Completing Preparations for esPIC

(1) Very quick: Connections between voltage and temperature equations

(2) A careful look at the nonlinear system

(3) "Nonlinear Lagging"

(4) Assigning ions in each cell: Computing Qval

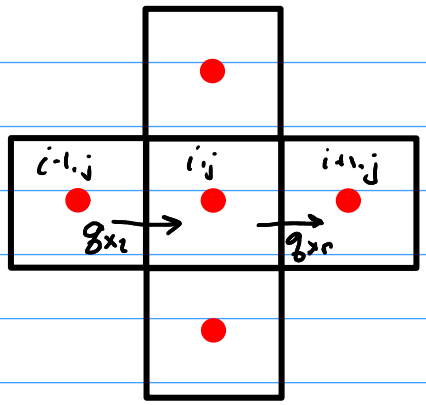
(5) Computing forces on each particle

(6) Sparse matrix format

(7) Neumann Boundary Conditions

(8) In-Class Code development: Sparse matrix, Neumann BCs, Qval, Forces

Voltage Equation is like the Temperature Equation



$$k\left(\frac{T_{i-1,j} - T_{i,j}}{\Delta x}\right) = q_{x_l}$$

$$k\left(\frac{T_{i,j} - T_{i+1,j}}{\Delta x}\right) = q_{x_r}$$

$$= q_{y_b}$$

$$= q_{y_t}$$

$$\frac{q_{x_l} - q_{x_r}}{\Delta x} + \frac{q_{y_b} - q_{y_t}}{\Delta y} = 0$$

$\underset{\sim}{q}$ is a vector

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0$$

Divergence of q: $\underset{\sim}{\nabla} \cdot \underset{\sim}{q} = 0$

Fourier's Law: $\underset{\sim}{q} = -\underset{\sim}{\nabla} T$

$$\nabla^2 T = 0$$

$\underset{\sim}{\nabla} \cdot \underset{\sim}{E} = \rho/\varepsilon$

$\underset{\sim}{E} = -\underset{\sim}{\nabla} V$

$\nabla^2 V = -\rho/\varepsilon$

LaplacianOnGrid...but RHS not zero anymore.

A Careful Look at this week's Nonlinear System

Our System: $\nabla^2 V = a n_i + b e^{cV}$ ← Voltage

↑ Number of ions

Neglect the ions, just for now: $\nabla^2 V = b e^{cV}$

$\nabla^2 \phi = b e^{c\phi}$

Approximate phi(x,y) using a finite difference mesh that has discrete values: $\phi_1, \phi_2, \ldots, \phi_{nField}$

Approximate the continuous phi with a bunch points:

$$\begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{nField} \end{bmatrix} = \underset{\sim}{\phi}$$

For the temperature equation, we solved this system:

$$\underset{\sim}{A}\,\underset{\sim}{\phi} = \underset{\sim}{b}$$

$$\underset{\sim}{A}\,\underset{\sim}{\phi} = \begin{bmatrix} BC \\ BC \\ \vdots \\ BC \\ 0 \\ 0 \\ 0 \\ \vdots \\ BC \end{bmatrix}$$

Our nonlinear system will have a non-zero right-hand side:

$$\underset{\sim}{A}\,\underset{\sim}{\phi} = \begin{bmatrix} BC \\ BC \\ \vdots \\ Qval_0 \\ Qval_1 \\ \vdots \\ Qval_n \\ BC \\ BC \end{bmatrix}$$

In our simplified system, Qval = $b e^{c\phi}$

$$\underset{\sim}{A}\,\underset{\sim}{\phi} = \underset{\sim}{b}(\underset{\sim}{\phi})$$

Nonlinear Lagging

We will be solving a transient problem...transient because the particles are moving transiently. Phi will adjust immediately (no time derivative in the phi equation). But the ni term will be changing with time.

↑ particle motion

- For time = 0 to endTime

  Compute the particle motion

  Update particle positions

  Form this system: current time step, previous time step

$$A\phi^{time\,new} = b(\phi^{time\,old})$$

  Yes, we are cheating.

Assigning Particles to Nodes/Cells

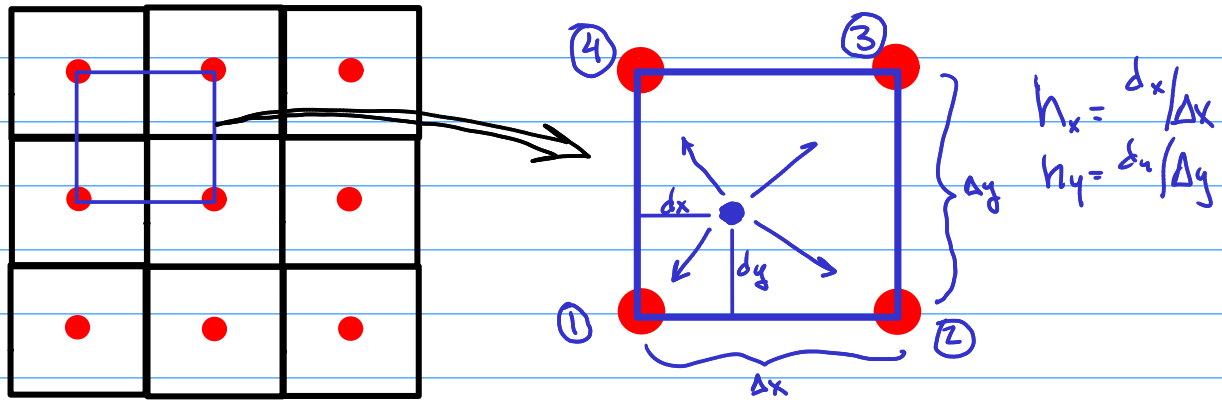
We need to compute the number of ions in the cell...ni

It appears on the right-hand side of our nonlinear system.

Problem: The numerics get jittery and unstable if we suddenly attribute an ion to the cell next door when it crosses the boundary.

It is better to smoothly transition the particle from one cell to the next.

We will use interpolation to assign particles to neighboring nodes. We will do the interpolation on the staggered mesh.



if $h_x = h_y = 0$ ... all weight of ptcls goes to lower left node

if $h_x = h_y = 1$ ... all weight goes to upper right

Compute the weights for each of the four nodes:

$w_1 = (1-h_x)(1-h_y)$

$w_2 = (h_x)(1-h_y)$

$w_3 = (1-h_x)(h_y)$

$w_4 = h_x h_y$

How much charge each ptcl represents (?)

Ths particle's ion density contribution to node (1) = $(w_1) \cdot (PTCL.Q_P)$

Computing Forces on Each Particle

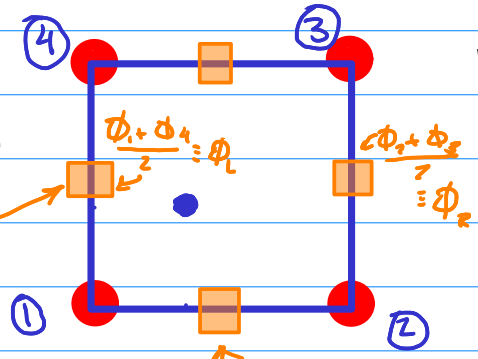
In our LaplacianOnGrid code, we wil be solving for voltage.
But the force on the ion is based on the electric field:

$$\vec{F}_{12} = \frac{q_1 q_2}{4\pi\varepsilon_0 r_{12}^2}\hat{r}_{12}$$

Φ we solve for it

$$\vec{F} = q\vec{E} = q\nabla V$$

We again use the staggered cell:



Assigned the average of 1 and 4

What is the electric field inside this cell? It is the negative of the gradient of voltage, V...phi

ParticleInCell.com

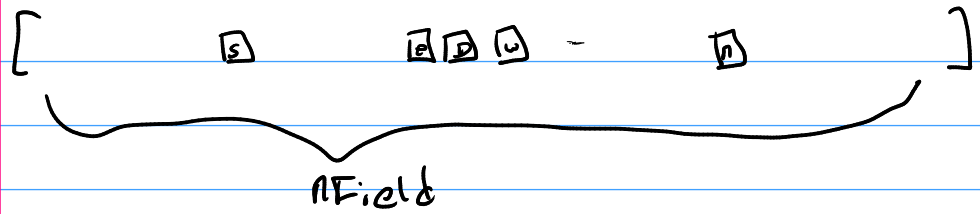
Assigned the average of 1 and 2

$$\frac{\partial V}{\partial x} = \frac{\phi_R - \phi_L}{\Delta x}$$

$$\frac{\partial V}{\partial y} = \frac{\phi_T - \phi_B}{\Delta y}$$

Sparse Matrix Format

Consider one row A in the system $\hat{A} * \tilde{phi} = \tilde{b}$



10 cells in the x-direction * 10 cells in the y-direction = 100 cells total

nField = 100

We have at most 5 non-zero entries in each row of the matrix.

Suppose:

$$A = \begin{bmatrix} 1 & 4 & 5 & 0 & 8 & 0 \\ 0 & 8 & 3 & 0 & 8 & 5 \\ 3 & 0 & 5 & 7 & 0 & 1 \\ 6 & 0 & 0 & 3 & 0 & 9 \\ 4 & 0 & 0 & 0 & 4 & 8 \\ 0 & 0 & 0 & 3 & 0 & 1 \end{bmatrix}$$

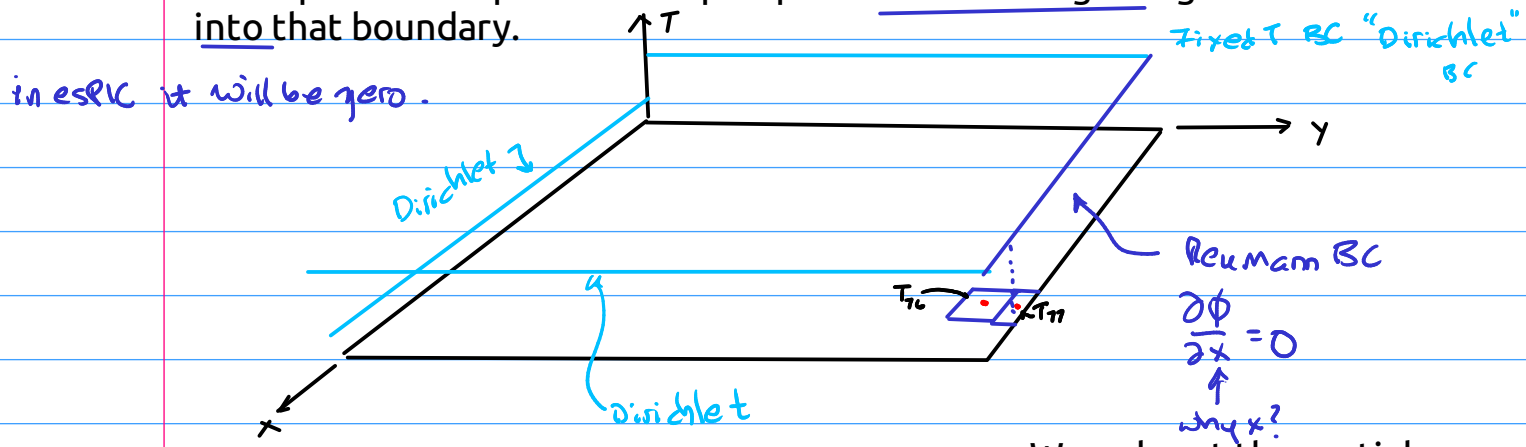
$$ACoef = \begin{bmatrix} 1 & 4 & 5 & 8 \\ 8 & 3 & 8 & 5 \\ 5 & 3 & 7 & 1 \\ 3 & 6 & 9 & 0 \\ 4 & 4 & 8 & 0 \\ 1 & 3 & 0 & 0 \end{bmatrix}$$

$$JCoef = \begin{bmatrix} 1 & 2 & 3 & 5 \\ 2 & 3 & 5 & 6 \\ 3 & 1 & 4 & 6 \\ 4 & 1 & 6 & 0 \\ 5 & 1 & 6 & 0 \\ 6 & 4 & 0 & 0 \end{bmatrix}$$

JCoef tells us the original columns in A for each entry.

Neumann Boundary Conditions

This boundary condition requires that the solution, phi, have specified slope from the perspective of heading straight into that boundary.



We only set the partial derivative w.r.t. x equal to zero on this boundary.

How do we enforce this BC?

$$\left.\frac{\partial T}{\partial x}\right|_{x_{max}} = 0 \rightsquigarrow T_{76} = T_{77}$$

$$\begin{bmatrix} \cdots & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} T_{76} \\ T_{77} \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix}$$

77 → col 76, col 77

In the matrix, we put a 1 in A[77,77] and a -1 in A[77,76], and a zero in b[77].