ODR s okrajovými podmínkami

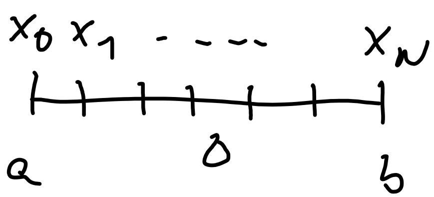
$$y'' = f(x, y, y') \qquad y(a) = \alpha \qquad y(b) = \beta$$

- metoda střelby

počáteční úloha $y(a) = \alpha \quad y'(a) = \lambda \xrightarrow{\text{poč. problém}} y(b) = g(\lambda)$

najdeme λ, pro kt. $y(b) = g(\lambda) = \beta$

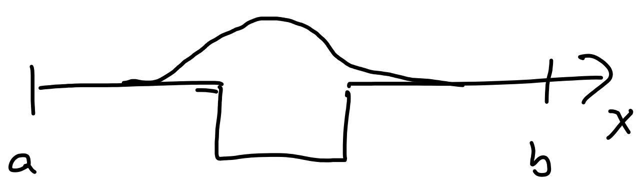
- metoda konečných diferencí



hledáme $y(x_j)$ $j = 0 \dots N$ → $N-1$ neznámé

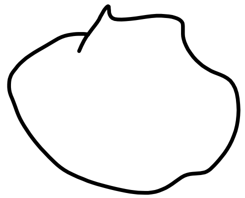
$$\frac{y_{j-1} - 2y_j + y_{j+1}}{\Delta^2} = f\left(x_j, y_j, \frac{y_{j+1} - y_{j-1}}{2\Delta}\right)$$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$$



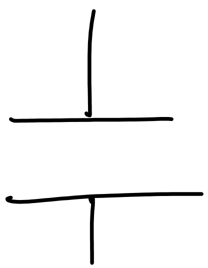
$$-\frac{\hbar^2}{2m\Delta^2}\left(\psi_{j-1} - 2\psi_j + \psi_{j+1}\right) + V(x_j)\psi_j = E\psi_j$$

PDR s okrajovými podmínkami



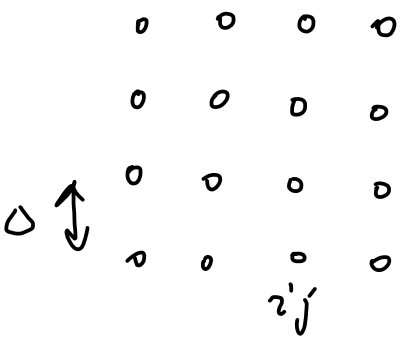
$\rho(\bar{r})$ → $$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0}$$ Poissonova rovnice

$$\bar{E} = -\nabla \phi$$



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

- metoda konečných diferencí



$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}$$ v místě ij

$$\frac{\partial^2 \phi}{\partial x^2} \approx \frac{\phi_{i-1,j} - 2\phi_{ij} + \phi_{i+1,j}}{\Delta^2}$$

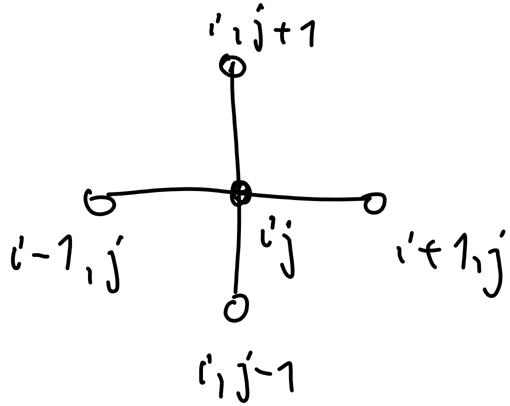
$$-\frac{1}{\Delta^2}\left(4\phi_{i,j}-\phi_{i-1,j}-\phi_{i+1,j}-\phi_{i,j-1}-\phi_{i,j+1}\right)=-\frac{\rho_{i,j}}{\varepsilon_0}$$

$$\frac{\partial^2\phi}{\partial x^2}\approx\frac{\phi_{i-1,j}-2\phi_{i,j}+\phi_{i+1,j}}{\Delta^2}$$

$$\frac{\partial^2\phi}{\partial y^2}\approx\frac{\phi_{i,j-1}-2\phi_{i,j}+\phi_{i,j+1}}{\Delta^2}$$

- iterační metody řešení řídké soustavy lin. rovnic

Laplaceova rce $\rightarrow$ $\phi_{i,j}=\frac{1}{4}\left(\phi_{i-1,j}+\phi_{i-1,j}+\phi_{i,j-1}+\phi_{i,j+1}\right)$



tabulka $\phi_{i,j}^{(n)}$

$\downarrow$ přiměrování   Jacobiho metoda

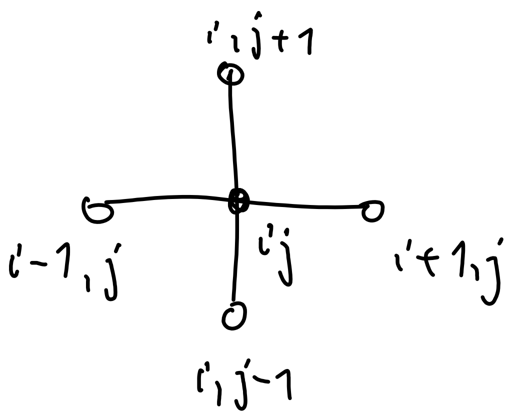
tabulka $\phi_{i,j}^{(n+1)}$

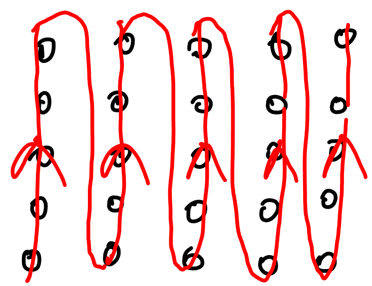
$$\phi_{i,j}^{(n+1)} = \frac{1}{4}\left(\phi_{i-1,j}^{(n)} + \phi_{i+1,j}^{(n)} + \phi_{i,j-1}^{(n)} + \phi_{i,j+1}^{(n)}\right)$$ Jacobiho metoda

$$\phi_{i,j}^{(n+1)} = \frac{1}{4}\left(\phi_{i-1,j}^{(n+1)} + \phi_{i+1,j}^{(n)} + \phi_{i,j-1}^{(n+1)} + \phi_{i,j+1}^{(n)}\right)$$ Gaussova-Seidelova

úspora paměti (2x)

a času (mnohokrát)





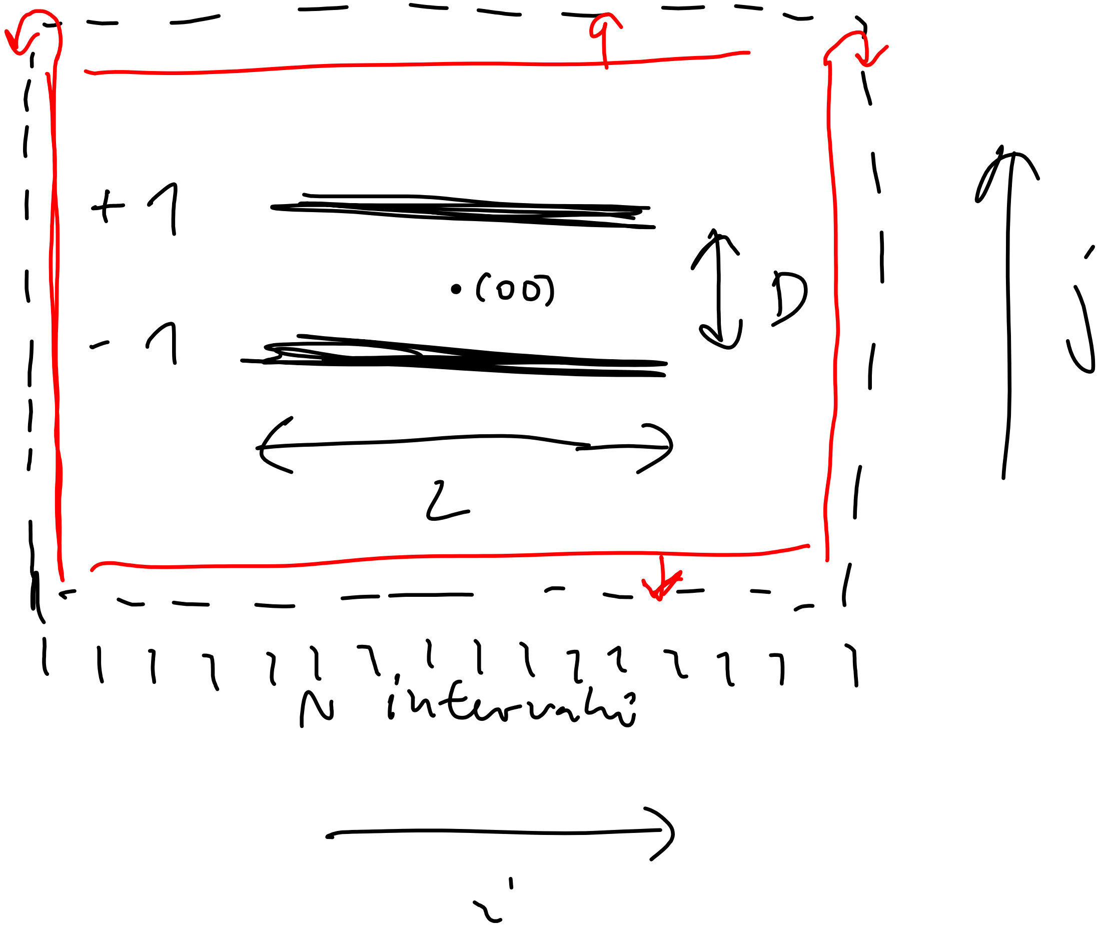
SOR

(Successive overrelaxation)

$$\phi^{(n+1)} = \phi^{(n)} + \left[\phi_{GS}^{(n+1)} - \phi^{(n)}\right]\omega$$

$0 < \omega < 2$

Laplaceova 2D $\quad \omega = \dfrac{2}{1 + \sin \pi \Delta}$



$i_1 \dots i_2$, j_1 j_2 desky

cython, numba