac{\epsilon_-}{2} |\nabla u_-|^2 - \epsilon_+ |\nabla u_+ \cdot n|^2 + \epsilon_- |\nabla u_- \cdot n|^2$$
Our Goal

A method has second order accuracy for both the solution and its gradient for complex interfaces
Classification of grid points

\[ G(x_i) = (g_1(x_i), g_2(x_i), \ldots, g_d(x_i)) \]
\[ g_k(x_i) = \begin{cases} 2, & \text{if } x_{i-e_k}, x_i \text{ and } x_{i+e_k} \text{ are in the same region;} \\ 0, & \text{if } x_{i-e_k} \text{ and } x_{i+e_k} \text{ are not in the region that } x_i \text{ belongs to;} \\ 1, & \text{otherwise.} \end{cases} \]

G(P) = (0, 1)
G(Q) = (0, 0)
G(R) = (0, 2)

RED: Exceptional points
Examples for exceptional points in 2D

(a) $G(x_i) = (0, 0)$

(b) $G(x_i) = (0, 1)$

(c) $G(x_i) = (0, 2)$
Examples for exceptional points in 3D

(a) $G(x_1) = (0, 0, 0)$
(b) $G(x_1) = (0, 0, 1)$
(c) $G(x_1) = (0, 0, 2)$
(d) $G(x_1) = (0, 1, 1)$
(e) $G(x_1) = (0, 1, 2)$
(f) $G(x_1) = (0, 2, 2)$

Local extreme
Oblique extreme
Saddle point
Complex Interfaces

Exceptional Points are usually exists for a complex interface. The number of exceptional points is usually $O(1)$. 
How do we solve them?

- Mesh refinement
- Flip domain
- Shift approximation
\[ \delta(\Gamma) := \inf_{x \in \Gamma} \{ r | \bar{B}_r(x) \cap \Gamma \text{ contains at least two nonempty disjoint subsets} \} \]
Mesh refinement conditions:

If the interface is smooth, closed, and bounded,

The cases $G(x) = (0, 0)$ and $(0, 2)$ disappear under the following conditions:

(i) $h < \frac{\delta(\Gamma)}{\sqrt{5}}$ and (ii) $\kappa_{\infty} h < \frac{4}{5}$
Flip domain: Introducing Ghost States

\[ \Omega^+ \]

\[ \Omega^- \]

\[ P = x_j \]

Ignore these two intersections

\[ \Omega^+ \]

\[ \Omega^- \]
\[-\varepsilon^+ \left( \frac{\partial^2 \tilde{u}_{i,j}}{\partial x^2} + \frac{\partial^2 \tilde{u}_{i,j}}{\partial y^2} \right) = \tilde{f}_{i,j} \]

\[\tilde{f}_{i,j} = \frac{1}{2} (f_{i+1,j} + f_{i-1,j}) + O(h^2).\]

\[\frac{\partial^2 \tilde{u}_{i,j}}{\partial x^2} = \frac{1}{h^2} (u_{i-1,j} - 2\tilde{u}_{i,j} + u_{i+1,j}) + O(h^2).\]

\[\frac{\partial^2 \tilde{u}_{i,j}}{\partial y^2} = L_{i,j,y}(u_{i,j-2}, u_{i,j-1}, \tilde{u}_{i,j}, u_{i,j+1}) + b_{i,j,y}[u] + c_{i,j,y}[\varepsilon \frac{\partial u}{\partial y}] + O(h),\]
Shift Approximation: Coupled with nearby Second order derivatives

\[ u_{xx}(x_i, y_j) \approx u_{xx}(x_i, y_{j-1}) \approx \frac{1}{h^2} (u_{i-1,j-1} - 2u_{i,j-1} + u_{i+1,j-1}) \]
## Summary of the Recipes

<table>
<thead>
<tr>
<th></th>
<th>Recipe 1 (shift)</th>
<th>Recipe 2 (flip)</th>
<th>Generic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G(x_i) = (0, 0)$</td>
<td>$-$</td>
<td>$\checkmark$</td>
<td>$-$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 1)$</td>
<td>$\Delta$</td>
<td>$\checkmark$</td>
<td>$\checkmark$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 2)$</td>
<td>$\checkmark$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 0, 0)$</td>
<td>$-$</td>
<td>$\checkmark$</td>
<td>$-$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 0, 1)$</td>
<td>$\Delta$</td>
<td>$\checkmark$</td>
<td>$\checkmark$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 0, 2)$</td>
<td>$\checkmark$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 1, 1)$</td>
<td>$\checkmark$</td>
<td>$\Delta$</td>
<td>$\checkmark$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 1, 2)$</td>
<td>$\checkmark$</td>
<td>$-$</td>
<td>$\checkmark$</td>
</tr>
<tr>
<td>$G(x_i) = (0, 2, 2)$</td>
<td>$\checkmark$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
</tbody>
</table>
Interface Problems

What is the problem caused by complex interfaces?

Numerical Results

Concluding Remarks
Numerical Results

We test for the following complex interfaces:

(I)          (II)          (III)          (IV)
Robustness Test in 2D for (I)

- $\epsilon^- : \epsilon^+ = 2 : 80$
- $\epsilon^- : \epsilon^+ = 1 : 1000$
- $\epsilon^- : \epsilon^+ = 1000 : 1$
Convergence Result in 2D for (I)

(a) Solution

(b) Grad

\[ \log_{10} \| u - u_e \|_\infty \]

\[ \log_{10} \| \nabla u - \nabla u_e \|_\infty \]

- Solution
  - slope = -2.37

- Gradient
  - slope = -1.88
Robustness Result in 2D for (II)
Convergence Result in 2D for (II)

<table>
<thead>
<tr>
<th>mesh</th>
<th>$|\nabla u - \nabla u_e|_{\infty, r}$ gradient</th>
<th>order</th>
<th>$|u - u_e|_{\infty}$ solution</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/320</td>
<td>1.63E-04</td>
<td></td>
<td>2.99E-06</td>
<td></td>
</tr>
<tr>
<td>1/640</td>
<td>3.26E-05</td>
<td>2.32</td>
<td>6.85E-07</td>
<td>2.13</td>
</tr>
<tr>
<td>1/1280</td>
<td>8.29E-06</td>
<td>1.97</td>
<td>1.78E-07</td>
<td>1.94</td>
</tr>
</tbody>
</table>
Convergence of Solution for (III)
Convergence of Gradient for (III)
Convergence Result for (IV)
Interface Problems

What is the problem caused by complex interfaces?

Numerical Results

Concluding Remarks
Concluding remarks

For Complex Interfaces
- Improved Coupling Interface is proposed with three recipes: Mesh refinement, Flip domain, and shift approximation
- Second order accuracy for the solution.
- The accuracy for the gradient of the solution is slightly lower than second order.
Thank you for your attention