Laplace Equation, Jacobi and SOR Methods

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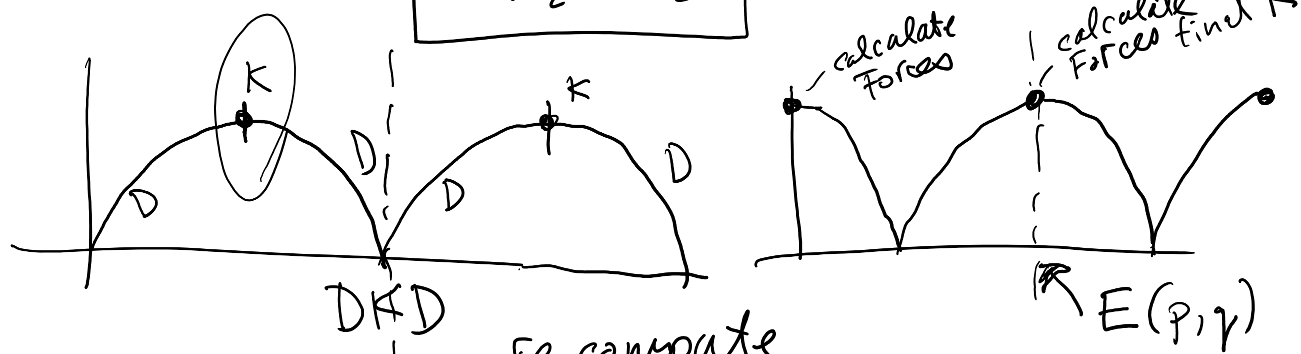
Leapfrog Variants $D_{\frac{1}{2}} K_1 D_{\frac{1}{2}}$

$$\boxed{K_{\frac{1}{2}} D_1 K_{\frac{1}{2}}} \qquad H = p^2 + q^2$$



Fe compute $V(q)$ to calculate the energy

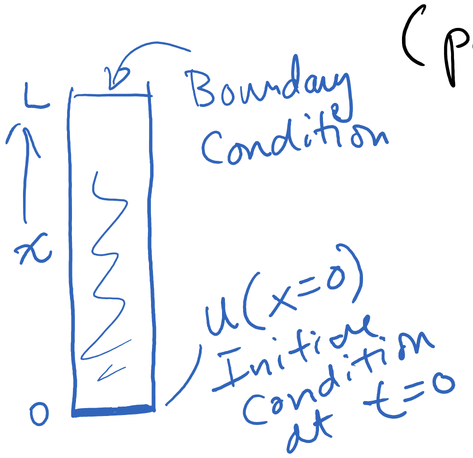
Partial Differential Equations

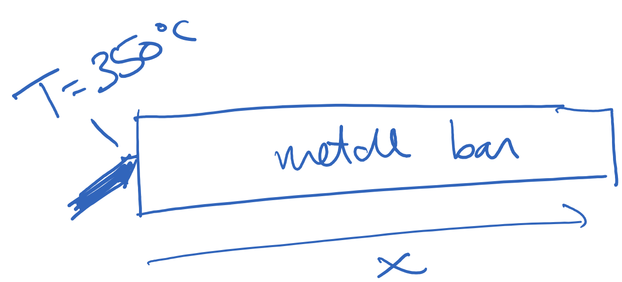
$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$ 1-D Wave Equation

(hyperbolic PDEs)

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$ 1-D Diffusion Equation

(parabolic PDE)





$$\partial^2 u \; + \; \partial^2 u = \rho(x,y)$$ Poisson Equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y) \quad \text{Poisson Equation}$$

(elliptic PDEs)

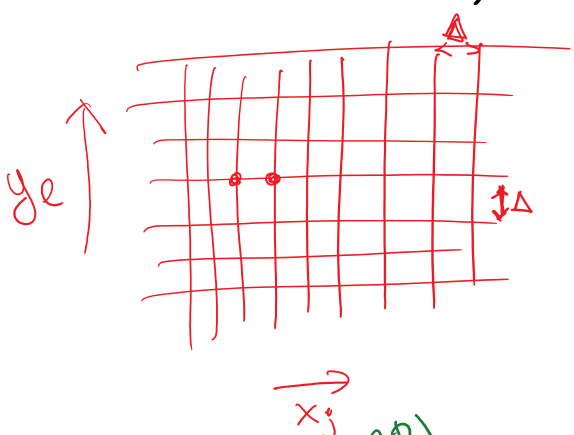
Only Boundary Conditions

Laplace Equation

$$\rho = 0 : \quad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad \boxed{\nabla^2 u = 0}$$

Electrostatic Potential in a Vacuum

$\Delta x, \Delta y$ to discretize the system

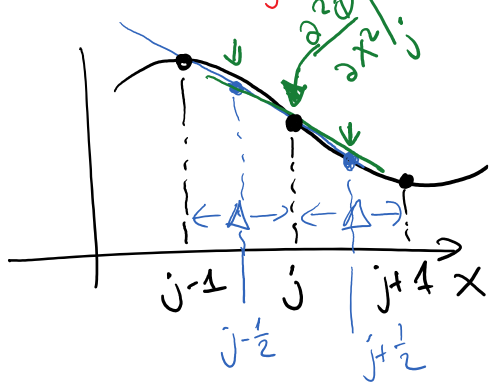


$$x_j = x_0 + j\Delta \qquad \Delta \text{ is the Grid spacing}$$

$$y_\ell = y_0 + \ell\Delta$$

$$j = 0, 1, 2, \dots J \; (N)$$

$$\ell = 0, 1, 2, \dots, L \; (N)$$



$$\left.\frac{\partial \phi}{\partial x}\right|_{j-\frac{1}{2}} \simeq \frac{\phi_j - \phi_{j-1}}{\Delta}$$

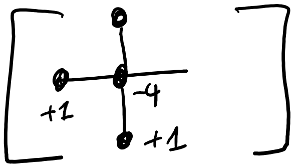
$$\left.\frac{\partial \phi}{\partial x}\right|_{j+\frac{1}{2}} \simeq \frac{\phi_{j+1} - \phi_j}{\Delta}$$

$$\frac{\partial^2 \phi}{\partial x^2} \simeq \frac{\left.\frac{\partial \phi}{\partial x}\right|_{j+\frac{1}{2}} - \left.\frac{\partial \phi}{\partial x}\right|_{j-\frac{1}{2}}}{\Delta}$$

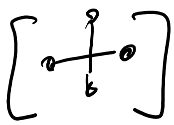
$$\boxed{\left.\frac{\partial^2 \phi}{\partial x^2}\right|_j \simeq \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{\Delta^2}}$$

$$\left.\frac{\quad}{\partial x^2}\right|_j = \frac{\quad}{\Delta^2}$$

$$\left[\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right]_{j,\ell} \cong \frac{\phi_{j+1,\ell}+\phi_{j-1,\ell}+\phi_{j,\ell+1}+\phi_{j,\ell-1}-4\phi_{j,\ell}}{\Delta^2}$$

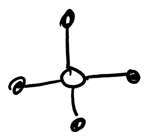
$\cong$ 

Grid operator for ∇^2
also called a Stencil

$\nabla^2\phi = 0$  $\phi = 0$

$$\frac{\phi_{j+1,\ell}+\phi_{j-1,\ell}+\phi_{j,\ell+1}+\phi_{j,\ell-1}-4\phi_{j,\ell}}{\Delta^2}=0$$

$$\boxed{\phi_{j,\ell}} = \frac{1}{4}\left(\phi_{j+1,\ell}+\phi_{j-1,\ell}+\phi_{j,\ell+1}+\phi_{j,\ell-1}\right)$$



Take the average of the neighboring points values.

Iterate until the change in $\phi_{j,\ell}$ over the grid is small!

Jacobi method: not fast, converges slowly!

$N_{iter} \sim \frac{1}{2} p N^2$ on an $N\times N$ grid to reduce the error by a factor of 10^{-p}

If you want 1 Volt of precision

with a 1000 V boundary condition
$p = 3$ and $N_{iter} \sim \frac{3}{2} N^2$

How many operations for 1 iteration

3 +, 1 *   4 ops per grid point
and there are N^2 grid points

$$4 N^2 \text{ ops / iteration}$$

$$N_{ops} \simeq \frac{3}{2} N^2 \times 4 N^2 = 6 N^4 \text{ operations!}$$
$$\mathcal{O}(N^4)$$

Faster is Successive Over Relaxation (SOR)

$$\phi_{j,l}^{(n+1)} = \boxed{\phi_{j,l}^{(n)}} + \frac{\omega}{4}\left(\phi_{j+1,l}^{(n)} + \phi_{j-1,l}^{(n)} + \phi_{j,l+1}^{(n)} + \phi_{j,l-1}^{(n)} - \boxed{4\,\phi_{j,l}^{(n)}}\right)$$

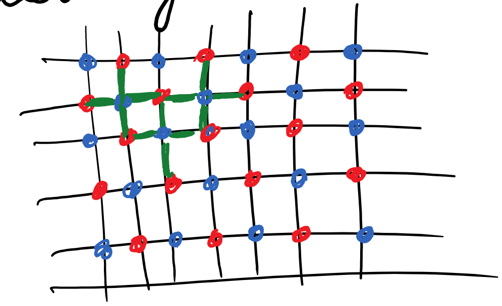
$\omega = 1 \Rightarrow$ Jacobi

$\omega > 1 \Rightarrow$ SOR $\omega \geqslant 2$ Unstable

If ω is optimal $\Rightarrow N_{iter} \sim \frac{1}{3} p N$!

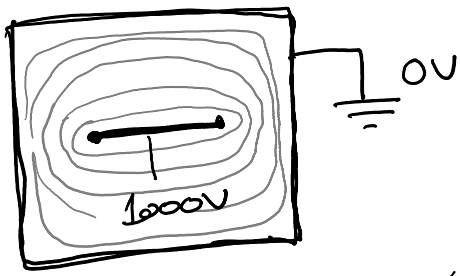
$\omega \simeq \dfrac{2}{1 + \pi/N}$ should work fairly well in many cases.

Implementing



Chessboard pattern update
First do all the blue points, then do all the red points

"An In-Place Algorithm"



For a "Boundary" Point we want $\phi_{j,l}^{(n+1)} = \phi_{j,l}^{(n)}$

For the other points we want to do the $\frac{\omega}{4}$ update!

~~if-then-else~~

slow

Use another Grid $R_{jl} = 0$ for a boundary jl

$R_{jl} = \frac{\omega}{4}$ for others

$$\phi_{jl}^{(n+1)} = \phi_{jl}^{(n)} + R_{jl} \cdot \left(\begin{smallmatrix} & +1 & \\ \cdot & -4 & \cdot \\ & \cdot & \end{smallmatrix} \right)$$

Loops over the chessboard is left to you to figure out.