Finding Efficient and Accurate Ways to Solve Interface Problems

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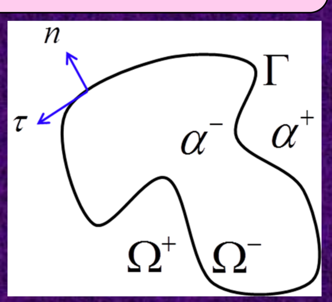
Abstract

Interface problems are a large class of problems that study the change of a physical quantity in Physics, Biology, Engineering, or Materials, such as heat or electrostatic potential, as it propagates across a material interface. Due to the irregularly shaped interface, solutions to interface problems can only be found numerically. However, for the very same reason, classical numerical methods cannot deliver accurate estimations, or may fail entirely. A new numerical method is necessary for solving interface problems efficiently and accurately. In this project, we present our recent study of a well-tuned matched Alternative Direction Implicit (ADI) method for solving two-dimensional interface problems with the most general of physical interface jump conditions. We also plan to present our recent improvements on the efficiency, accuracy, and stability of the proposed method.

Parabolic Interface Problems and Their Applications

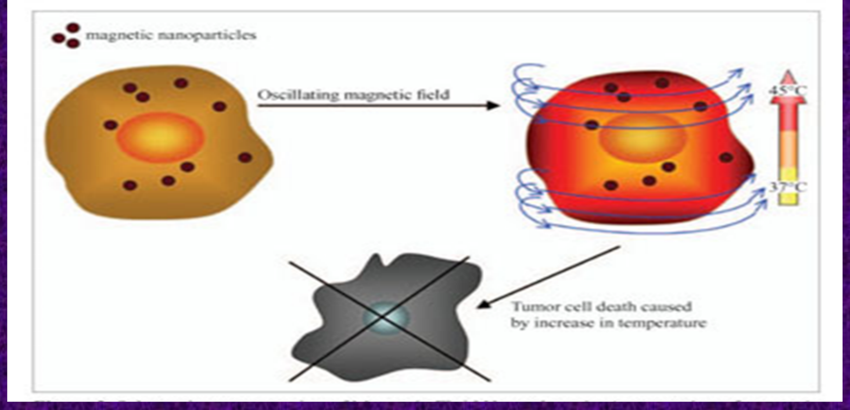
The parabolic interface problems are mathematically described by:



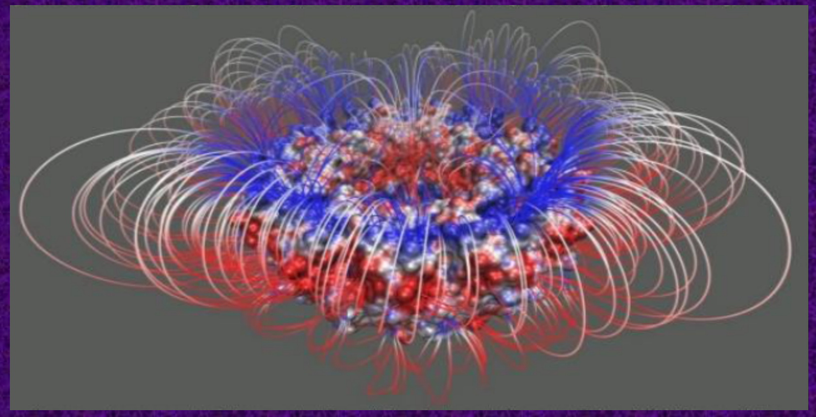
$$\frac{\partial u}{\partial t} = \nabla \cdot (\alpha \nabla u) + f \text{ in } \Omega = \Omega^- \cup \Omega^+ \quad (1)$$

$$[u] = u^+ - u^- = \phi(s,t), [\alpha u_n] = \alpha^+ \frac{\partial u^+}{\partial n} - \alpha^- \frac{\partial u^-}{\partial n} = \psi(s,t). \quad (2)$$

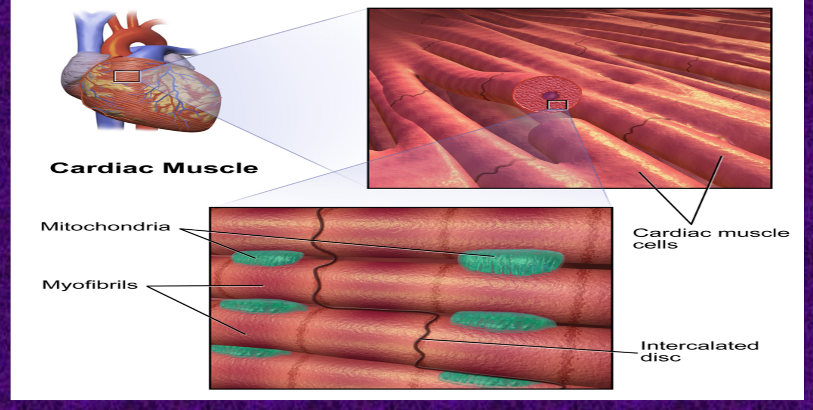
where $u(x,t)$ is a function of interest, α is the diffusion coefficient, and f is a source. Proper boundary conditions are prescribed on $\partial\Omega$. The domain Ω is split into two media Ω^- and Ω^+ by a material interface Γ. Across the interface Γ, the diffusion coefficient α is discontinuous, while the source term f may be even singular.



Penne's Bioheat Equation which is used in Magnetic Hyperthermia, a promising cancer treatment



Poisson-Boltzmann Equation for modeling electrostatic interactions of complicated protein molecules



The **Cable Equation** which is used to model electric potentials in Cardiac muscle cells

A Matched Alternative Direction Implicit Method

- **Temporal Discretization - Douglas ADI scheme**

$$\left(\frac{1}{\alpha} - \Delta t \delta_{xx}\right) u_{i,j}^{*} = \left(\frac{1}{\alpha} + \Delta t \delta_{yy}\right) u_{i,j}^{k} + \frac{\Delta t}{\alpha} f_{i,j}^{k+1}, \quad (3)$$

$$\left(\frac{1}{\alpha} - \Delta t \delta_{yy}\right) u_{i,j}^{k+1} = \frac{1}{\alpha} u_{i,j}^{*} - \Delta t \delta_{yy} u_{i,j}^{k} \quad (4)$$

Δt - time increment δ_{xx}, δ_{yy} - finite difference operators in x- and y- directions

- **Spatial Discretization – Matched Interface and Boundary (MIB) method**
  - Use the standard central difference formula on grids away from the interface

$$\delta_{xx} u_{i,j}^{k} := \frac{1}{h^2}\left(u_{i-1,j}^{k} - 2u_{i,j}^{k} + u_{i+1,j}^{k}\right) \quad (5)$$

$$\delta_{yy} u_{i,j}^{k} := \frac{1}{h^2}\left(u_{i,j-1}^{k} - 2u_{i,j}^{k} + u_{i,j+1}^{k}\right) \quad (6)$$

  - Incorporate the derived jump conditions

$$[\alpha u_x] = \psi cos\theta - sin\theta(\alpha^+ - \alpha^-) \boldsymbol{u_\tau^+} - sin\theta[\alpha^- \phi_\tau] := \bar{\psi} \quad (7)$$

$$[\alpha u_y] = \psi sin\theta + cos\theta(\alpha^+ - \alpha^-) \boldsymbol{u_\tau^+} - cos\theta[\alpha^- \phi_\tau] := \hat{\psi} \quad (8)$$

to correct the central difference formula on grids close to the interface

$$\delta_{xx} u_{i,j}^{k} := \frac{1}{h^2}\left(\tilde{u}_{i-1,j}^{k} - 2u_{i,j}^{k} + u_{i+1,j}^{k}\right) \text{ or } \delta_{xx} u_{i,j}^{k} := \frac{1}{h^2}\left(u_{i-1,j}^{k} - 2u_{i,j}^{k} + \tilde{u}_{i+1,j}^{k}\right) \quad (9)$$

$$\delta_{yy} u_{i,j}^{k} := \frac{1}{h^2}\left(\tilde{u}_{i,j-1}^{k} - 2u_{i,j}^{k} + u_{i,j+1}^{k}\right) \text{ or } \delta_{yy} u_{i,j}^{k} := \frac{1}{h^2}\left(u_{i,j-1}^{k} - 2u_{i,j}^{k} + \tilde{u}_{i,j+1}^{k}\right) \quad (10)$$

where $\tilde{u}_{i,j}^{k+1}$ and $\tilde{u}_{i,j+1}^{k+1}$ are additional "fictitious values" on grids.

- **u_τ^+ Approximation**

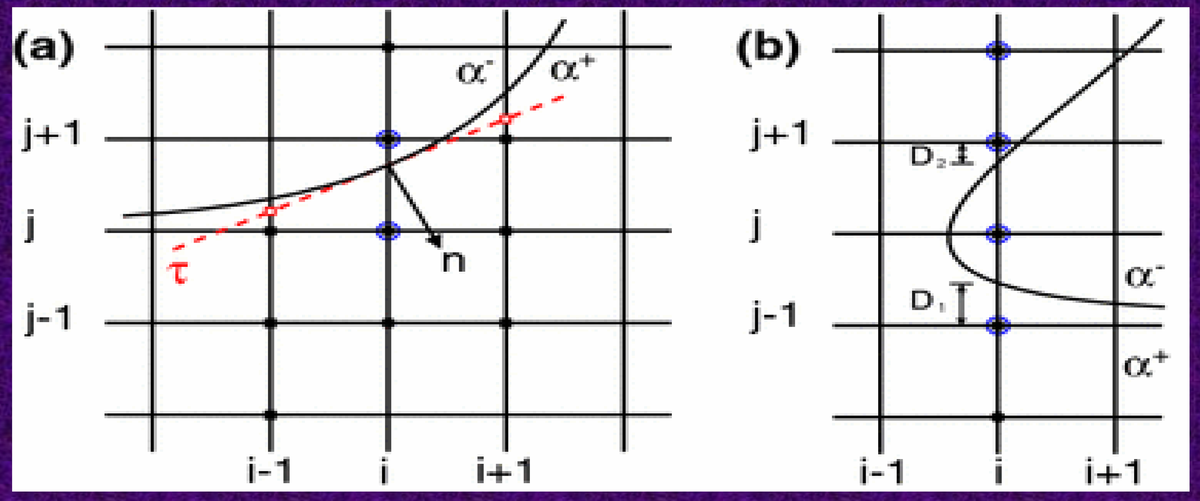
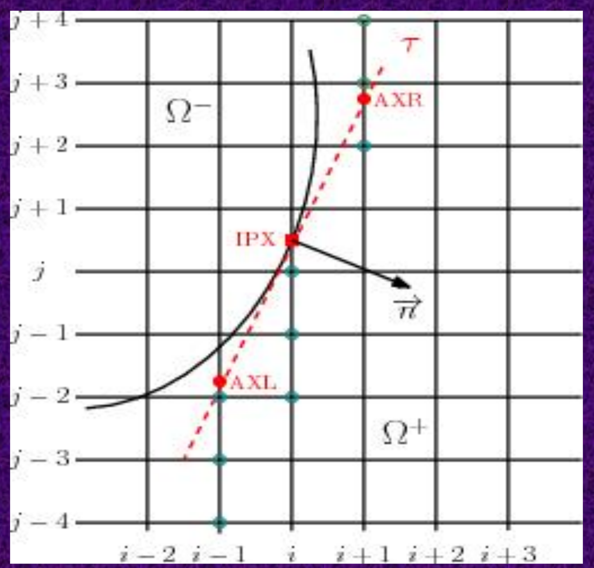
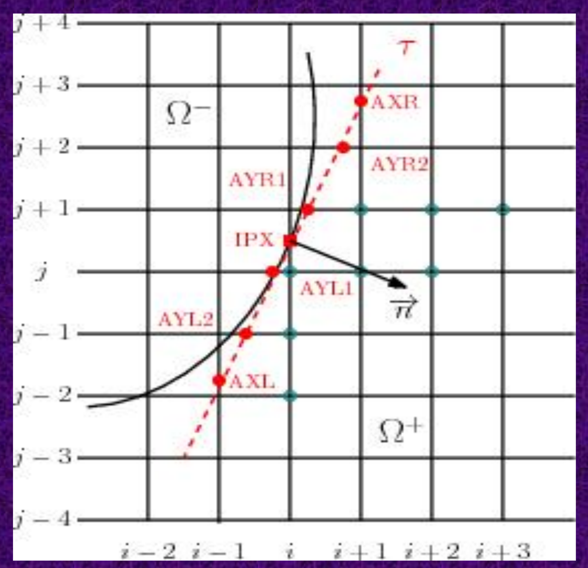
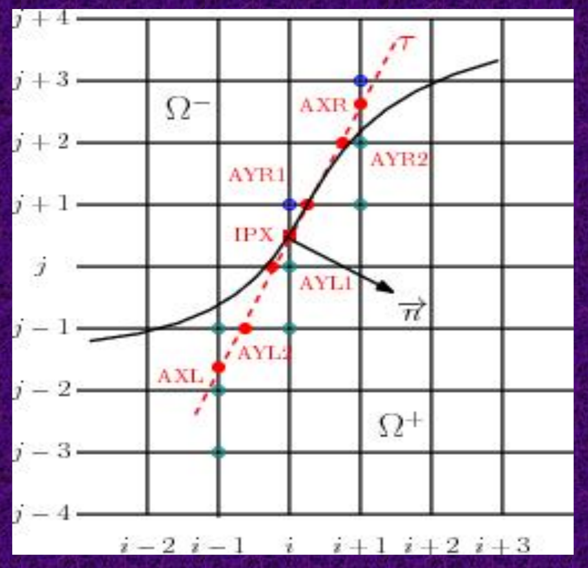


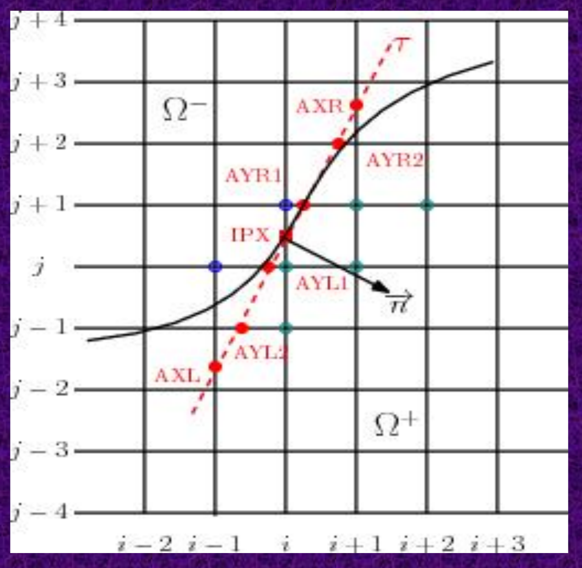
Illustration of the MIB grid partitions. **(a)** For a regular interface. **(b)** For a corner point. In both figures, the jump conditions will be discretized by using fictitious (**open circles**) and function values (**filled circles**). In (a), the approximation of u_τ^+ is also shown, i.e., it is approximated by two auxiliary values (**open squares**), then interpolated by six function values (**filled squares**).

- **Recent Improvements**
  a) Improve the temporal discretization formula by including the Peaceman-Rachford ADI method along with the Douglas ADI method.
  b) Improve the approximation of u_τ^+ by using additional auxiliary points in the y direction
  c) Make spatial approximations in both Ω^+ and Ω^- by utilizing u_τ^- in addition to u_τ^+.

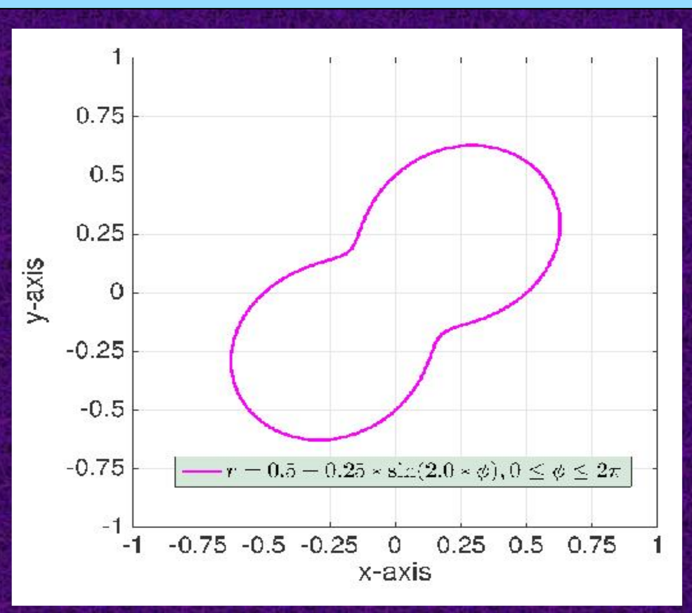


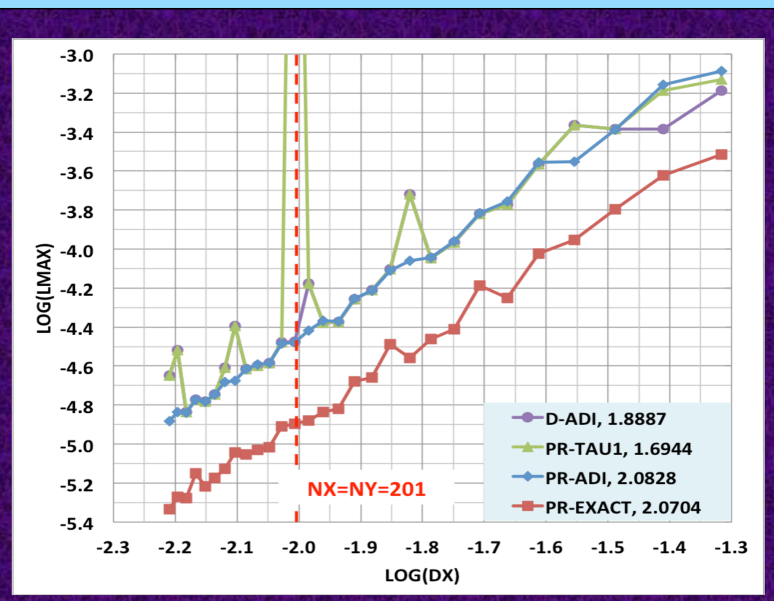


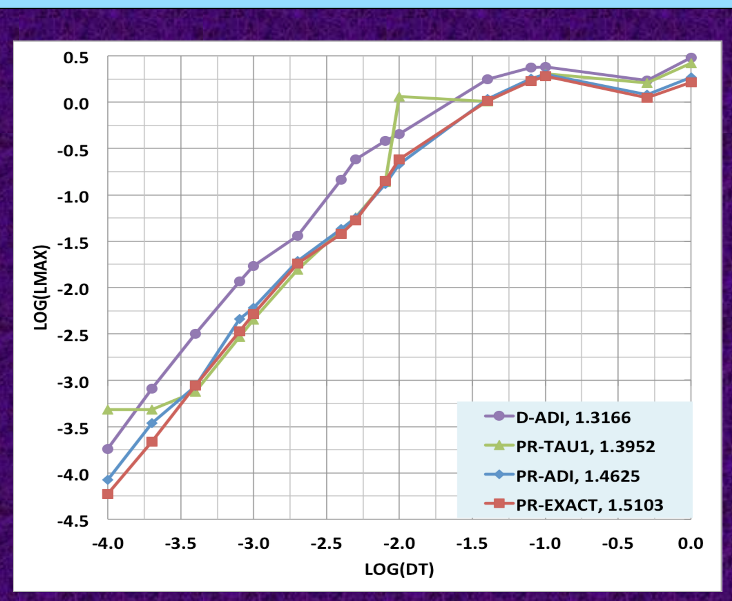


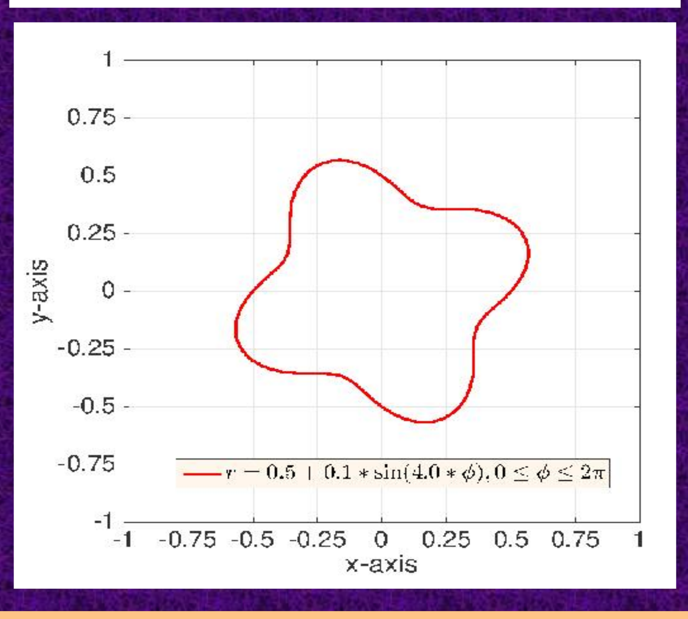


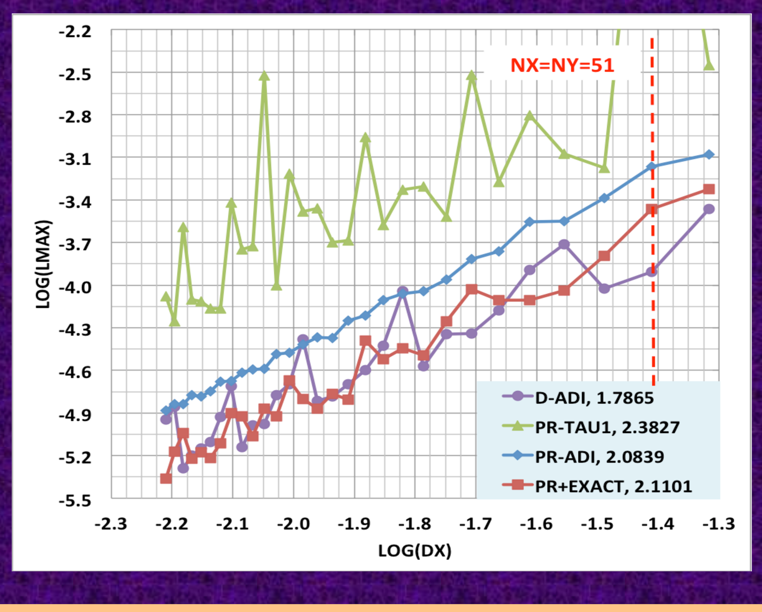
Numerical Experiments

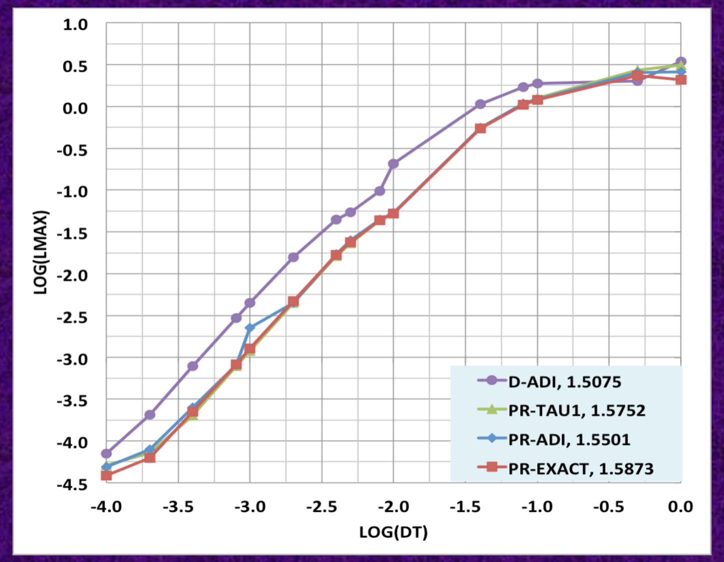












References

[1] Zhao S. (2015) A Matched Alternating Direction Implicit (ADI) Method for Solving the Heat Equation with Interfaces. Journal of Scientific Computing (2015) 63: 118. doi:10.1007/s10915-014-9887-0

[2] Li C. and Zhao S. (2016) A Matched Peaceman Rachford ADI Method for Solving Parabolic Interface Problems. Journal of Applied Mathematics and Computation. Accepted.

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