Parallelization of simulations of physical processes

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Parallel Computing
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Content:

- Poisson’s equation.
- Heat equation.
- Schrodinger equation.
    - 1D Time-independent Schrodinger Equation
    - 1D Time-dependent Schrodinger Equation

Poisson's equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Poisson's equation

Poisson's equation: $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$ in the [0,1]×[0,1] square domain

Boundary conditions: $u(x,0) = x, \quad u(x,1) = x - 1, \quad u(0,y) = -y, \quad u(1,y) = 1 - y.$

Lowest-order finite-difference representation →

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) \simeq \frac{1}{\Delta x}\left(\frac{\partial u}{\partial x}(x_{i+1}, y_j) - \frac{\partial u}{\partial x}(x_{i-1}, y_j)\right)$$

$$\simeq \frac{1}{\Delta x}\left(\frac{1}{\Delta x}(u(x_{i+1}, y_j) - u(x_i, y_j)) - \frac{1}{\Delta x}(u(x_i, y_j) - u(x_{i-1}, y_j))\right)$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \simeq \left(\frac{1}{\Delta^2}(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j})\right)$$

Poisson's equation

Diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

Forward Time-Centered Space differencing (FTCS)

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{\Delta t}{\Delta^2}(u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n} - 4u_{i,j}^{n})$$

Timestep $\Delta t = \Delta^2/4$

$$u_{i,j}^{n+1} = \frac{1}{4}(u_{i+1,j}^{n} + u_{i-1,j}^{n} + u_{i,j+1}^{n} + u_{i,j-1}^{n})$$

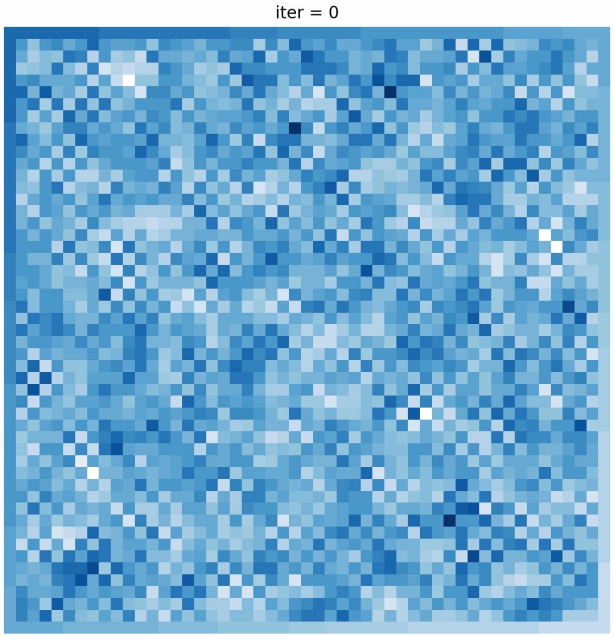
Jacobi method

$$u_{ij}^{k} = 0.25(u_{i-1,j}^{k} + u_{i,j-1}^{k} + u_{i,j+1}^{k} - u_{i+1,j}^{k})$$

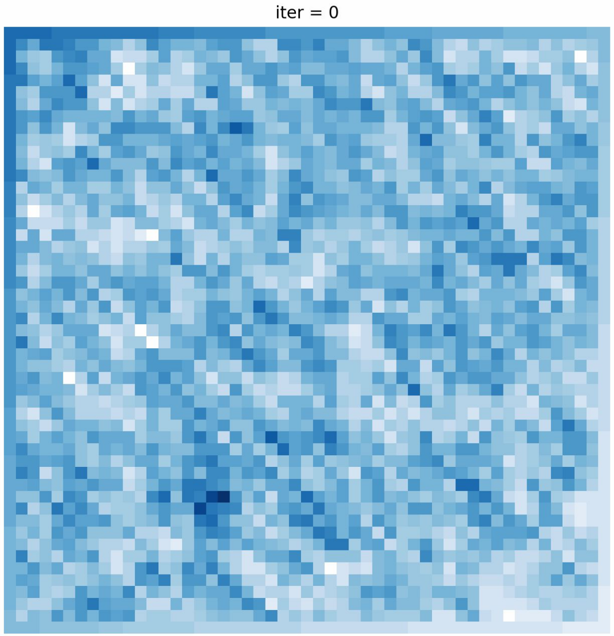
Gauss-Seidel method

Poisson's equation

Jacobi

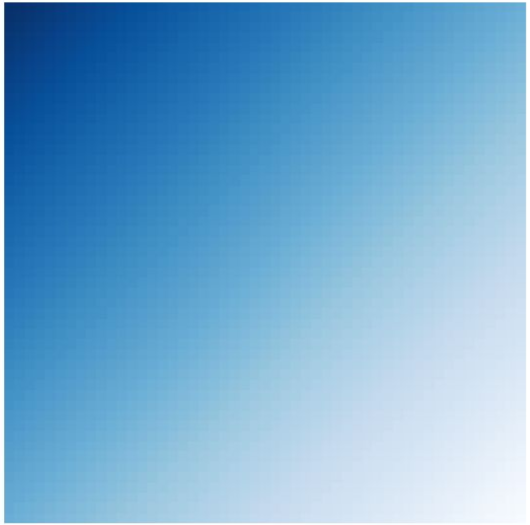


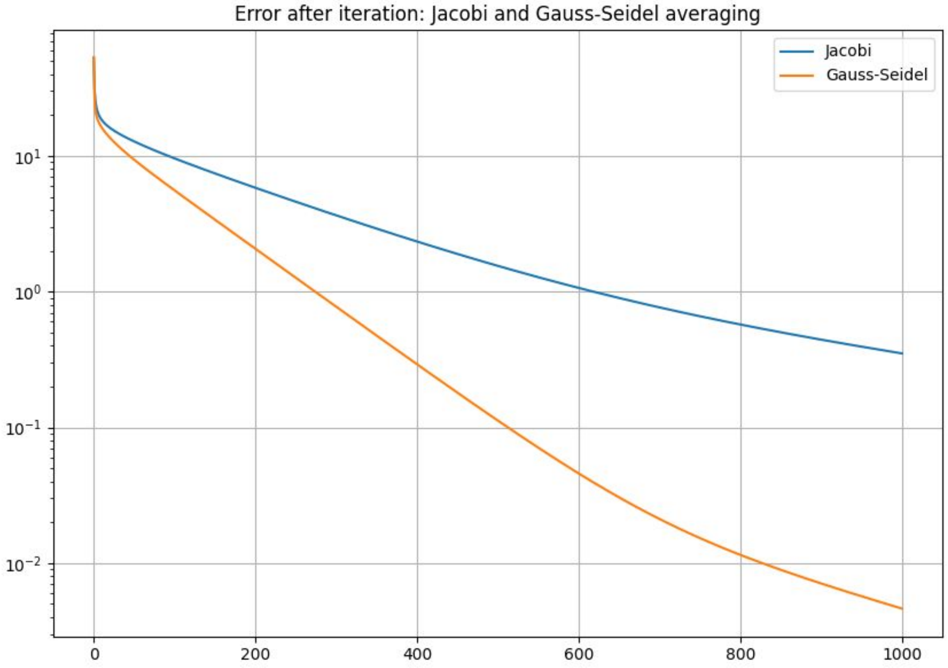
Gauss-Seidel



Poisson's equation

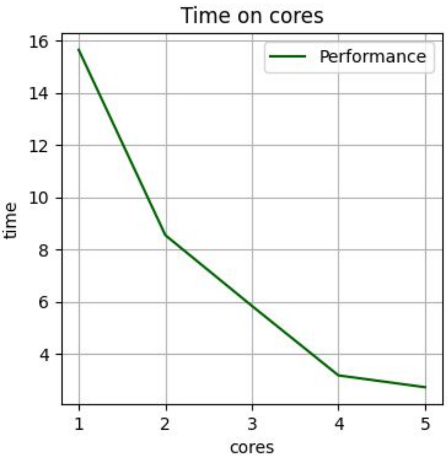
Direct solution

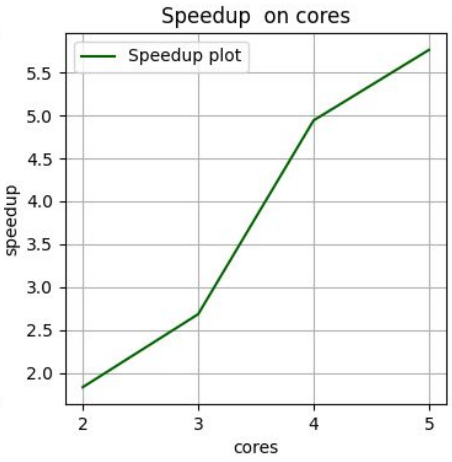




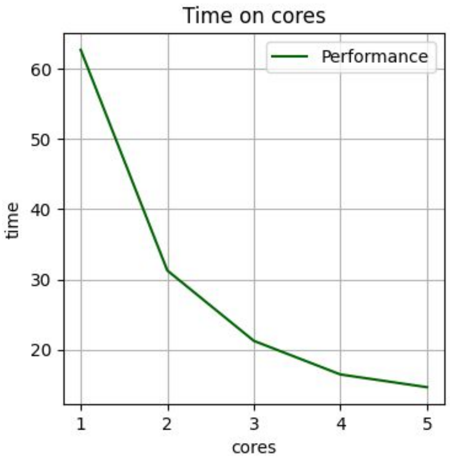
Poisson’s equation

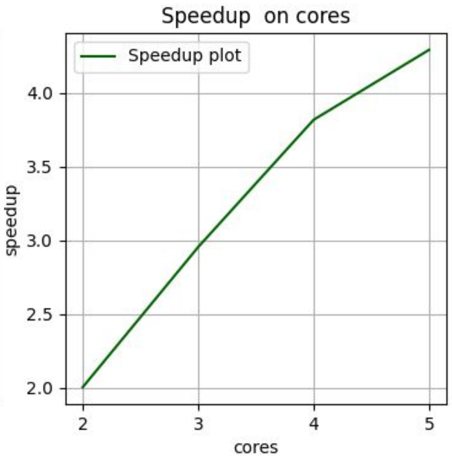
Jacobi





Gauss-Seidel





Heat equation

$$\frac{\partial u}{\partial t} - \alpha \nabla^2 u = 0$$

Heat equation

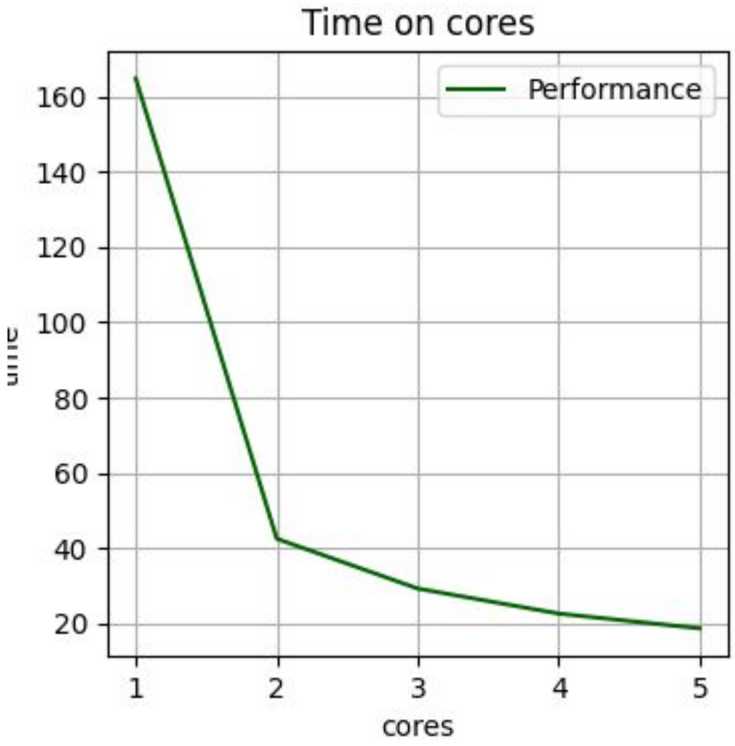
Heat equation is basically a partial differential equation

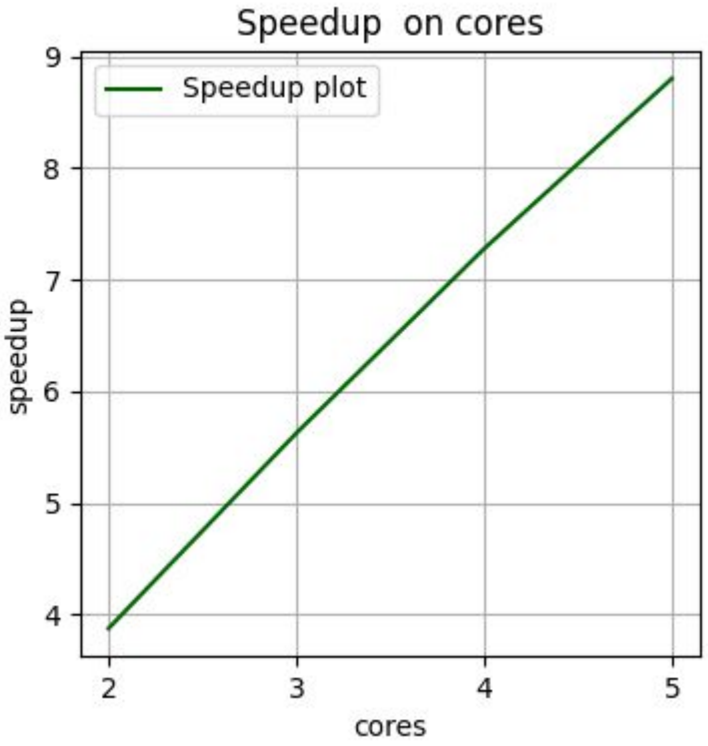
$$\frac{\partial u}{\partial t} - \alpha \nabla u = 0 \qquad \frac{\partial u}{\partial t} - \alpha \left(\frac{\partial^2 u}{\partial x} + \frac{\partial^2 u}{\partial y} \right) = 0 \qquad \Delta t \leq \frac{\Delta x^2}{4\alpha}$$

$$\frac{u_{i,j}^{k+1} - u_{i,j}^{k}}{\Delta t} - \alpha \left(\frac{u_{i+1,j}^{k} - 2u_{i,j}^{k} + u_{i-1,j}^{k}}{\Delta x^2} + \frac{u_{i,j+1}^{k} - 2u_{i,j}^{k} + u_{i,j-1}^{k}}{\Delta y^2} \right) = 0$$

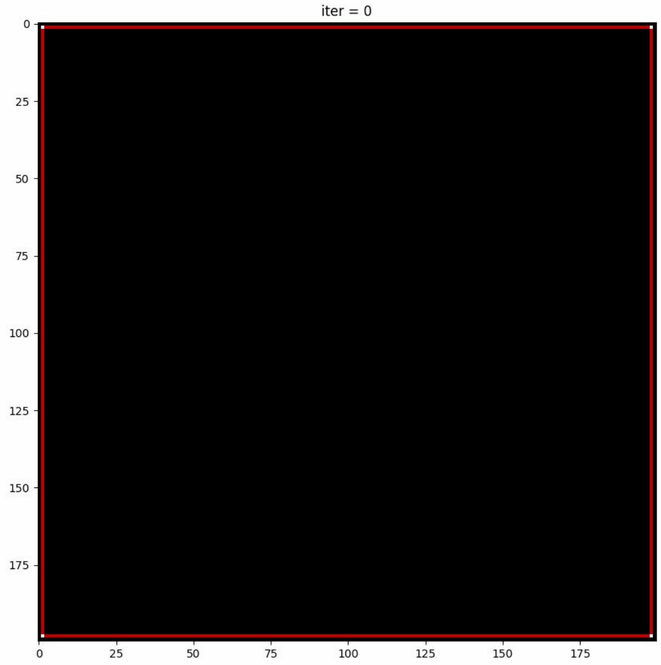
$$u_{i,j}^{k+1} = \gamma(u_{i+1,j}^{k} + u_{i-1,j}^{k} + u_{i,j+1}^{k} + u_{i,j-1}^{k} - 4u_{i,j}^{k}) + u_{i,j}^{k} \qquad \gamma = \alpha \frac{\Delta t}{\Delta x^2}$$

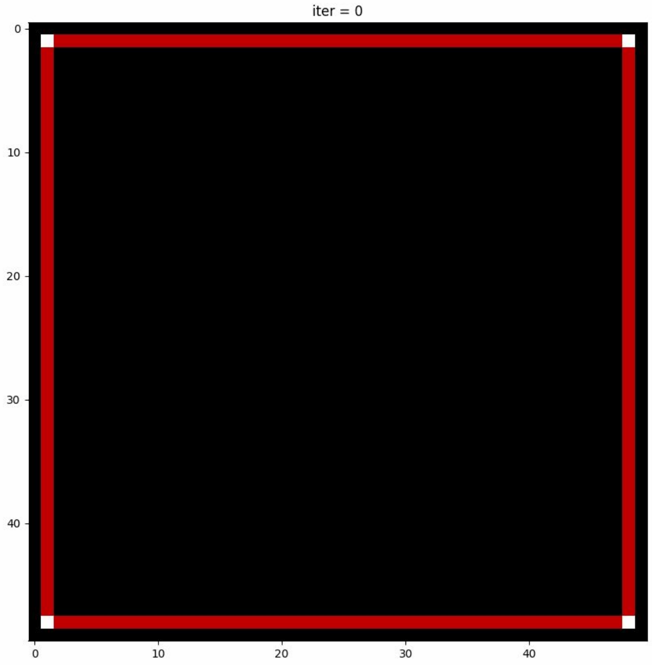
Heat equation





Heat equation





Schrodinger equation

$$i\hbar \frac{\partial \psi(x,y,z,t)}{\partial t} = \hat{H}\psi(x,y,z,t)$$

Schrodinger equation

$$i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = \hat{H}\psi(x,y,z,t)$$

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

$$\hat{U} = U$$

$$\hat{T} = \frac{\hat{p}^2}{2m},\ \hat{p} = -i\hbar\nabla$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{U} = \frac{(-i\hbar\nabla)^2}{2m} + \hat{U} = -\frac{\hbar^2}{2m}\Delta + \hat{U}$$

$$\boxed{i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(x,y,z,t) + U(x,y,z,t)\psi(x,y,z,t)}$$

Time-Independent Schrodinger equation

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

Time-Independent Schrodinger equation

$$U(x,y,z,t) = U(x,y,z) \longrightarrow$$

Stationary Schrodinger equation

Since the Hamilton operator in the equation does not depend explicitly on time

$$\psi(x,y,z,t) = \psi(x,y,z)\cdot\psi(t)$$

$$\psi(x,y,z,t) = \psi(x,y,z)\cdot\psi(t) \longrightarrow i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = \hat{H}\psi(x,y,z,t)$$

$x,y,z \rightarrow r$

$$i\hbar\frac{\partial}{\partial t}(\psi(r)\cdot\psi(t)) = \hat{H}(\psi(r)\cdot\psi(t))$$

$$\boxed{i\hbar\frac{1}{\psi(t)}\frac{\partial}{\partial t}\psi(t) = \frac{1}{\psi(r)}\hat{H}\psi(r)}$$

Time-Independent Schrodinger equation

$$i\hbar\frac{1}{\psi(t)}\frac{\partial}{\partial t}\psi(t)=\frac{1}{\psi(r)}\hat{H}\psi(r)=E$$

$$i\hbar\frac{1}{\psi(t)}\frac{\partial}{\partial t}\psi(t)=E$$

$$\frac{\partial\psi(t)}{\psi(t)}=\frac{E}{i\hbar}\partial t$$

$$ln\psi(t)=\frac{E}{i\hbar}t+lnC$$

$$\psi(t)=e^{\frac{E}{i\hbar}t}C$$

$$C=1.$$

$$\psi(t)=e^{\frac{E}{i\hbar}t}$$

$$\boxed{\psi(r,t)=\psi(r)\cdot e^{\frac{E}{i\hbar}t}}$$

$$i\hbar\frac{\partial\psi(r,t)}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi(r,t)+U(r,t)\psi(r,t)$$

$$i\hbar\frac{\partial}{\partial t}(\psi(r)\cdot e^{\frac{E}{i\hbar}t})=-\frac{\hbar^2}{2m}\Delta(\psi(r)\cdot e^{\frac{E}{i\hbar}t})+U(r)\psi(r)\cdot e^{\frac{E}{i\hbar}t}$$

$$i\hbar\cdot\psi(r)\frac{\partial e^{\frac{E}{i\hbar}t}}{\partial t}=-\frac{\hbar^2}{2m}\cdot e^{\frac{E}{i\hbar}t}\cdot\Delta\psi(r)+e^{\frac{E}{i\hbar}t}\cdot U(r)\psi(r)$$

$$i\hbar\cdot\psi(r)\cdot e^{\frac{E}{i\hbar}t}\cdot\frac{E}{i\hbar}=-\frac{\hbar^2}{2m}\cdot e^{\frac{E}{i\hbar}t}\cdot\Delta\psi(r)+e^{\frac{E}{i\hbar}t}\cdot U(r)\psi(r)$$

$$\psi(r)\cdot E=-\frac{\hbar^2}{2m}\cdot\Delta\psi(r)+U(r)\psi(r)$$

$$-\frac{\hbar^2}{2m}\cdot\Delta\psi(r)+U(r)\psi(r)-\psi(r)\cdot E=0$$

$$\boxed{\Delta\psi(r)+\psi(r)\cdot\frac{2m}{\hbar^2}(E-U(r))=0}\rightarrow$$

Stationary Schrodinger equation

Schrödinger equation in a one-dimensional field

1D case: $$\frac{\partial^2}{\partial x^2}\psi(x) + \frac{2m}{\hbar^2}(E - U(x)) \cdot \psi(x) = 0$$

$$U(x) = \begin{cases} 0 & \text{при } 0 < x < L \\ \infty & \text{при } x \leq 0, x \geq L \end{cases}$$

We consider the case of $0 < x < L$

$$U(x) = 0 \longrightarrow \boxed{\frac{\partial^2 \psi(x)}{\partial x^2} + \psi(x) \cdot \frac{2m}{\hbar^2} E = 0}$$

Boundary conditions: $$\psi(x = 0) = \psi(x = L) = 0$$

1D TISE. Analytical Solution

$$\frac{\partial^2\psi(x)}{\partial x^2} + \psi(x)\cdot\frac{2m}{\hbar^2}E = 0 \quad k^2 = \frac{2m}{\hbar^2}E$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + \psi(x)\cdot k^2 = 0$$

$$\psi'' + k^2\psi = 0$$

$$\psi(x) = C_1 coskx + C_2 sinkx, \text{ where } k = \frac{\sqrt{2mE}}{\hbar}$$

Let's use boundary condition

$$\psi(x=0) = C_1 cos(k\cdot 0) + C_2 sin(k\cdot 0) = C_1$$

$$\psi(x=0) = 0 \rightarrow C_1 = 0$$

$$\psi(x) = C_2 sinkx$$

$$\psi(x=L) = C_2 sin(kx) = C_2 sin(k\cdot L) = 0$$

$$sin(k\cdot L) = 0$$

$$kL = \pi n, n \in Z$$

$$k = \frac{\pi n}{L}, n = 1, 2, 3...., \text{ т.е.} n \in Z$$

Using the normalization condition

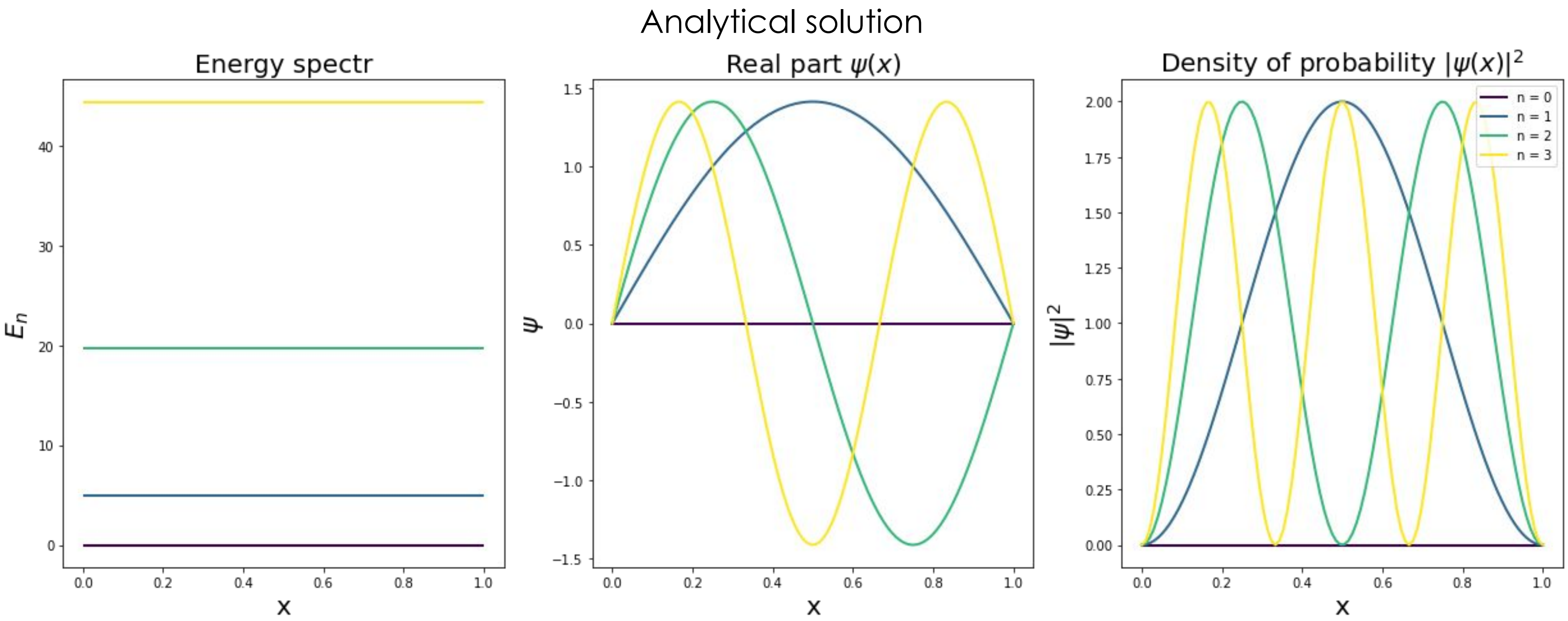
$$\int_0^L |\psi_n(x)|^2 dx = 1$$

$$C_2 = \sqrt{\frac{2}{L}} \longrightarrow \psi(x) = C_2 sinkx$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{\pi n}{L}x\right), \text{ при } E_n = \frac{\hbar^2\pi^2 n^2}{2m}, n = 1, 2, 3....}$$

1D TISE. Analytical Solution

1D Time-independent Schrodinger Equation



1D TISE. Numerical Solution

$$\frac{\partial^2}{\partial x^2}\psi(x) + \frac{2m}{\hbar^2}(E - U(x))\cdot\psi(x) = 0$$

Boundary conditions: $\psi(x=0) = \psi(x=L) = 0$

Let’s rewrite it as

$$-\frac{1}{2}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{m}{\hbar^2}U(x)\psi(x) = \frac{m}{\hbar^2}E\psi(x)$$

Let's make a replacement: $y = \frac{x}{L}$

$$dx^2 = L^2 d\left(\frac{x^2}{L^2}\right) = L^2 d\left(\left(\frac{x}{L}\right)^2\right) = L^2 dy^2$$

$$-\frac{1}{2}\frac{\partial^2\psi(y)}{L^2\partial y^2} + \frac{m}{\hbar^2}U(y)\psi(y) = \frac{m}{\hbar^2}E\psi(y)$$

$$\boxed{-\frac{1}{2}\frac{\partial^2\psi(y)}{\partial y^2} + L^2\frac{m}{\hbar^2}U(y)\psi(y) = L^2\frac{m}{\hbar^2}E\psi(y)}$$

$$\boxed{-\frac{1}{2}\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta y^2} + L^2\frac{m}{\hbar^2}U_j\psi_j = L^2\frac{m}{\hbar^2}E\psi_j}$$

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

$$\begin{cases} -\frac{1}{2\Delta y^2}\psi_2 + \left(\frac{1}{\Delta y^2} + L^2\frac{m}{\hbar^2}U_j\right)\psi_1 - \frac{1}{2\Delta y^2}\psi_0 = L^2\frac{m}{\hbar^2}E\psi_1 \\ -\frac{1}{2\Delta y^2}\psi_3 + \left(\frac{1}{\Delta y^2} + L^2\frac{m}{\hbar^2}U_j\right)\psi_2 - \frac{1}{2\Delta y^2}\psi_1 = L^2\frac{m}{\hbar^2}E\psi_2 \\ \dots \\ -\frac{1}{2\Delta y^2}\psi_N + \left(\frac{1}{\Delta y^2} + L^2\frac{m}{\hbar^2}U_j\right)\psi_{N-1} - \frac{1}{2\Delta y^2}\psi_{N-2} = L^2\frac{m}{\hbar^2}E\psi_{N-1} \end{cases}$$

1D TISE. Numerical Solution

$$\begin{bmatrix} \left(\frac{1}{\Delta y^2}+L^2\frac{m}{\hbar^2}U_1\right) & -\frac{1}{2\Delta y^2} & 0 & \dots & 0 & 0 \\ -\frac{1}{2\Delta y^2} & \left(\frac{1}{\Delta y^2}+L^2\frac{m}{\hbar^2}U_2\right) & -\frac{1}{2\Delta y^2} & 0 & \dots & 0 \\ 0 & -\frac{1}{2\Delta y^2} & \left(\frac{1}{\Delta y^2}+L^2\frac{m}{\hbar^2}U_3\right) & -\frac{1}{2\Delta y^2} & \dots & 0 \\ & & \dots & \dots & & \\ & & \dots & \dots & & \\ 0 & & \dots & 0 & -\frac{1}{2\Delta y^2} & \left(\frac{1}{\Delta y^2}+L^2\frac{m}{\hbar^2}U_{N-1}\right) \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \\ \psi_{N-1} \end{bmatrix} = L^2\frac{m}{\hbar^2}E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \vdots \\ \\ \psi_{N-1} \end{bmatrix}$$

$$A\psi = b\psi$$

eigenvalues

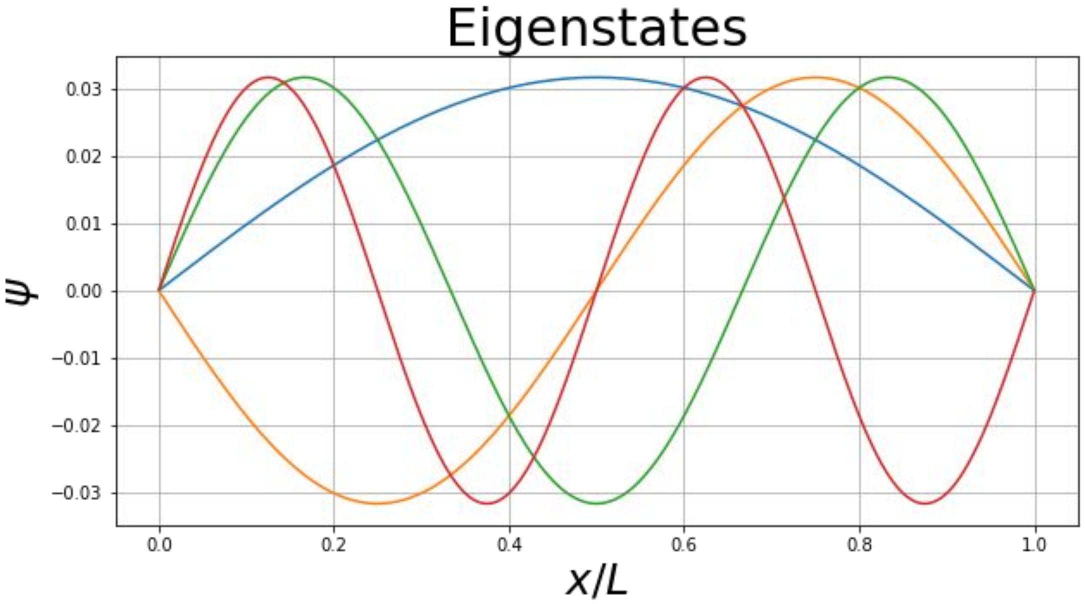
eigenvectors

1D TISE. Numerical Solution

1D Time-independent Schrodinger Equation

Numerical solution

Finding eigenvectors
via skype.linalg
Wall time: 553 ms

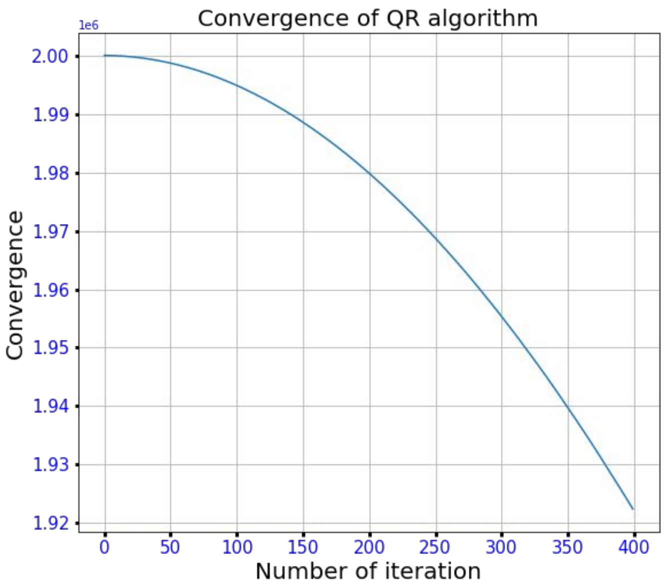


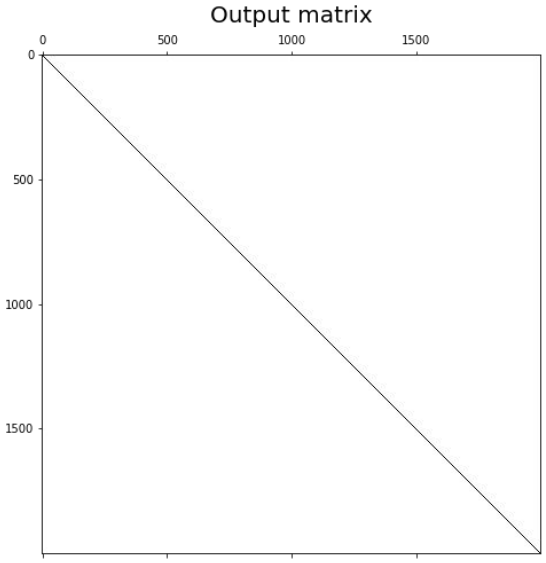
Schrodinger equation

1D Time-independent Schrodinger Equation

Numerical solution

Finding eigenvalues
via QR algorithm
Wall time: 10min 59s





Time-dependent Schrodinger equation

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(r,t) + U(r,t)\psi(r,t)$$

Schrodinger equation

$$i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = \hat{H}\psi(x,y,z,t)$$

Time-independent Hamiltonian $\longrightarrow$ $\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{U}(x)$

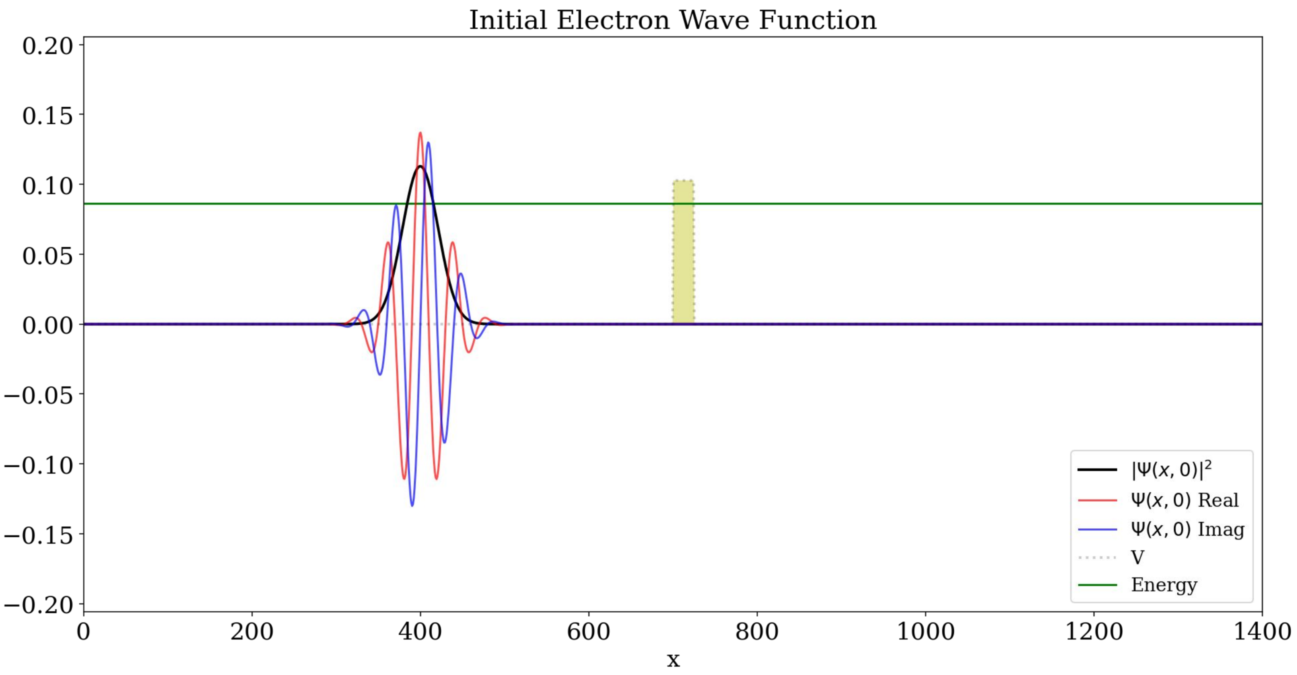
$$M = \left(1 - \frac{dt}{2i}H\right)^{-1}\left(1 + \frac{dt}{2i}H\right)$$

$$\psi(x,t+dt) = M \cdot \psi(x,t)$$

Schrodinger equation

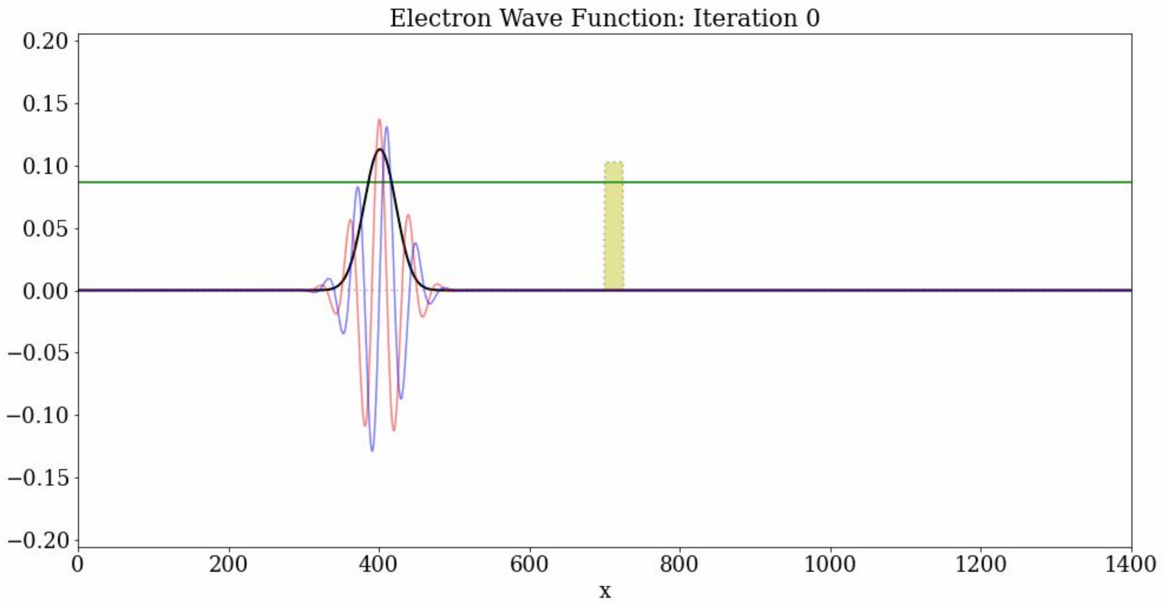
$$\psi(x,t=0) = e^{-\frac{1}{2}\left(\frac{x-5}{\sigma_0}\right)^2} e^{ik_0 x}$$

1D Time-dependent Schrodinger Equation



Schrodinger equation

1D Time-dependent Schrodinger Equation



Our Team

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P R E S E N T A T I O N