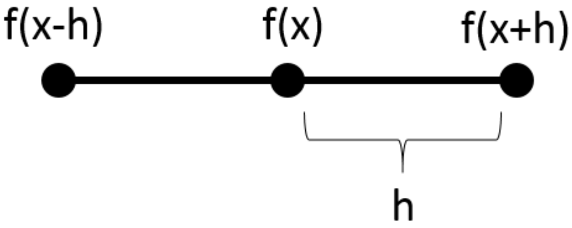
Adaptive Mesh Refinement for the Smoothed Boundary Method

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.

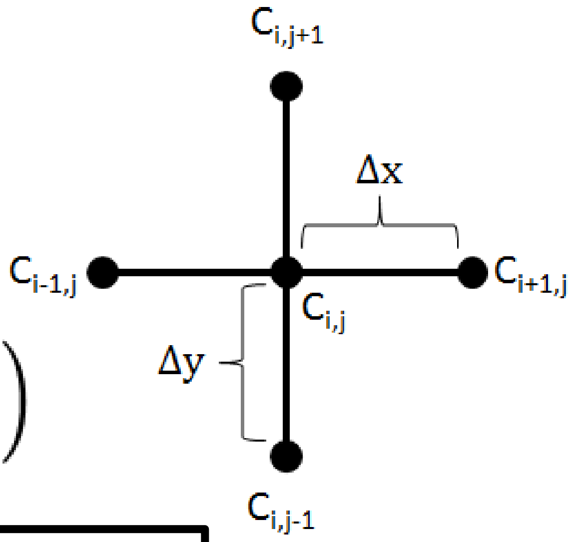
Derived from a Taylor Series, the first and second derivatives can be approximated (in 1D):



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

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:

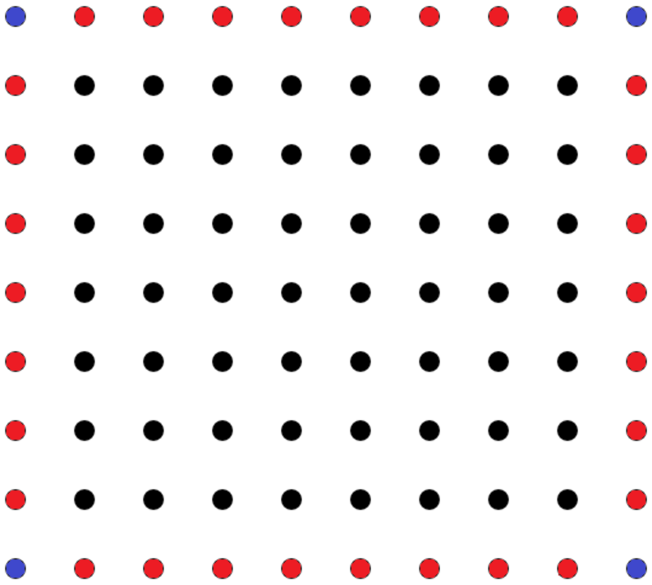
$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D\left(\frac{C_{i-1,j}^{n} - 2C_{i,j}^{n} + C_{i+1,j}^{n}}{\Delta x^2} + \frac{C_{i,j-1}^{n} - 2C_{i,j}^{n} + C_{i,j+1}^{n}}{\Delta y^2}\right)$$

Ultimately comes down to:

New Concentration = Old Concentration + time_step*change

Note: Concentration depends on its neighbors!

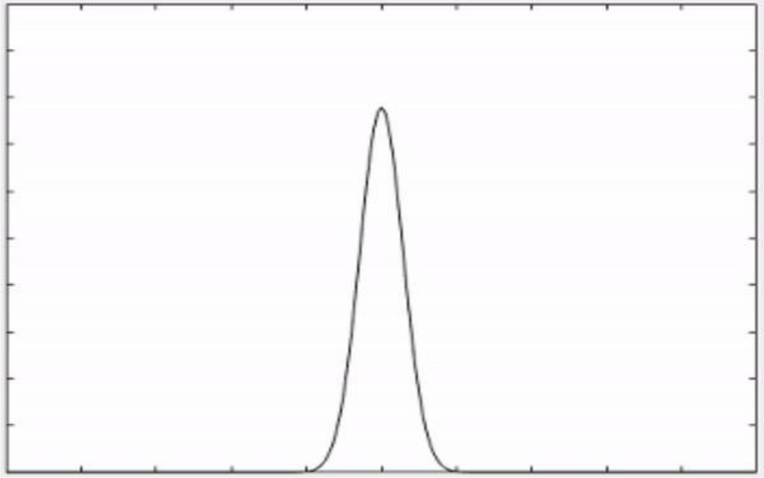
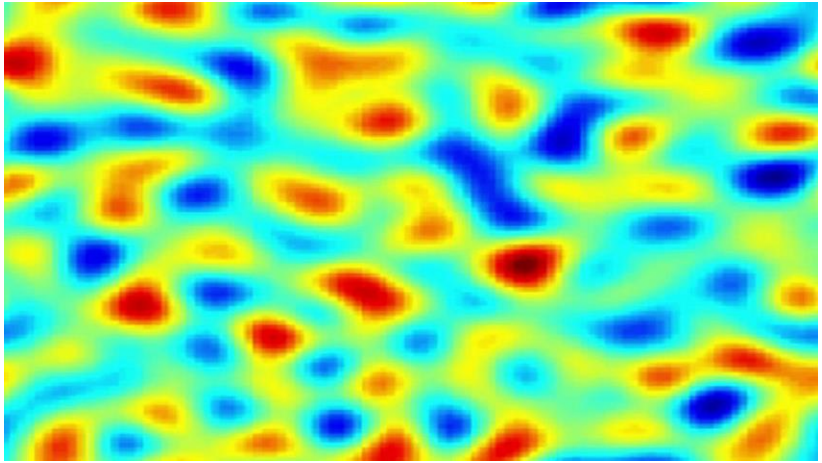
Issues: Boundary Conditions



Black points have 4 neighbors

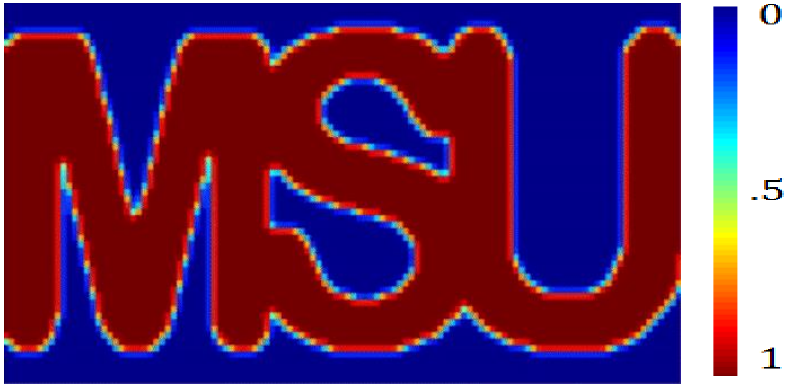
Others have 3 or less

Solution: Ghost Points

Diffusion Equation (1D)	Cahn-Hilliard Phase Field Model (2D)
$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$	$$\frac{\partial C}{\partial t} = M\nabla^2\left(\frac{W}{2}c(1-c)(1-2c) - \varepsilon^2\nabla^2 c\right)$$
	

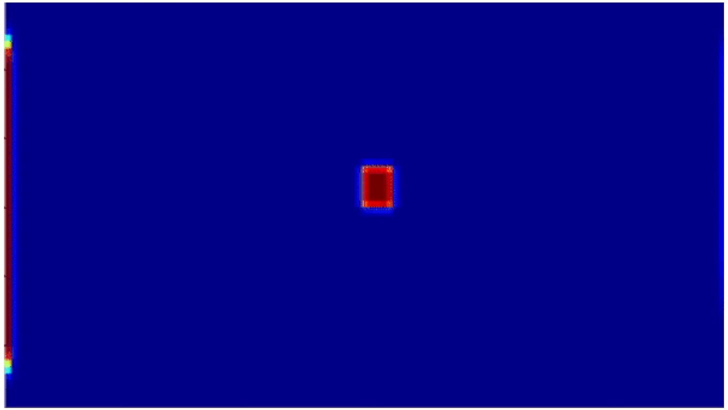
Smoothed Boundary Method

Diffusion Smoothing
(Continuous Function)

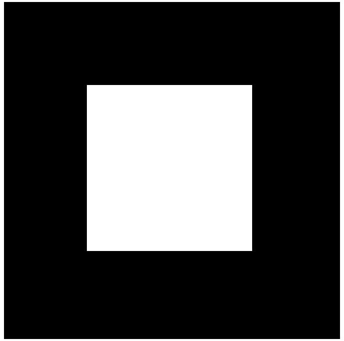


ψ

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

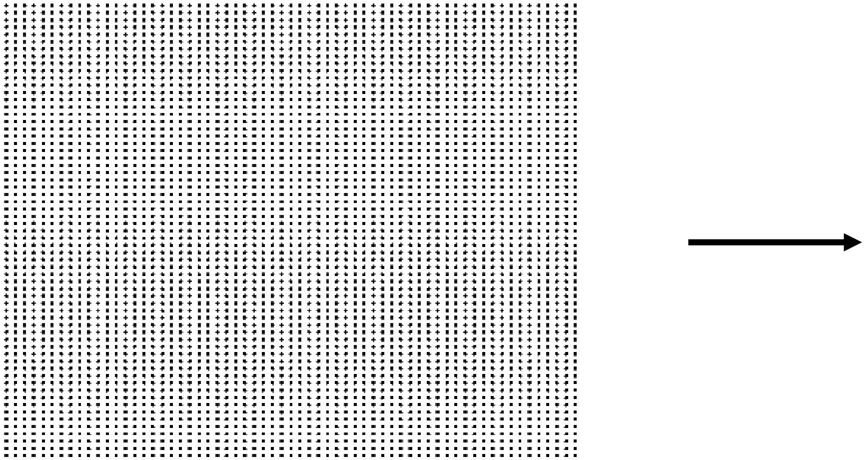


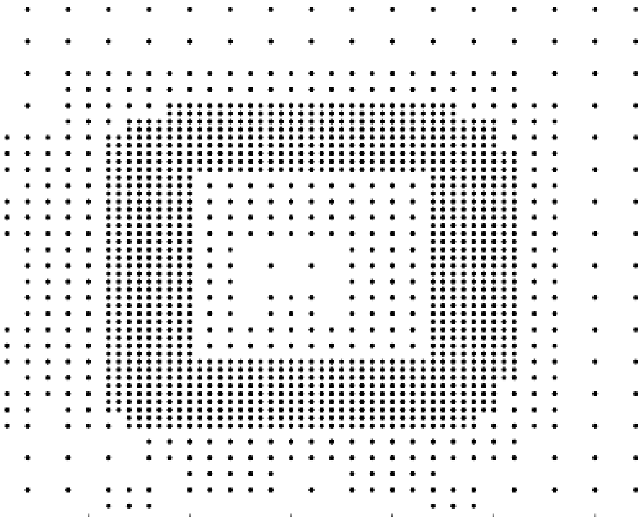
Adaptive Mesh Refinement Algorithm



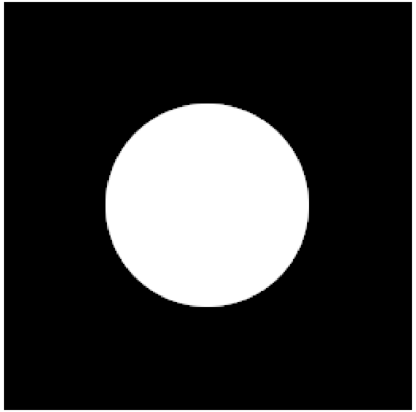
Bottom-Up Approach

Focuses grid points on
the interface of geometry

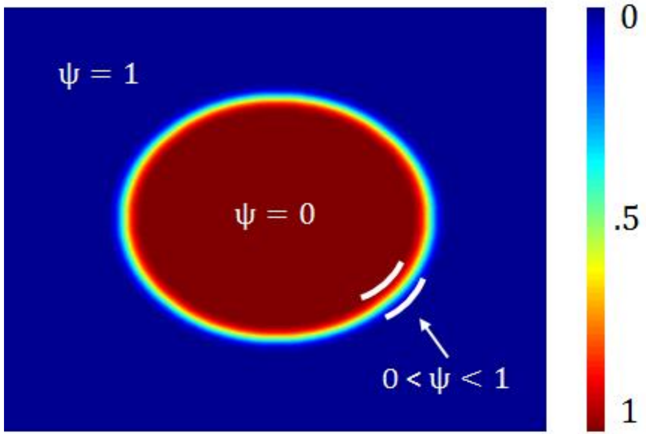




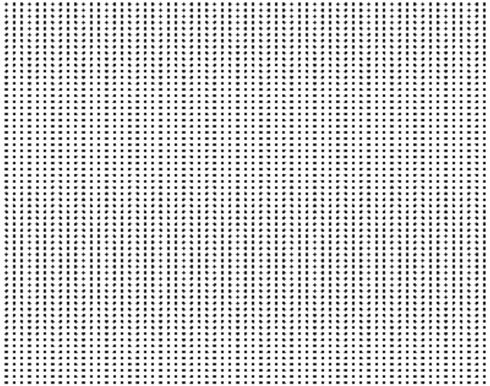
Bottom-Up Approach

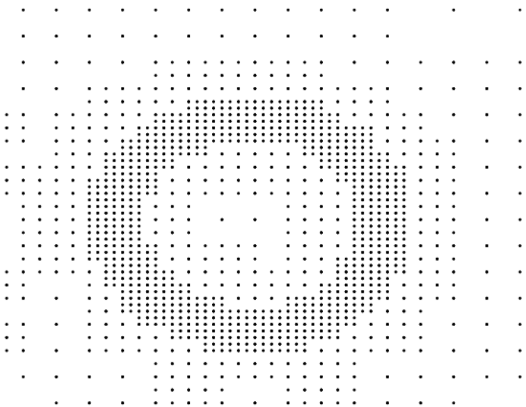


Diffusion Smoothing

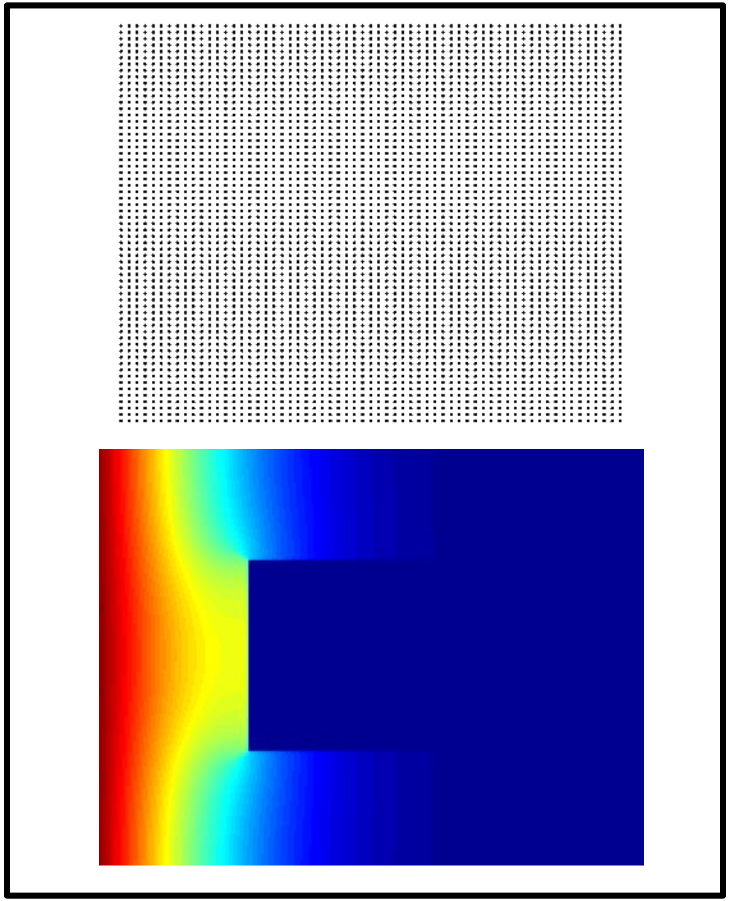


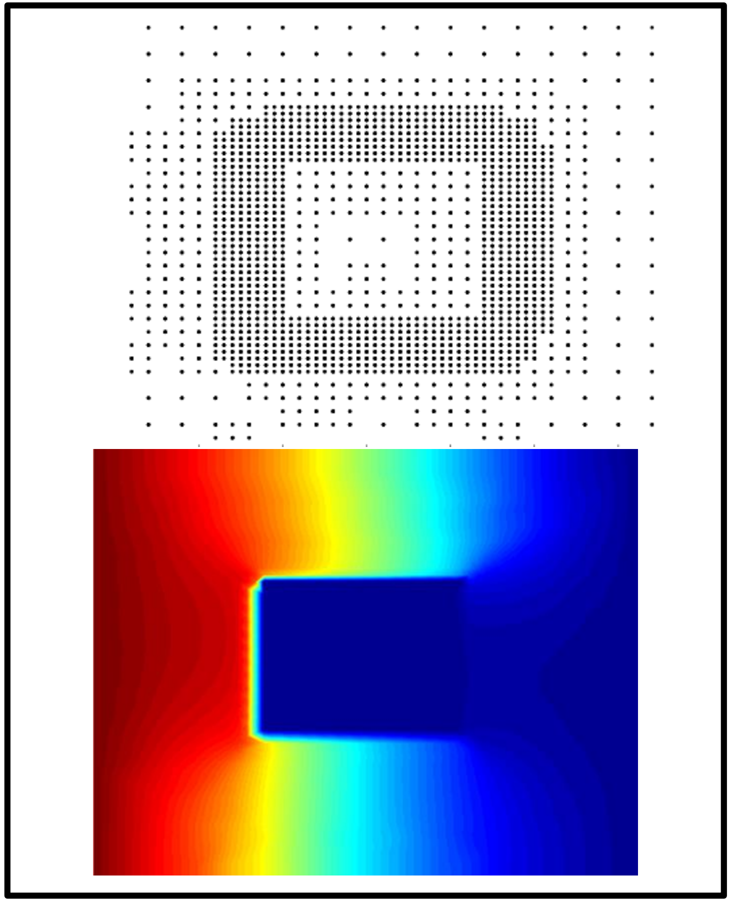
$$|\nabla\psi|$$



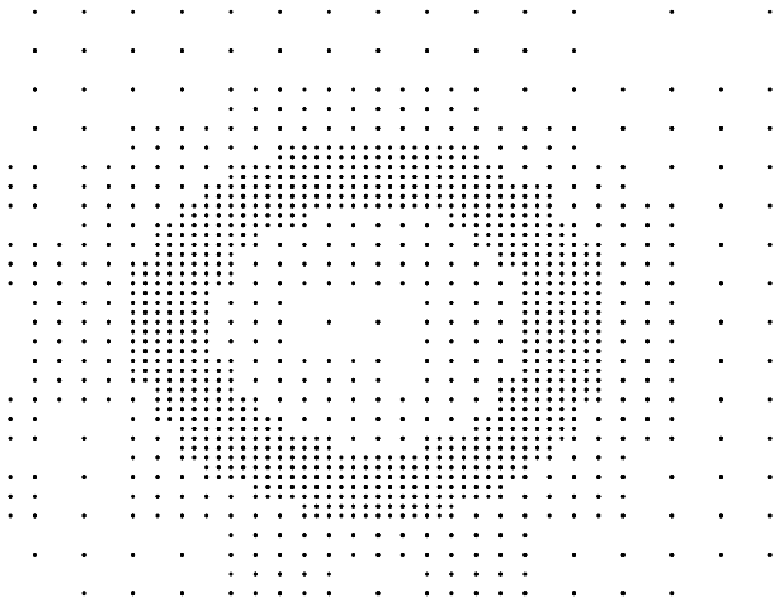


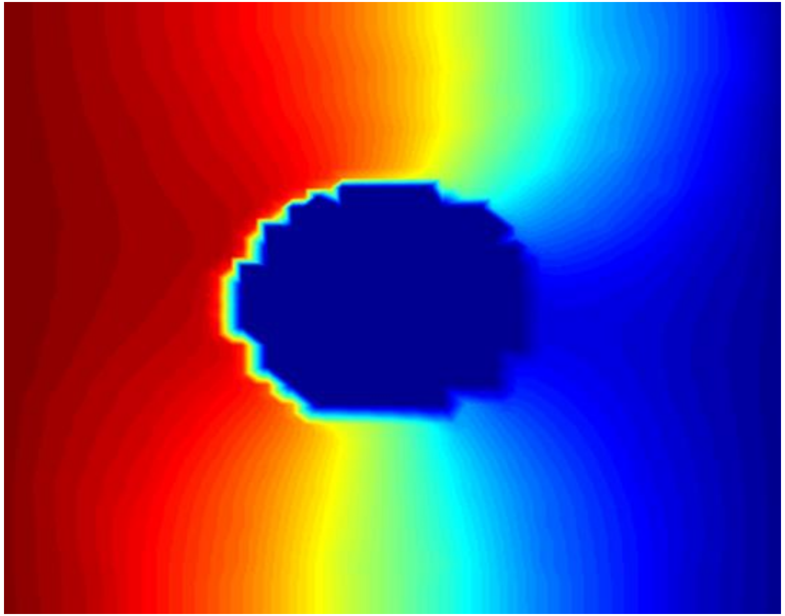
Simple Geometry Case





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