

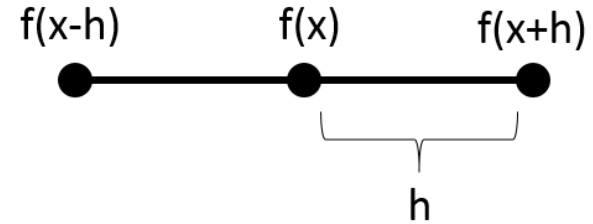
Adaptive Mesh Refinement for the Smoothed Boundary Method

Kendell Crowley, Kieran Fitzmaurice,
Mentor: Dr. Hui-Chia Yu

First and Foremost: Finite Difference Method

- Entire basis used for the numerical solution of differential equations.

Derived from a Taylor Series, the first and second derivatives can be approximated (in 1D):



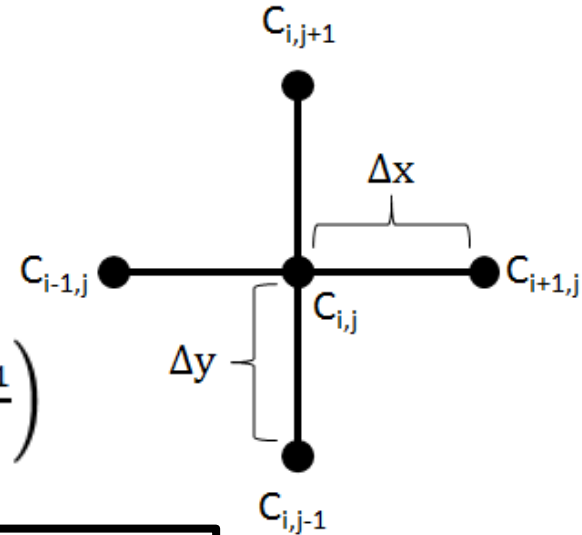
First Derivative: $f'(x)$	$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$
Second Derivative: $f''(x)$	$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$

Example: Diffusion Partial Differential Equation in 2D

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

Discretization:

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

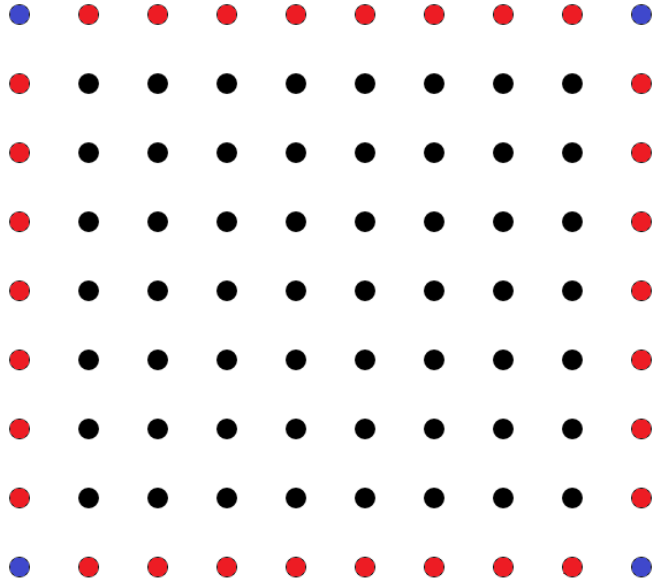


Ultimately comes down to:

New Concentration = Old Concentration + time_step * change

Note: Concentration depends on its neighbors!

Issues: Boundary Conditions



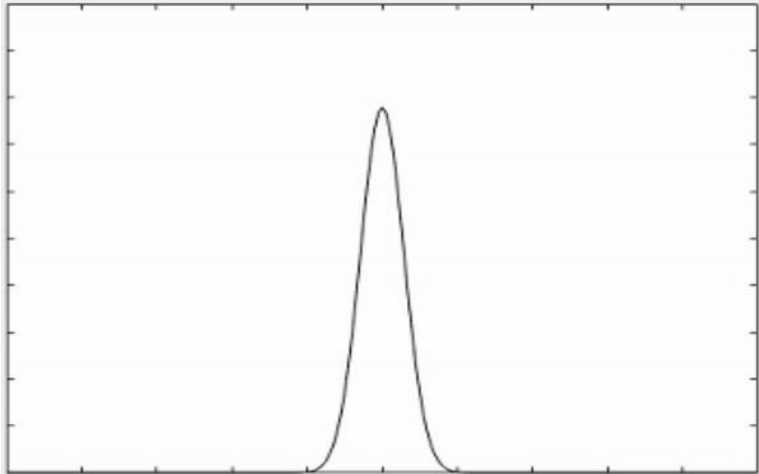
Black points have 4 neighbors

Others have 3 or less

Solution: Ghost Points

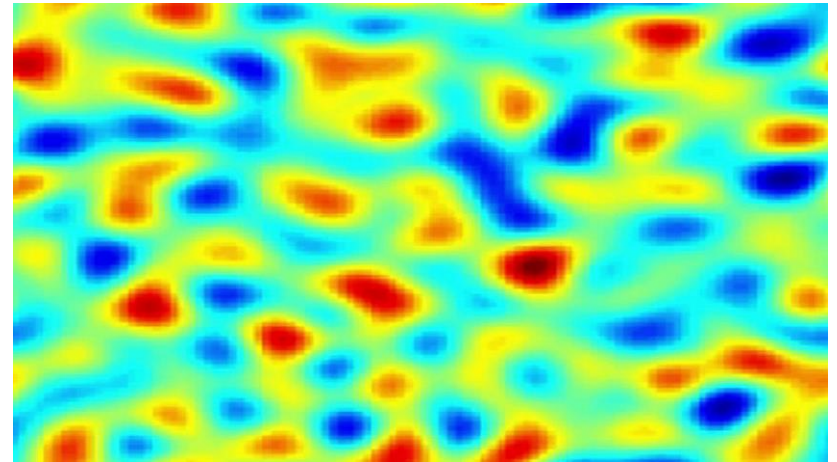
Diffusion Equation (1D)

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$



Cahn-Hilliard Phase Field Model (2D)

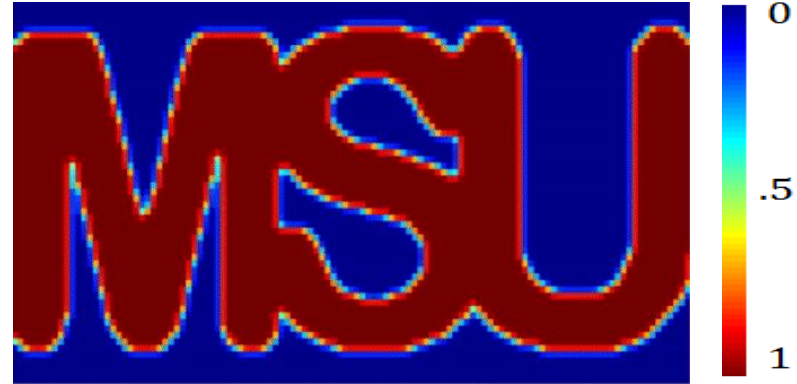
$$\frac{\partial C}{\partial t} = M \nabla^2 \left(\frac{W}{2} c(1-c)(1-2c) - \varepsilon^2 \nabla^2 c \right)$$



Smoothed Boundary Method

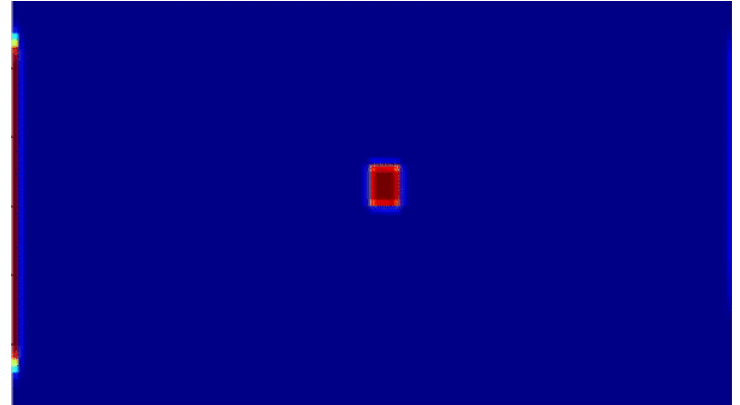
MSU

Diffusion Smoothing
(Continuous Function)



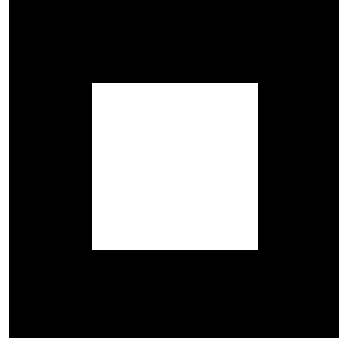
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$$\frac{\partial C}{\partial t} = \frac{1}{\psi} \nabla \cdot (\psi D \nabla C)$$

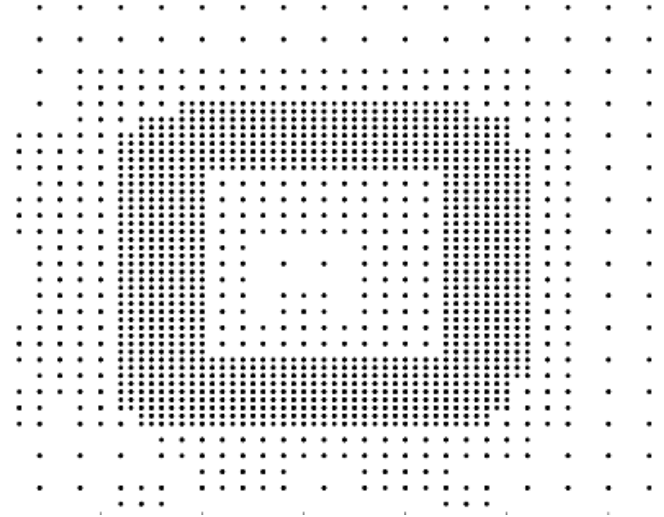
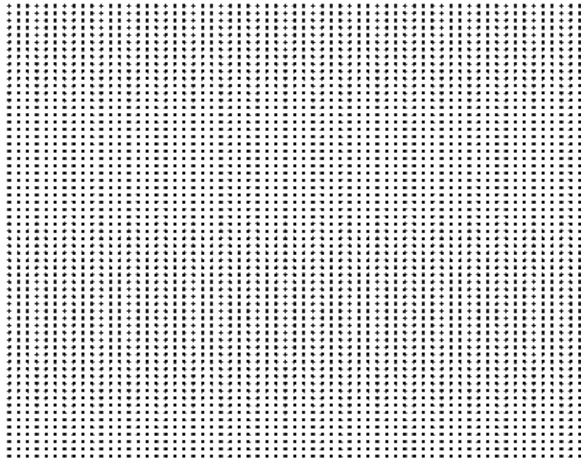


Adaptive Mesh Refinement Algorithm

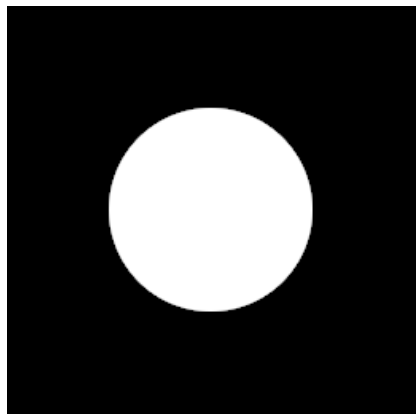
Bottom-Up Approach



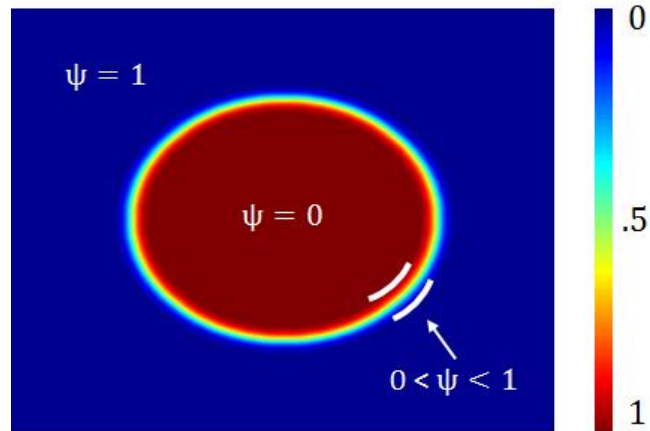
Focuses grid points on the interface of geometry



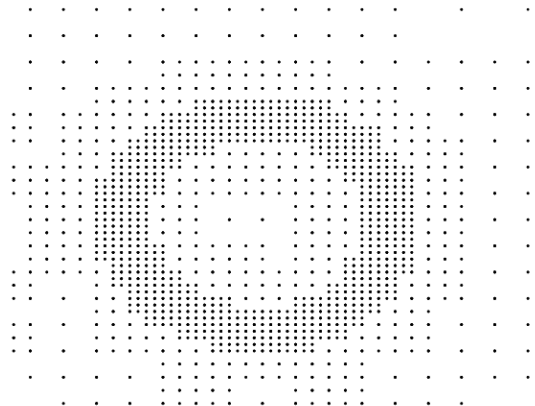
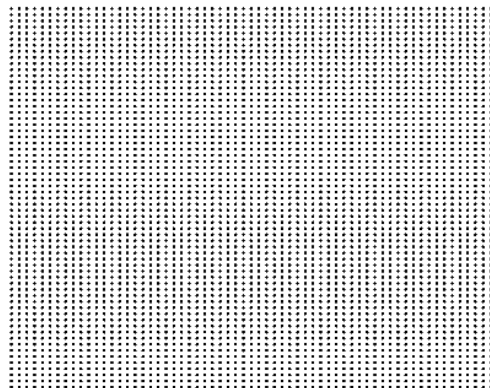
Bottom-Up Approach



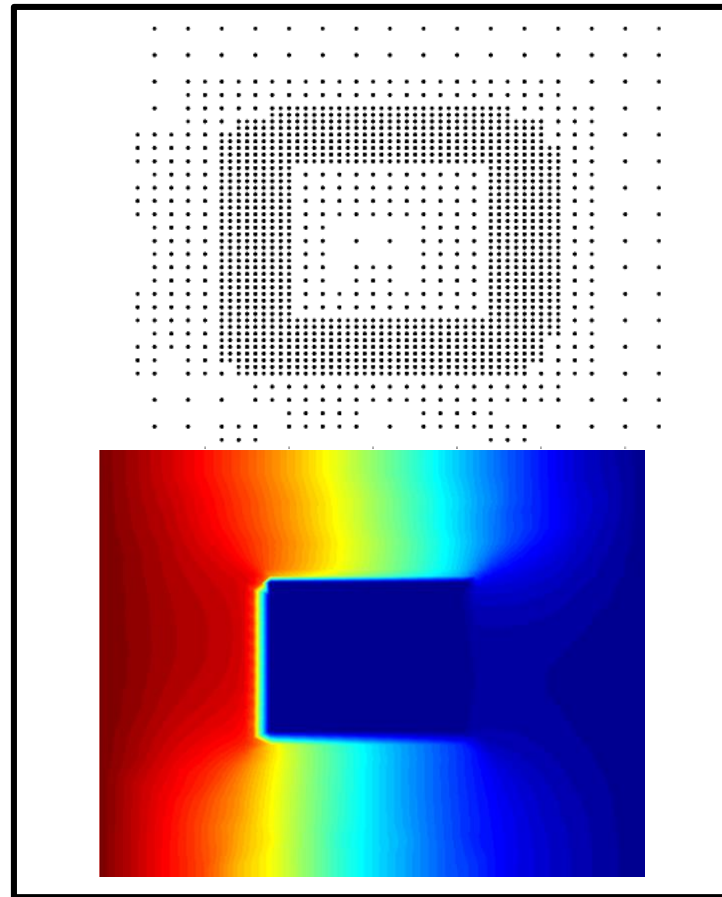
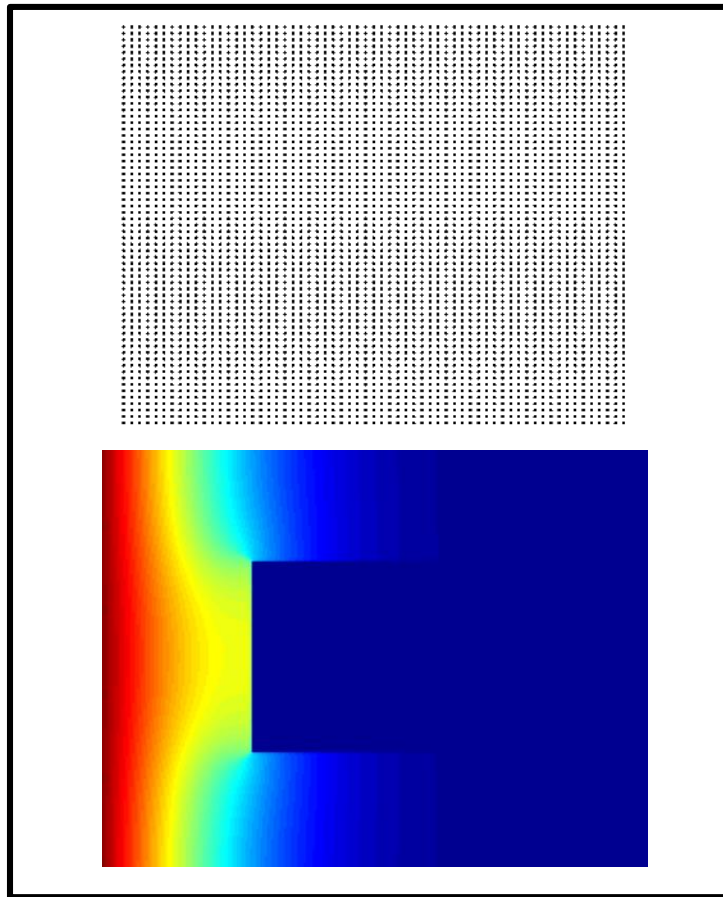
Diffusion Smoothing



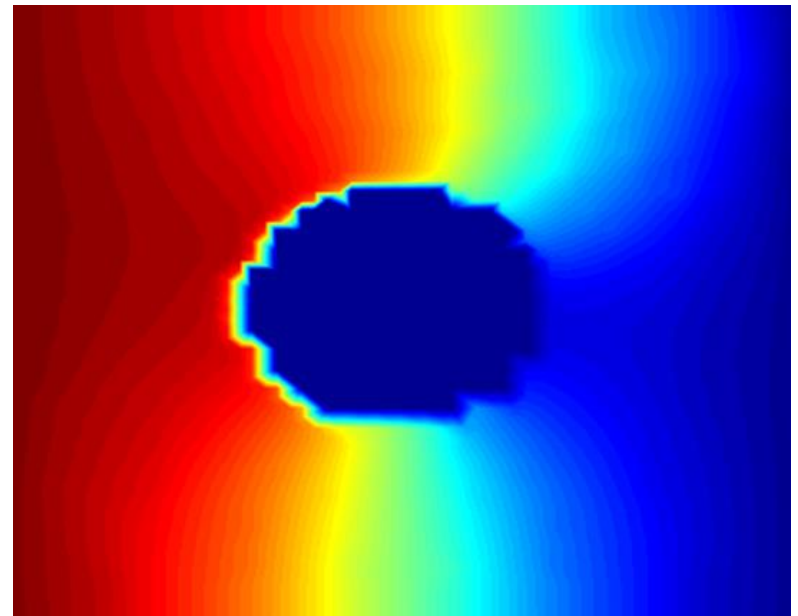
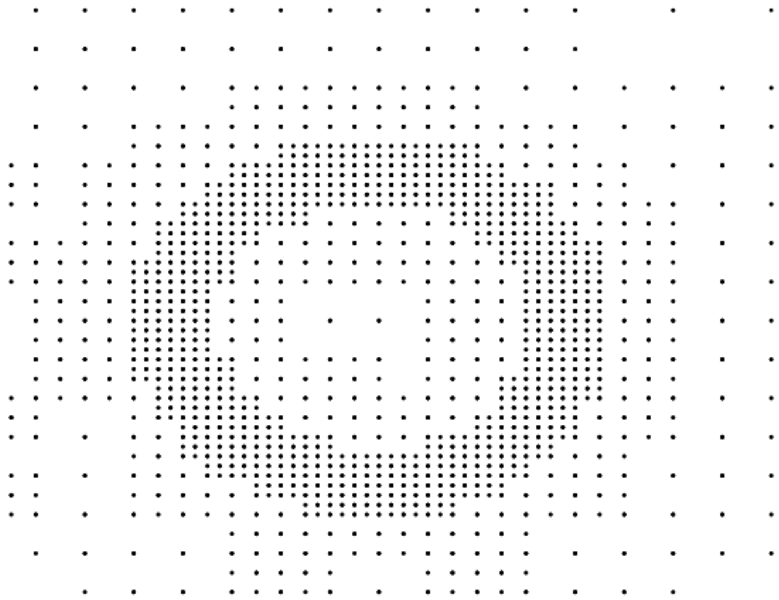
$$|\nabla\psi|$$



Simple Geometry Case



Applying the Smoothed Boundary Method and Adaptive Mesh Refinement allows simulation of diffusion through complex geometries.



Future:

- The SBM and AMR techniques will ultimately be used to simulate the diffusion process in a battery electrode, which contains complicated geometries.
- Run simulations on a larger scale
- 3D simulations

