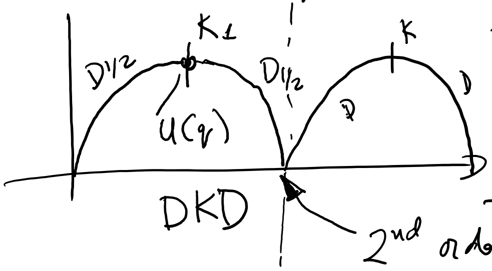
Variants of Leapfrog

Umbrela diagrams

$D_{1/2} K_1 D_{1/2}$

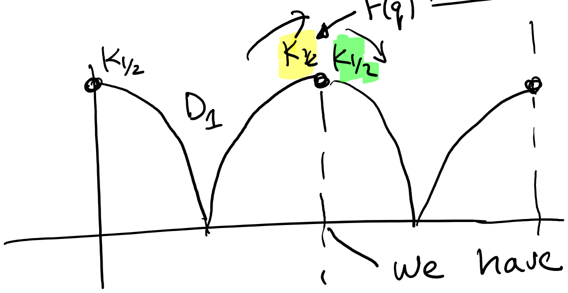
$$\boxed{K_{1/2} D_1 K_{1/2}}$$

$$H = p^2 + q^2$$



2nd order accurate ✓

$E = T + \boxed{U(q)}$ recompute this part! $O(N^2)$



we have U(q)

After $K_{1/2}$ we calculate Kinetic Energy using velocities and simply add $U(q)$ which can be calculated with the Forces. Only 1 $O(N^2)$ Force loops.

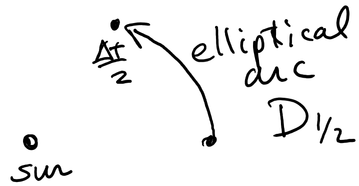
$H = \underline{\underline{T}} + \underline{\underline{U}}$

each is analytical to solve

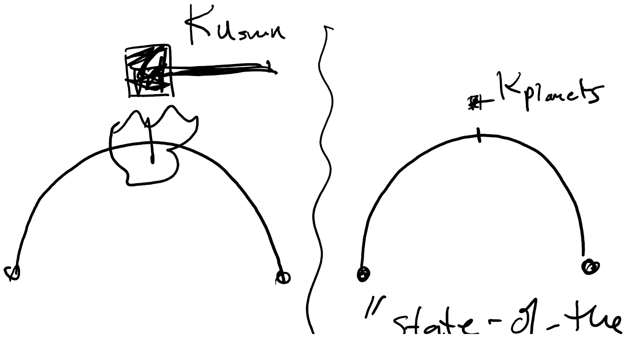
Solar System Hamiltonian

$H = T + U = H_{P-S} + H_{P-P}$

Kepler 2-body problem



$H_{P-P} \rightarrow$ forces due to planets only



Stength of the Kick is 1/1000 the strength in T+U decomposition.

1000x more accurate

"state-of-the-art"

1000x more accurate

"state-of-the-art"

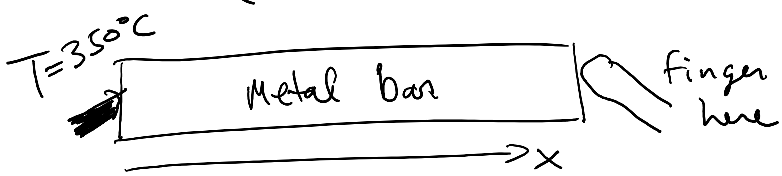
Partial Differential Equations (PDEs)

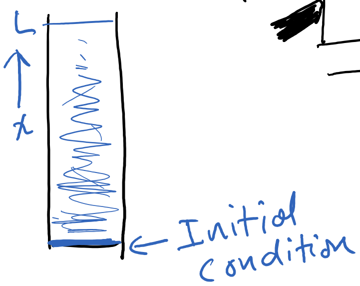
$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$ 1-D Wave equation

(hyperbolic PDE) CLASS

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

(CLASS: parabolic PDE)





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

(CLASS: elliptic PDEs)

- Only Boundary Conditions (BCs)

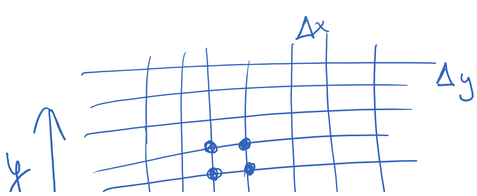
$\rho = 0$: $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$ continuous equation

$$\boxed{\nabla^2 u = 0}$$ Laplace Equation

Electrostatic Potential in a Vacuum

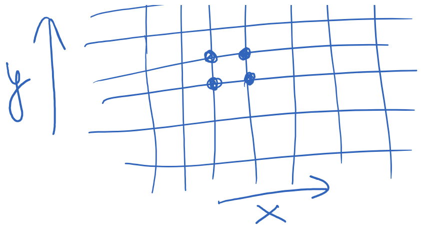
We want to discretize the system.

$\Delta x, \Delta y$: grid spacing



$x_j = x_0 + j\Delta \qquad \Delta \equiv \Delta x \equiv \Delta y$

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

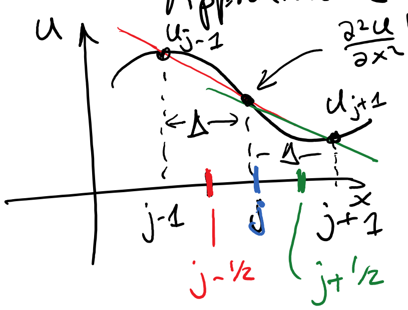


$x_j = x_0 + j\Delta \qquad \Delta \equiv \Delta x \equiv \Delta y$

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

$\left.\begin{array}{l} j = 0, 1, 2, \cdots, J \\ \ell = 0, 1, 2, \cdots, L \end{array}\right\} N$

Approximate $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ on the grid.



$$\left.\frac{\partial u}{\partial x}\right|_{j-1/2} \cong \frac{u_j - u_{j-1}}{\Delta}$$

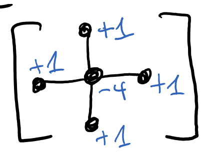
$$\left.\frac{\partial u}{\partial x}\right|_{j+1/2} \cong \frac{u_{j+1} - u_j}{\Delta}$$

Substitute!

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_j \cong \frac{\left.\frac{\partial u}{\partial x}\right|_{j+1/2} - \left.\frac{\partial u}{\partial x}\right|_{j-1/2}}{\Delta}$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_j \cong \frac{1}{\Delta^2}\left[u_{j+1} - 2u_j + u_{j-1}\right]$$

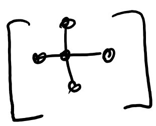
$$\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right] \cong \frac{1}{\Delta^2}\left[u_{j+1,\ell} + u_{j-1,\ell} + u_{j,\ell+1} + u_{j,\ell-1} - 4u_{j\ell}\right]$$

$\nabla^2 u \cong \frac{1}{\Delta^2}$ 

stencil for ∇^2

---

the equation: $\nabla^2 \phi = 0$ Continuous

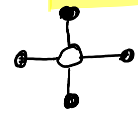
 $\phi = 0$ Disrete

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

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

Take the average

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

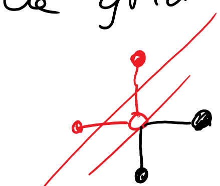


Take the average of the 4 neighbor points.

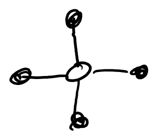
We have to iterate this until the change in $\phi_{j,\ell}$ over the grid is small!

$$\phi^{(n+1)}_{j,\ell} = \frac{1}{4}\left(\phi^{(n)}_{j+1,\ell} + \phi^{(n+1)\,(n)}_{j-1,\ell} + \phi^{(n)}_{j,\ell+1} + \phi^{(n+1)\,(n)}_{j,\ell-1}\right)$$

One sweep over the grid is one iteration.



Gauss-Seidel Method



Jacobi Method very slow: needs a lot of iterations.

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

ϕ is potential in volts. 1 volt precision with 1000 V boundary condition

$$N_{iter} = \frac{3}{2} N^2$$

How many operations for 1 iteration

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

$4N^2$ ops / iteration

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

$$\mathcal{O}(N^4)$$

Successive Over Relaxation (SOR-method) // over do it a bit*

$\phi^{(n+1)}$ ... (n) ($\phi^{(n)}$ ... $\phi^{(n)}$ + ... $4\phi^{(n)}$)

"over do it a bit"

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

$\omega = 1 \Rightarrow$ Jacobi

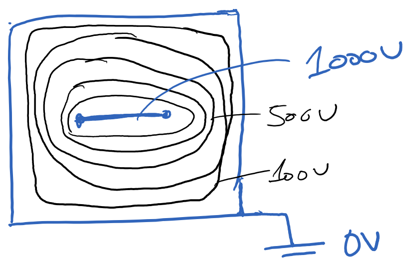
$\omega > 1 \Rightarrow$ SOR $(\omega < 2)$

Unstable

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

$\omega \approx \dfrac{2}{1 + \pi/N}$ } should work fairly well in most problems.

SOR $\Rightarrow \Theta(N^3)$



BCs are blue here
0V and 1000V

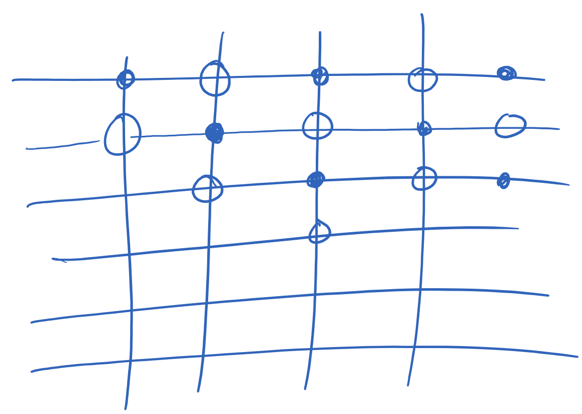
we want $\phi_{jl}^{(n+1)} = \phi_{jl}^{(n)}$

for the other points we want update $\frac{\omega}{4}(\;)$

Use another grid of values

$$R_{jl} = \begin{cases} 0, & \text{for a boundary } jl \\ \frac{\omega}{4}, & \text{for other } jl \end{cases}$$

$$\phi_{jl}^{(n+1)} = \phi_{jl}^{(n)} + R_{jl} \cdot \left(\;\right)$$



Sweep in a chess-board pattern.

1 iteration = sweep over black and sweep over white points