Adaptive Mesh Refinement for the Smoothed Boundary Method

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Introduction

Simulating diffusion through **complex geometries** is a difficult task, especially at a **sharp interface**. Therefore, implementing a smoothed boundary method **(SBM)** to the **diffusion equation** allows a **straightforward simulation.** To further **improve numerical accuracy,** an adaptive mesh refinement **(AMR)** algorithm is incorporated to create **refined** grid points at the interface, and **coarser** grid points everywhere else.

Objective

- Simulate diffusion through a simple geometry with both a sharp and diffuse interface along with a uniform mesh grid and an AMR
- Compare the diffusion results against the sharp interface to determine the accuracy of the SBM and AMR implementation
- Simulate diffusion through a complex geometry incorporating the SBM and an AMR

Methods

2D Diffusion Equation:

$$\frac{\partial C}{\partial t} = D\nabla^2 C = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$

2D Discretization:

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D\left(\frac{C_{i-1,j}^{n} - 2C_{i,j}^{n} + C_{i+1,j}^{n}}{\Delta x^2} + \frac{C_{i,j-1}^{n} - 2C_{i,j}^{n} + C_{i,j+1}^{n}}{\Delta y^2}\right)$$

Smoothed Boundary Method:

$$\frac{\partial C}{\partial t} = \frac{1}{\psi}\nabla \cdot (\psi D \nabla C)$$

1D Discretization:

$$\frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta t} = \frac{D}{\psi_i^n} * \frac{\left(\frac{C_{i+1}^{n} - C_{i}^{n}}{\Delta x} * \frac{\psi_{i+1}^{n} + \psi_{i}^{n}}{2}\right) - \left(\frac{C_{i}^{n} - C_{i-1}^{n}}{\Delta x} * \frac{\psi_{i-1}^{n} + \psi_{i}^{n}}{2}\right)}{\Delta x}$$

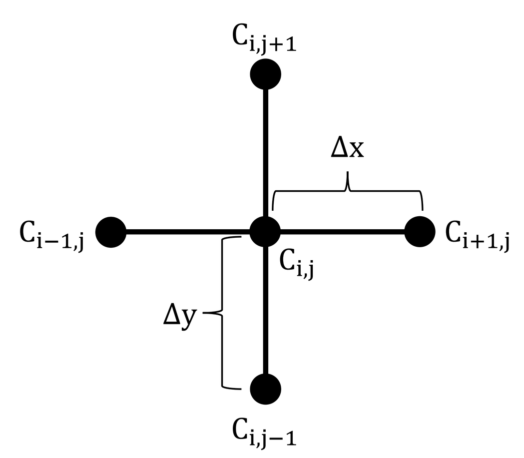

Fig. 1: Finite Difference Scheme

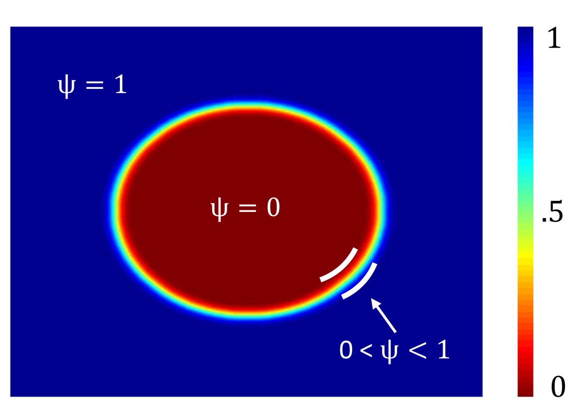

Fig. 2: Smoothed/Diffuse Boundary

Adaptive Mesh Refinement:

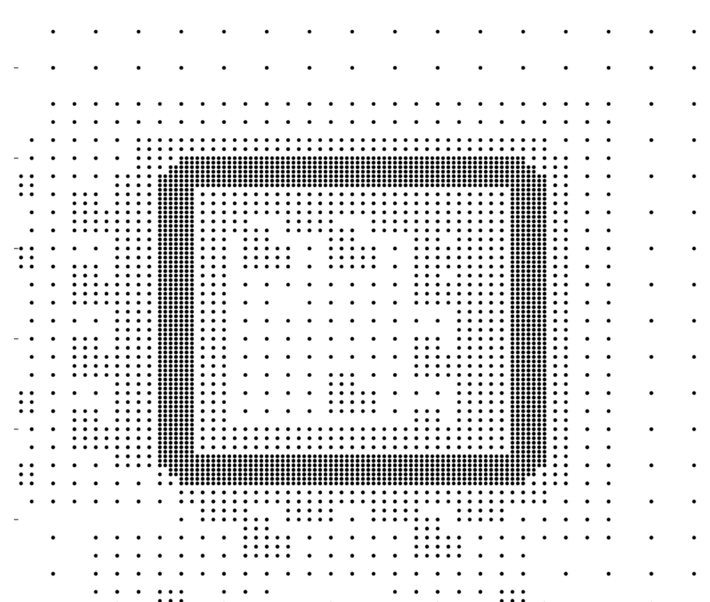

Fig. 3: AMR for a simple geometry

Starting with a refined grid, coarsening occurs everywhere except at the interface of the geometry. Coarsening depends on psi (ψ). A restriction was made to ensure that each point does not have neighbors which are too coarse; therefore, the finite difference scheme can be easily implemented.

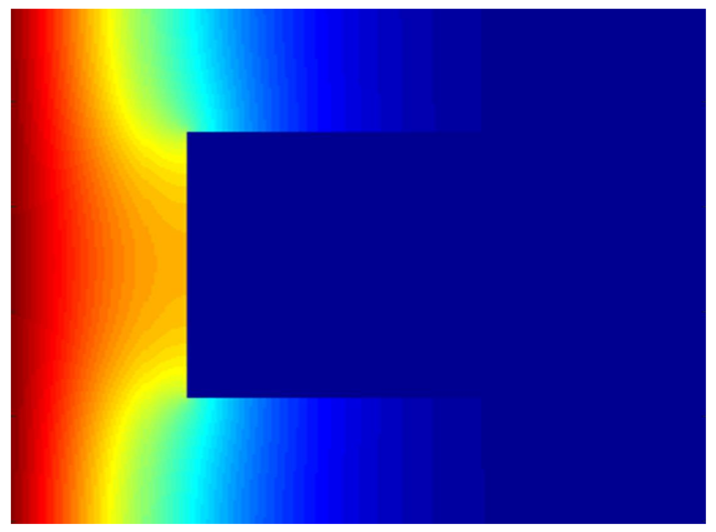

Fig. 4: Sharp Interface Diffusion

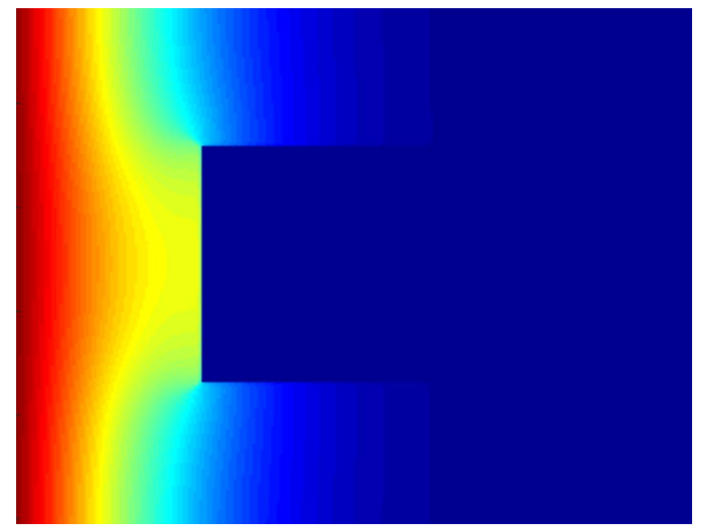

Fig. 5: Diffuse Interface SBM Diffusion

The figures above showcase diffusion through a simple geometry with a uniform grid after 10 seconds. A constant injection of concentration was imposed on the left side. Figure 4's interface is sharp and contains No-Flux boundary conditions around the interface. Figure 5's interface is smoothed and the SBM was implemented, replacing the No-Flux boundary condition.

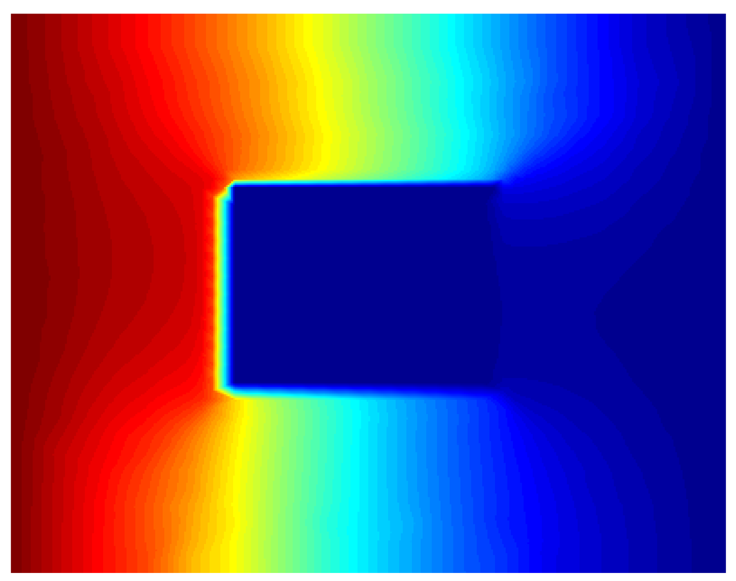

Fig. 6: Diffuse Interface AMR & SBM Diffusion

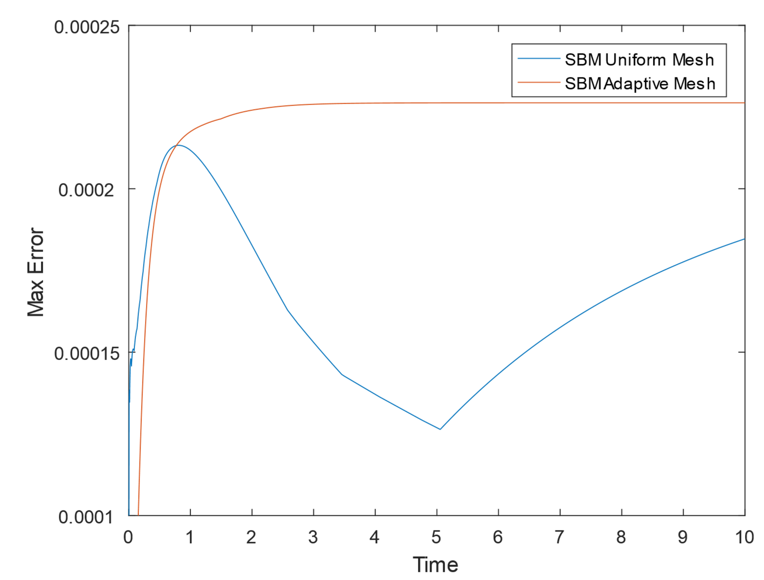

Fig. 7: Error in Diffusion

Figure 6 displays diffusion through a simple geometry using a smoothed boundary at the interface and an adaptive mesh refinement grid shown in Figure 3. Figure 7 compares the difference in concentration values over time from Figures 5 and 6 with the sharp interface diffusion from Figure 4.

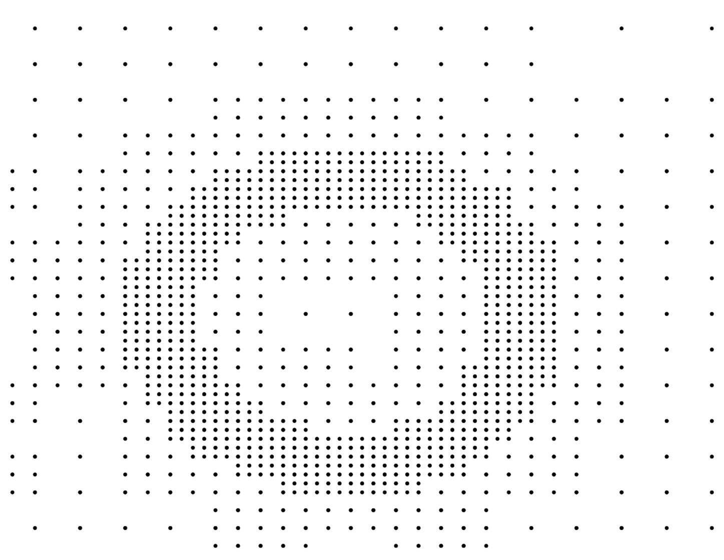

Fig. 8: AMR for a complex geometry

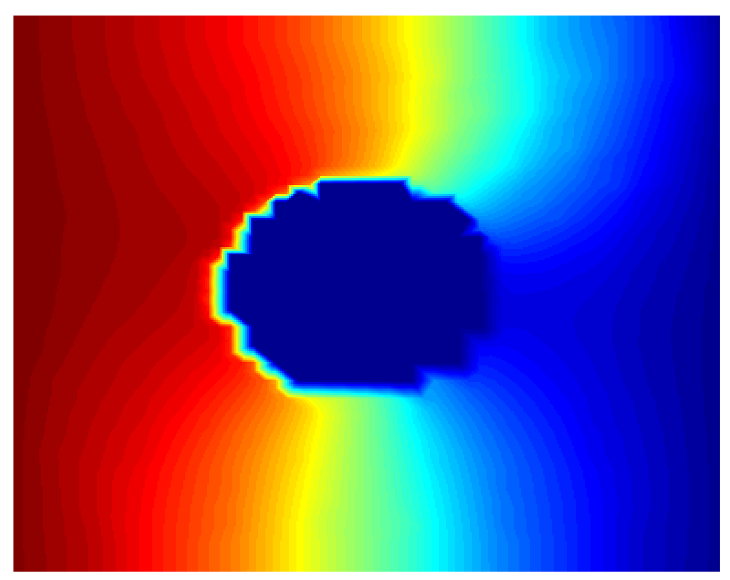

Fig. 9: Diffusion through a complex geometry

With the implementation of a SBM and an AMR, diffusion through a complex geometry can be modeled, as shown in Figure 9. The adaptive mesh refinement used for the complex geometry can be seen in Figure 8.

Discussion

For the simple geometry example, three separate diffusion simulations were ran. The base case occurred in Figure 4, where the interface of the square was sharp and no SBM was applied. The other two simulations, both with a SBM applied and one with an AMR were compared against the base case; Figure 7 displays those results.

At the beginning of the diffusion, the errors are very little because the interface has not been contacted. However, the error continues to rise as the diffusion reaches and hits the interface. This is due to the SBM implementation slightly changing the diffusion.

The AMR diffusion in both the simple and complex geometry cases is not exactly symmetrical and requires further examination to provide a more accurate simulation, thus affecting the error results.

Conclusion

Through the use of creating an adaptive mesh refinement algorithm and applying the smoothed-boundary method to the diffusion equation, simulation of diffusion through a complex geometry was achieved. To compare the accuracy of the methods incorporated, simulations of diffusion through a simple geometry were compared.

Running the simulations on a larger scale in both size and time would contribute to further information for the implementation of the SBM and AMR on complex geometries.

For the future, the SBM and AMR techniques will ultimately be used to simulate the diffusion process in a battery electrode, which contains complicated geometries.

Acknowledgements

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