Time evolution simulation of the quantum mechanical wave function in 3D space

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- Structure and composition of carbon nanostructures
- Tunneling through carbon nanostructures
- Etc.

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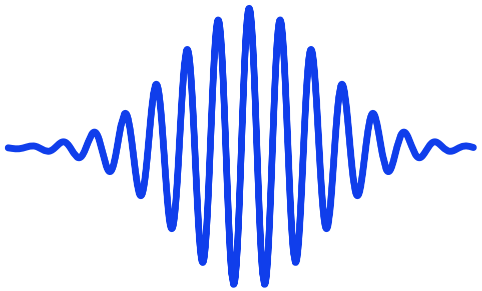
Outline

1. Introduction to wave packet dynamics
2. Simulation method
3. Visualization method
4. Presentation of results

Wave packet dynamics

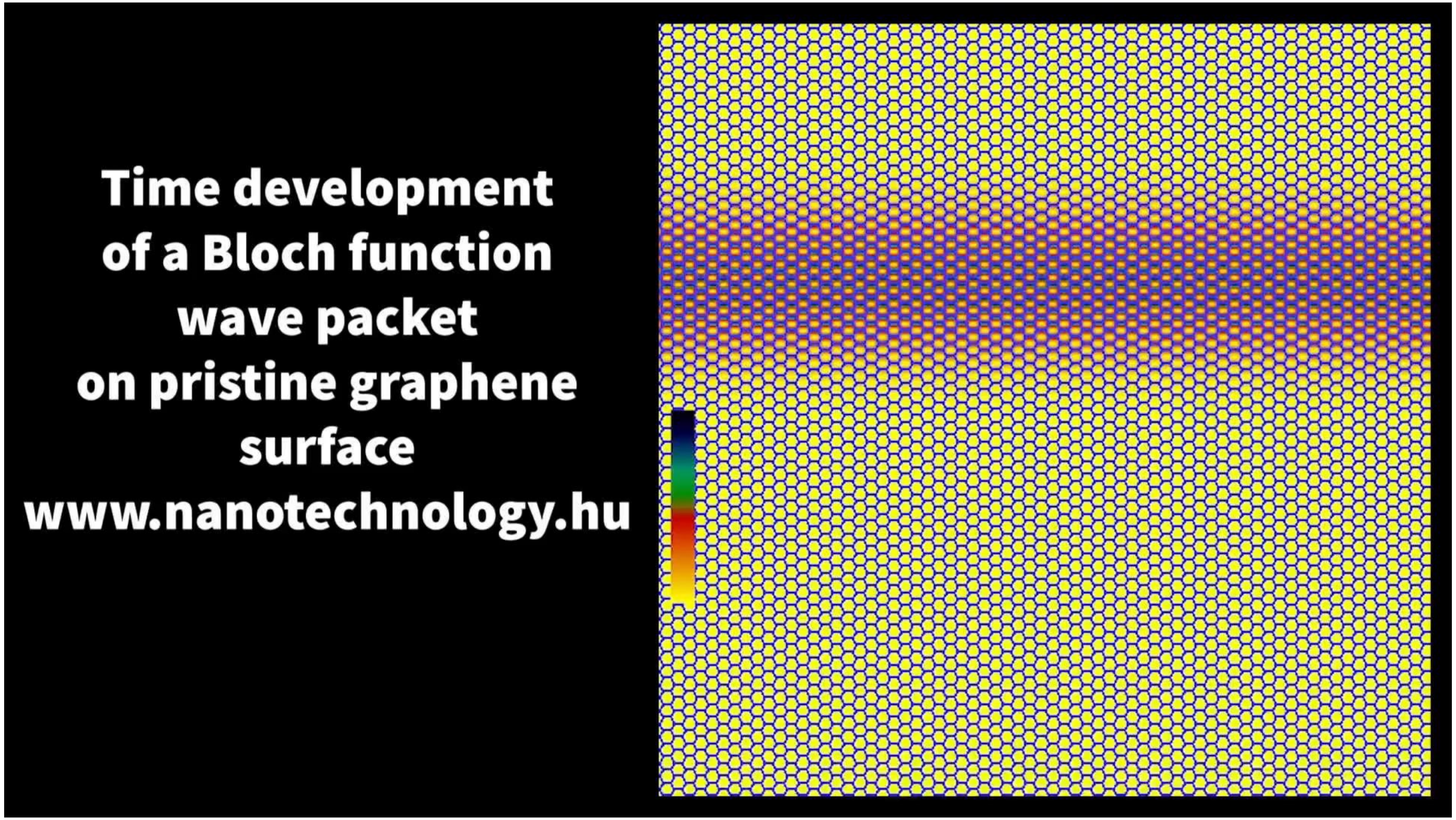


Wave packet

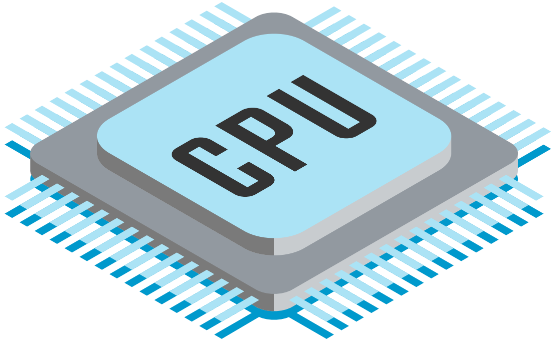
Modeled system

Canvas

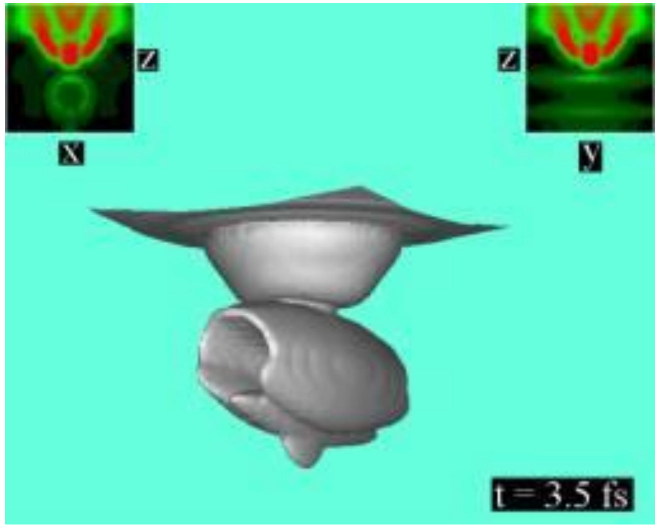
Wave packet scattering in defected graphene



Motivation

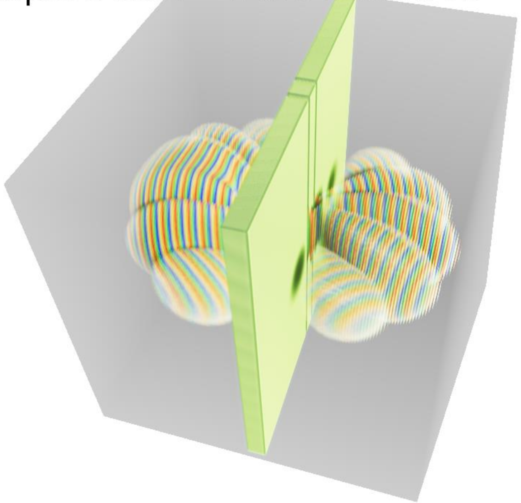


Faster



Advanced visuals

Elapsed time = 12.90 ħ/Hartree = 0.31 fs



Possible simulation methods

$$i\hbar \frac{d}{dt}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right]\psi(\vec{r},t)$$

$$\psi(\vec{r},t) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\psi(\vec{r},t_0)$$

$$\psi(\vec{r},t_n) = e^{-\frac{i}{\hbar}\hat{H}(\delta t)}\psi(\vec{r},t_{n-1})$$

How to calculate numerically?

- Split-operator Fourier method
- Finite Difference Time Domain

Fourier transform of the derivative

$$\mathcal{F}\left[\frac{d}{dx}f\right] = ik\mathcal{F}[f]$$

$$\mathcal{F}\left[\frac{d^2}{dx^2}f\right] = -k^2\mathcal{F}[f]$$

Operator separation

$$\psi(\vec{r}, t_n) = e^{-\frac{i}{\hbar}\hat{H}\delta t}\psi(\vec{r}, t_{n-1})$$

$$e^{-\frac{i}{\hbar}\hat{H}\delta t} = e^{-\frac{i}{\hbar}(\hat{K}+\hat{V})\delta t}$$

$$e^{-\frac{i}{\hbar}(\hat{K}+\hat{V})\delta t} \approx e^{-\frac{i}{\hbar}\hat{K}\delta t/2} e^{-\frac{i}{\hbar}\hat{V}\delta t} e^{-\frac{i}{\hbar}\hat{K}\delta t/2}$$

Error of the approximation is $\mathcal{O}(\delta t^3)$.

Split-operator Fourier method

$$\psi(\vec{r}, t_n) \approx e^{-\frac{i}{\hbar}\hat{K}\delta t/2} e^{-\frac{i}{\hbar}\hat{V}\delta t} e^{-\frac{i}{\hbar}\hat{K}\delta t/2} \psi(\vec{r}, t_{n-1})$$

$$\mathcal{F}$$

$$\times\, e^{-\frac{ik^2\hbar\delta t}{4m}}$$

$$\mathcal{F}^{-1}$$

$$\times\, e^{-\frac{i}{\hbar}V(\vec{r})\delta t}$$

$$\mathcal{F}$$

$$\times\, e^{-\frac{ik^2\hbar\delta t}{4m}}$$

$$\mathcal{F}^{-1}$$

FDTD method: power series expansion

$$\psi(\vec{r}, t_{n+1}) = e^{-\frac{i}{\hbar}\hat{H}\delta t}\psi(\vec{r}, t_n) = \sum_{k=0}^{\infty} S_k(\vec{r}, t_n)$$

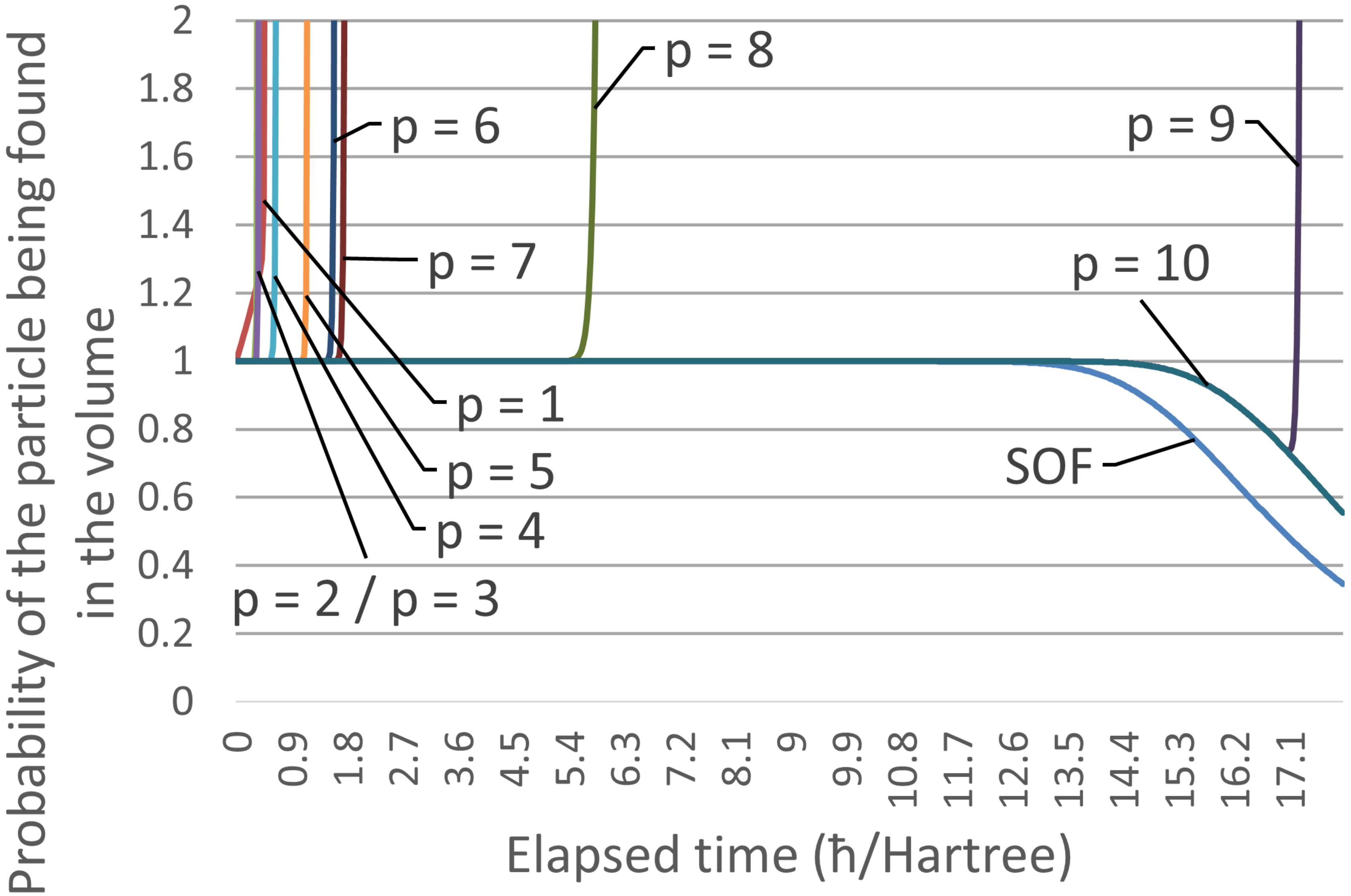
$$S_k(\vec{r}, t_n) = \frac{-\frac{i}{\hbar}\hat{H}\delta t}{k} S_{k-1}(\vec{r}, t_n) = \frac{i\delta t}{k}\left[\frac{\hbar}{2m}\Delta S_{k-1}(\vec{r}, t_n) - \frac{V(\vec{r})}{\hbar} S_{k-1}(\vec{r}, t_n)\right]$$

$k = 1,2,3, \ldots$

$$S_0(\vec{r}, t_n) = \Psi(\vec{r}, t_n)$$

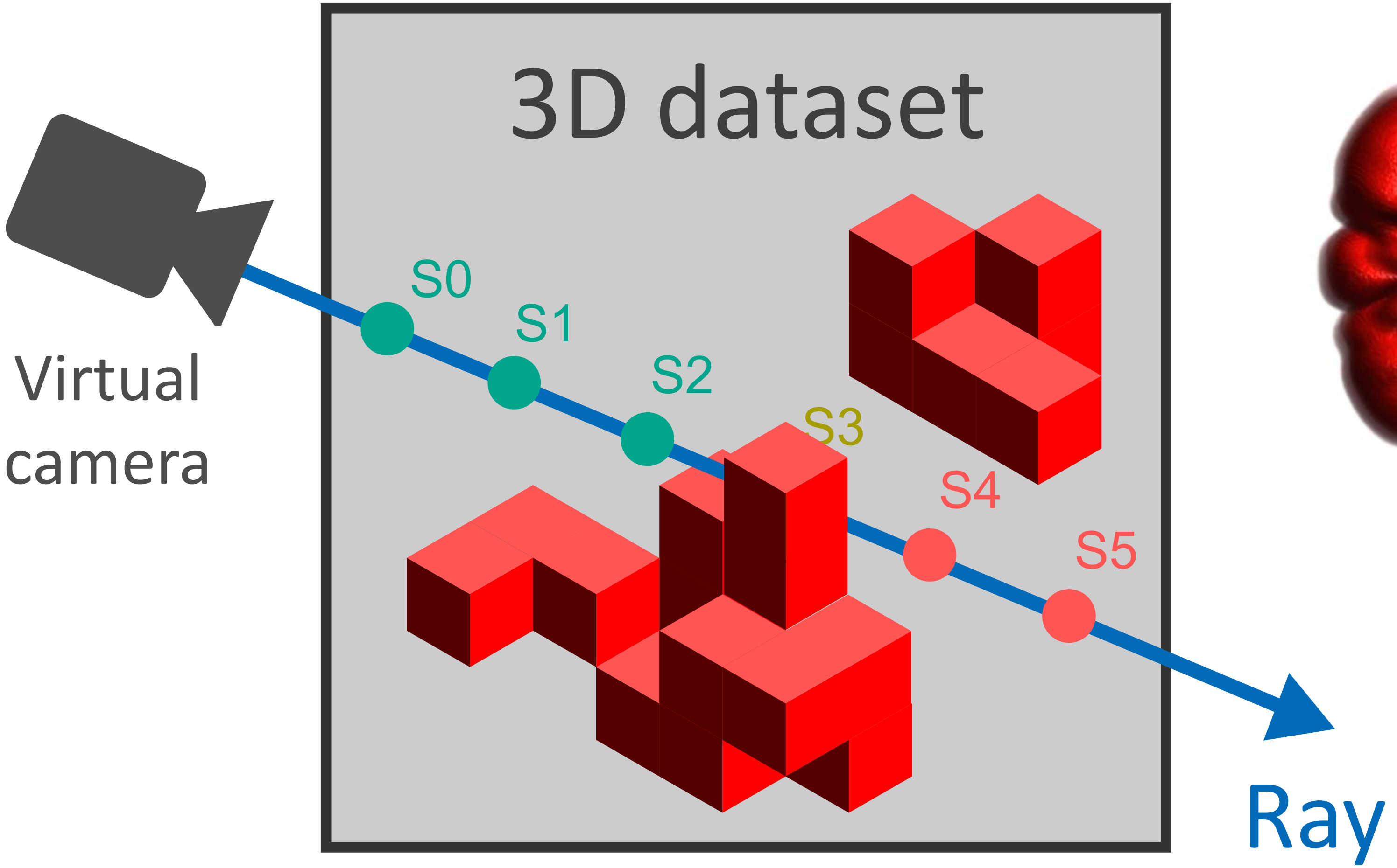
Evolution of the integrated probability density over simulated time

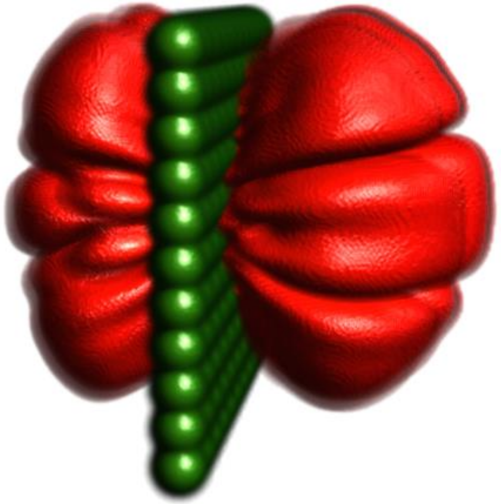
$$\mathbb{P}_{\mathcal{V}} = \int_{\mathcal{V}} |\psi(\vec{r},t)|^2 d\vec{r}$$



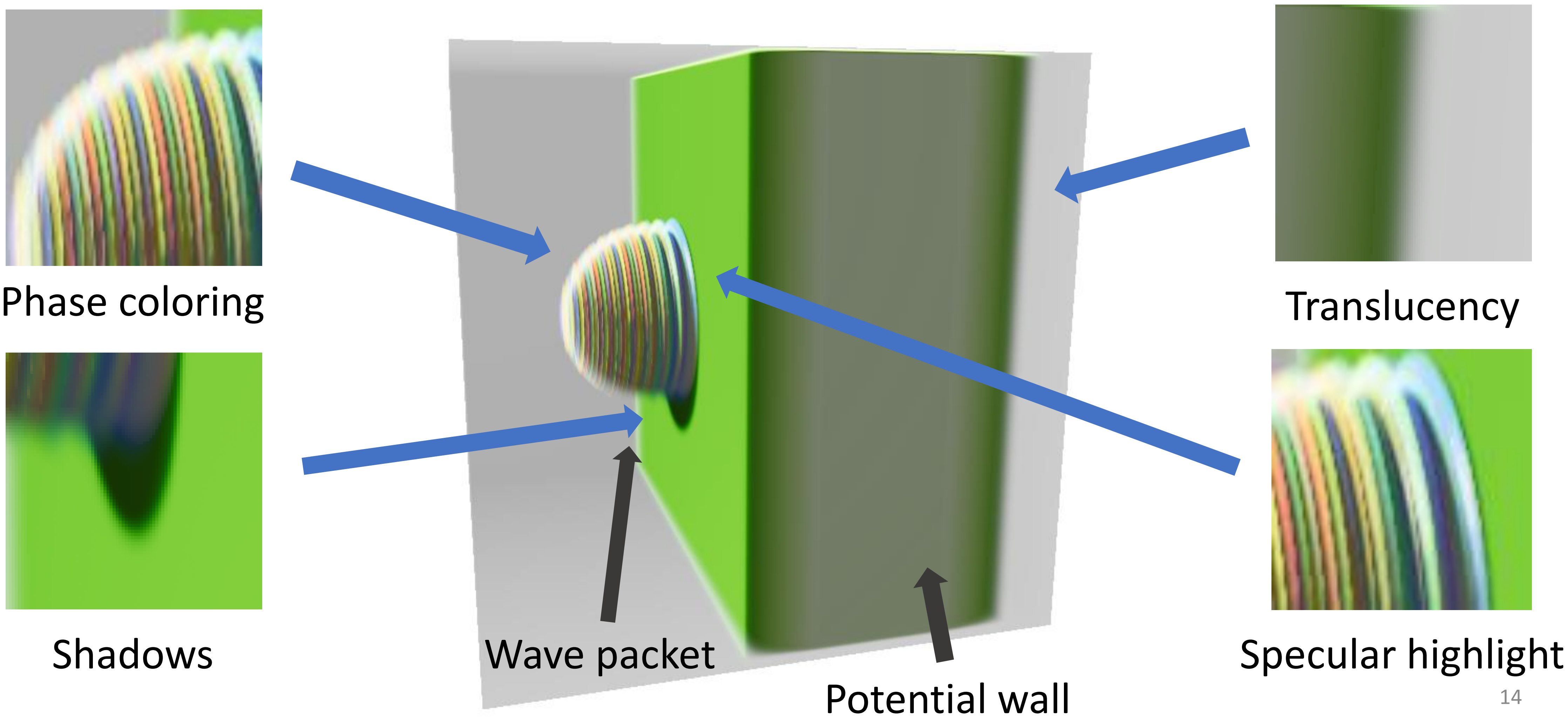
Ray marching

To visualize: $\rho(\vec{r}, t) = |\psi(\vec{r}, t)|^2$ probability density





Advanced visualization techniques



My implementation

- A program written in Python
- The 3D FFT calculation and the large complex valued tensor multiplications are carried out on the GPU using **CUDA**.
- Mathematics: **Numpy, Cupy**
- Visualization: **Vispy**
- Custom CUDA kernels for some calculations
- Custom GLSL shader for ray marching

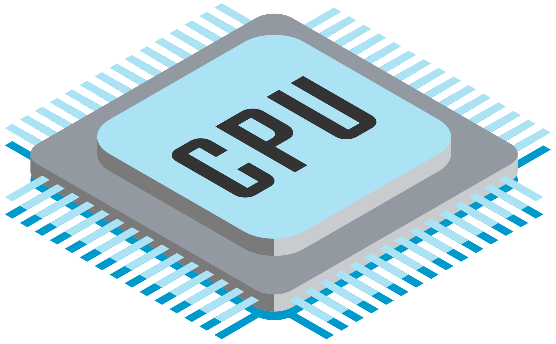
github.com/
TheFlyingPiano99/
WaveFunctionSimPython

Achieved speed-up

- $\times$ 50 **speed-up** compared to the previous implementation
- $512 \times 512 \times 512$ voxels simulated with the speed of $\sim$0.5 **iteration / second**.

Input size	CPU-only Avg. [iter/s]	GPU accelerated Avg. [iter/s]	Avg. speed up
$128 \times 128 \times 128$	1.1	11.5	$\times$10.45
$256 \times 256 \times 256$	0.09	6.5	$\times$72.22
$512 \times 512 \times 512$	0.01	0.5	$\times$50.00

Achieved speed-up



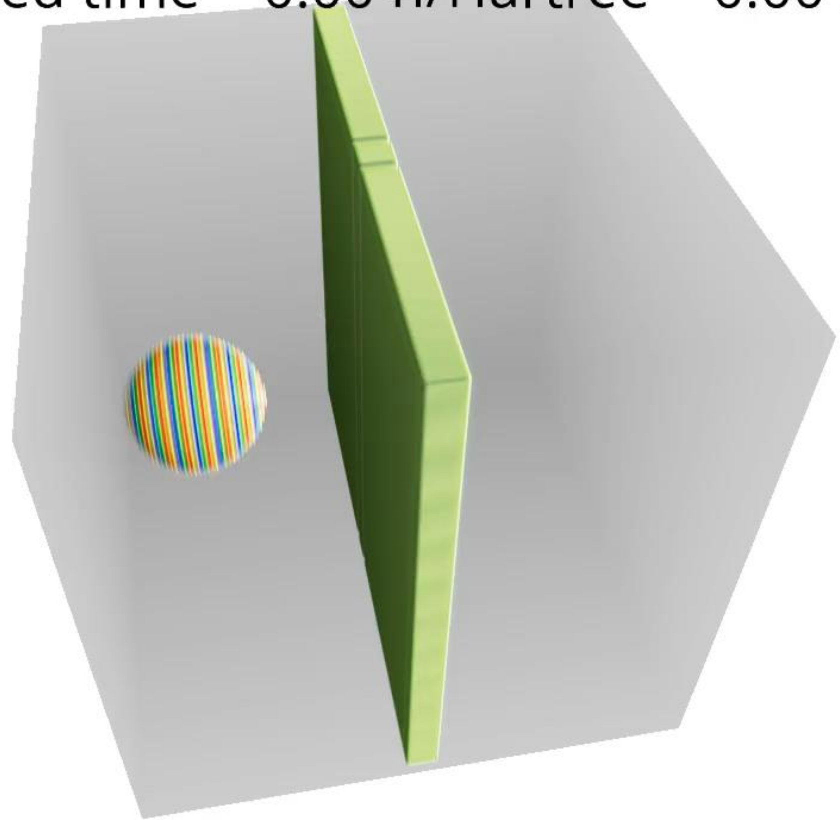
AMD Ryzen 5 6600H

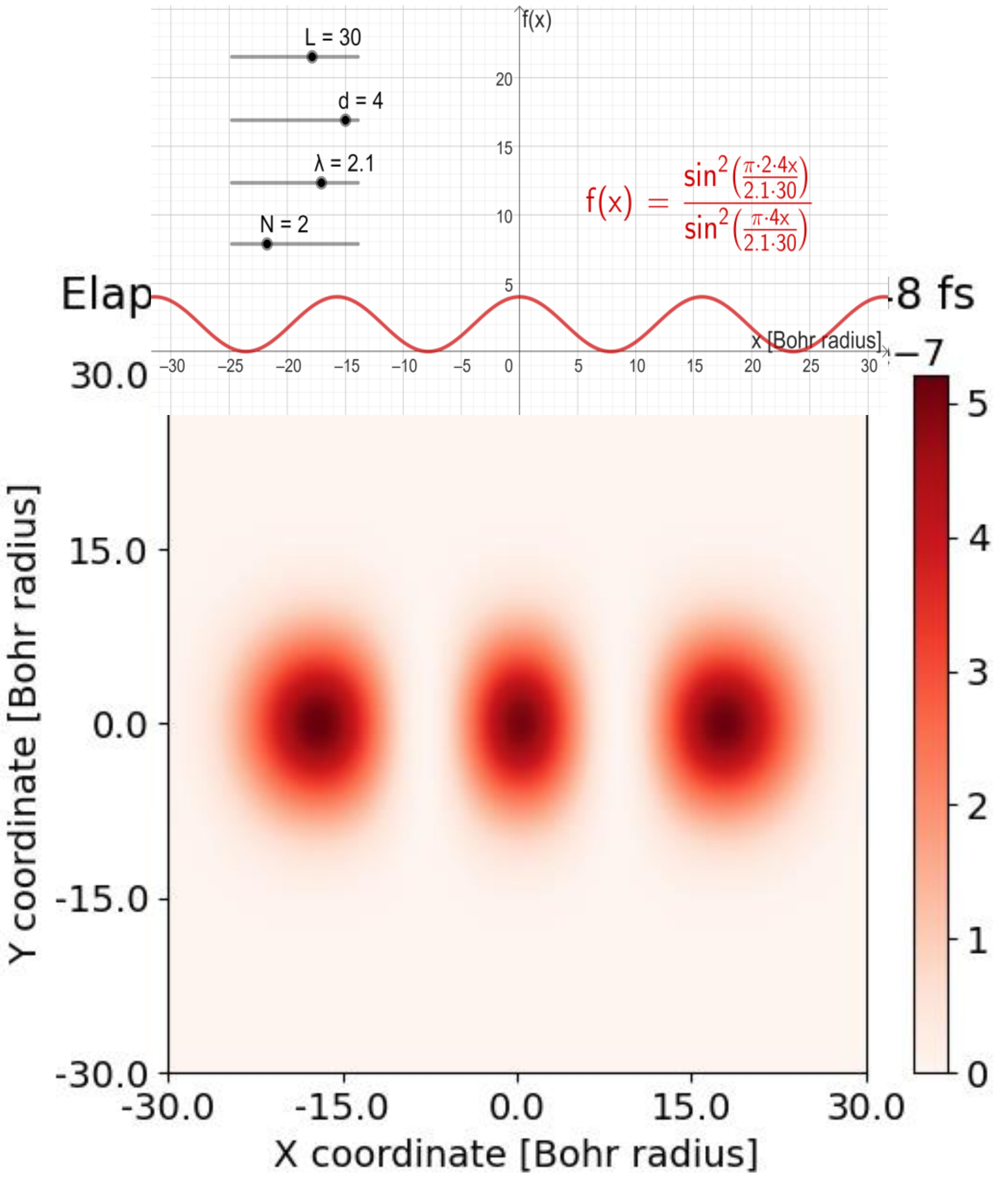
$50\times$

NVIDIA GeForce RTX 3050 Ti Laptop GPU

Double-slit simulation

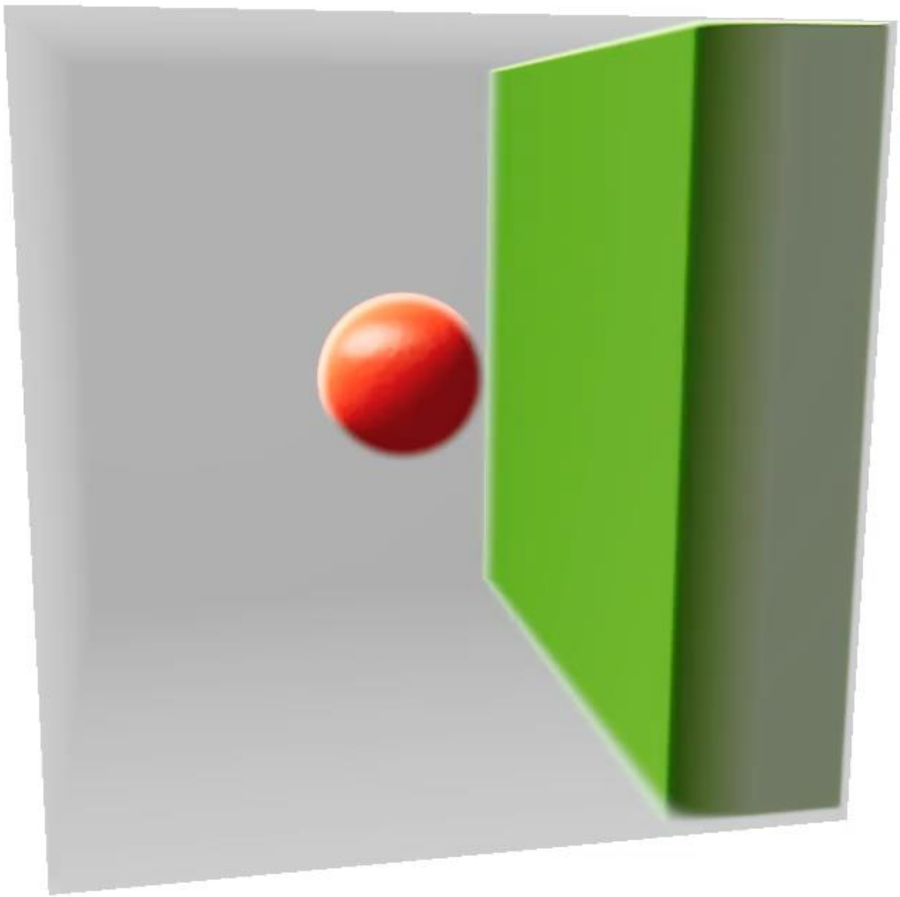
Elapsed time = 0.00 ħ/Hartree = 0.00 fs



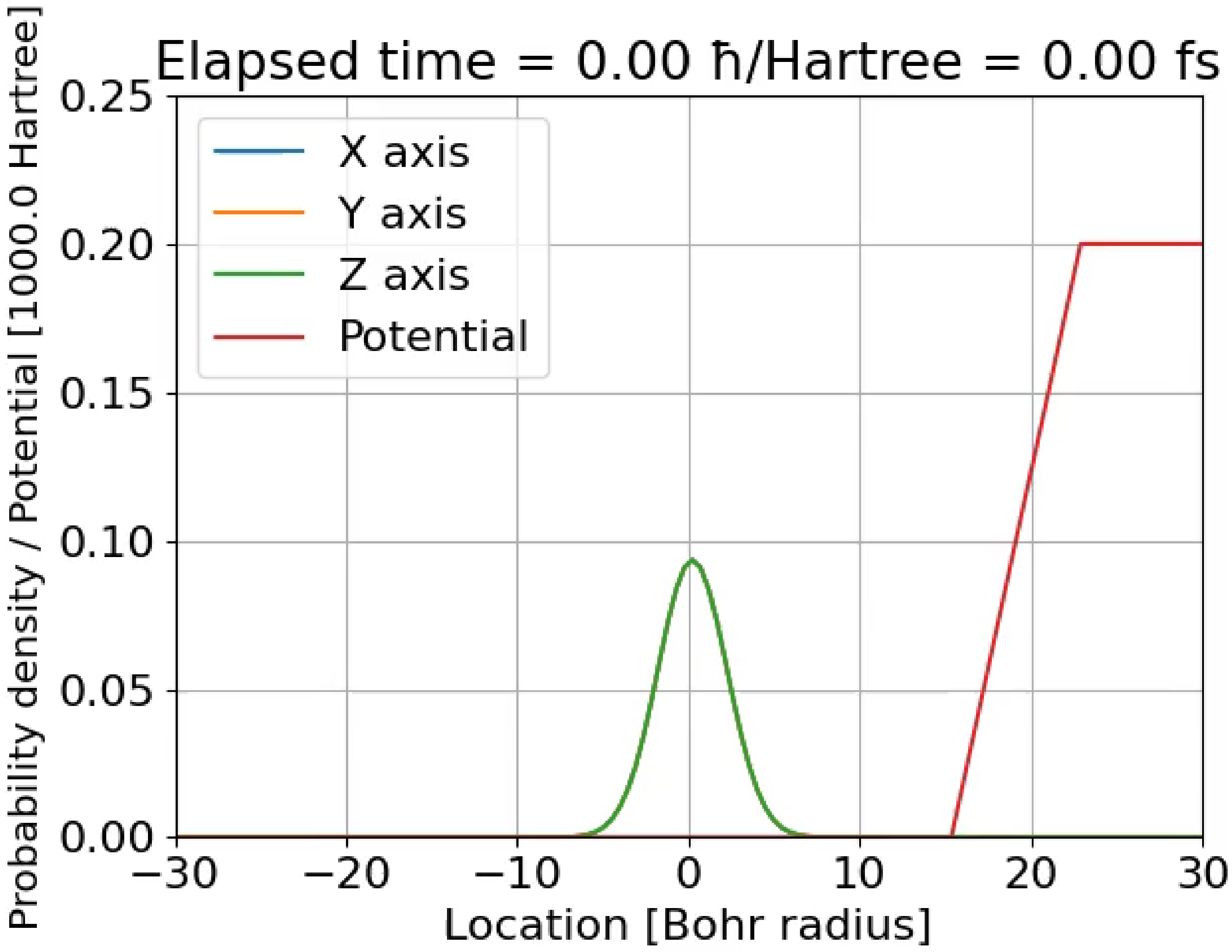


WP pushed by a moving potential wall

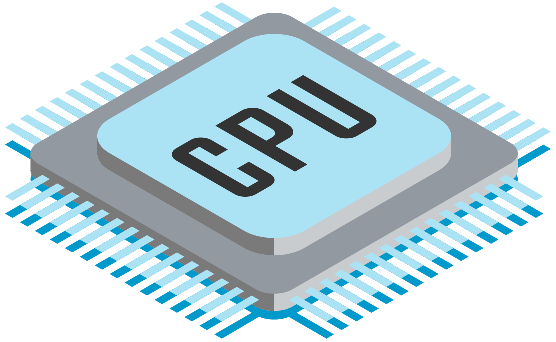
Elapsed time = 0.00 ħ/Hartree = 0.00 fs



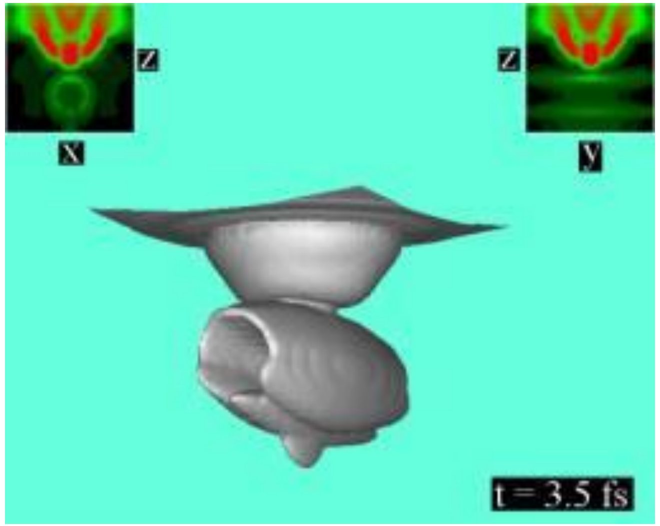
WP pushed by a moving potential wall



Summary

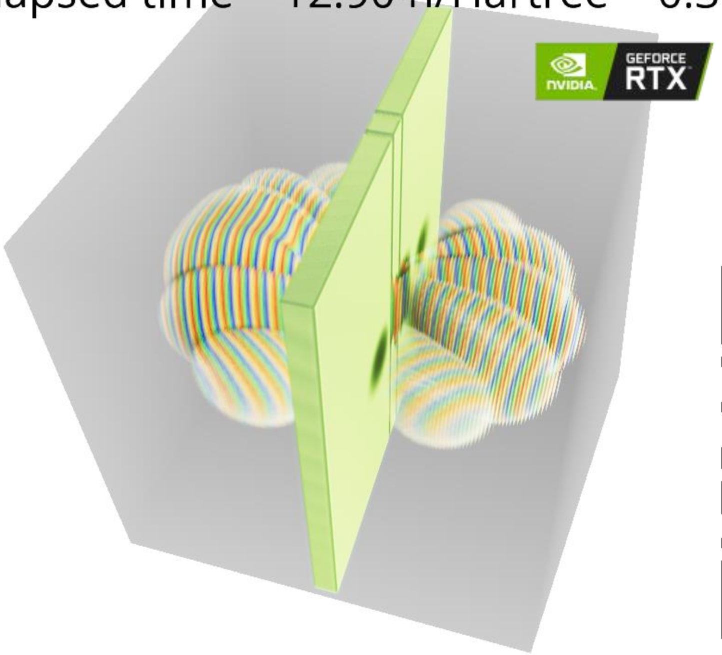


50 × faster



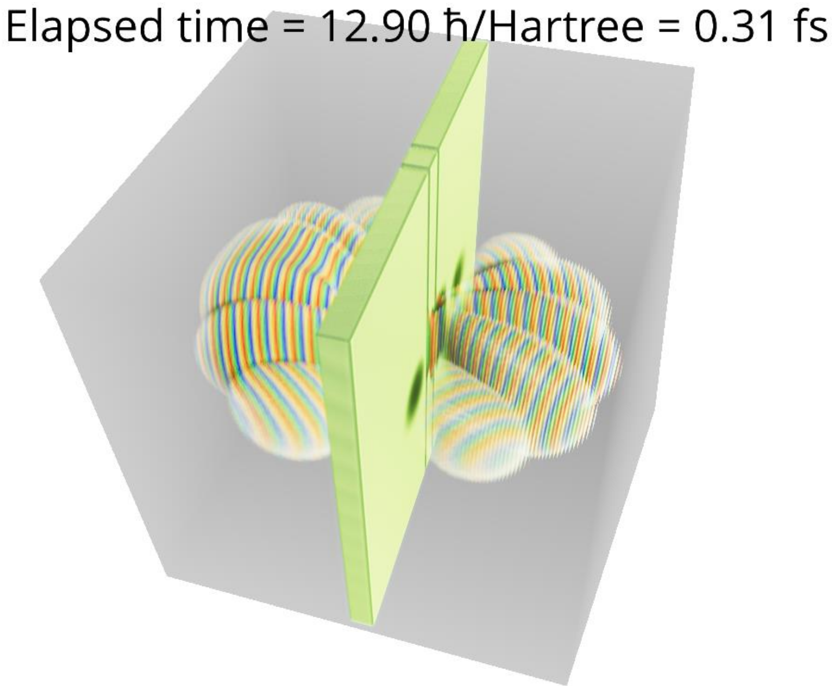
Ray traced

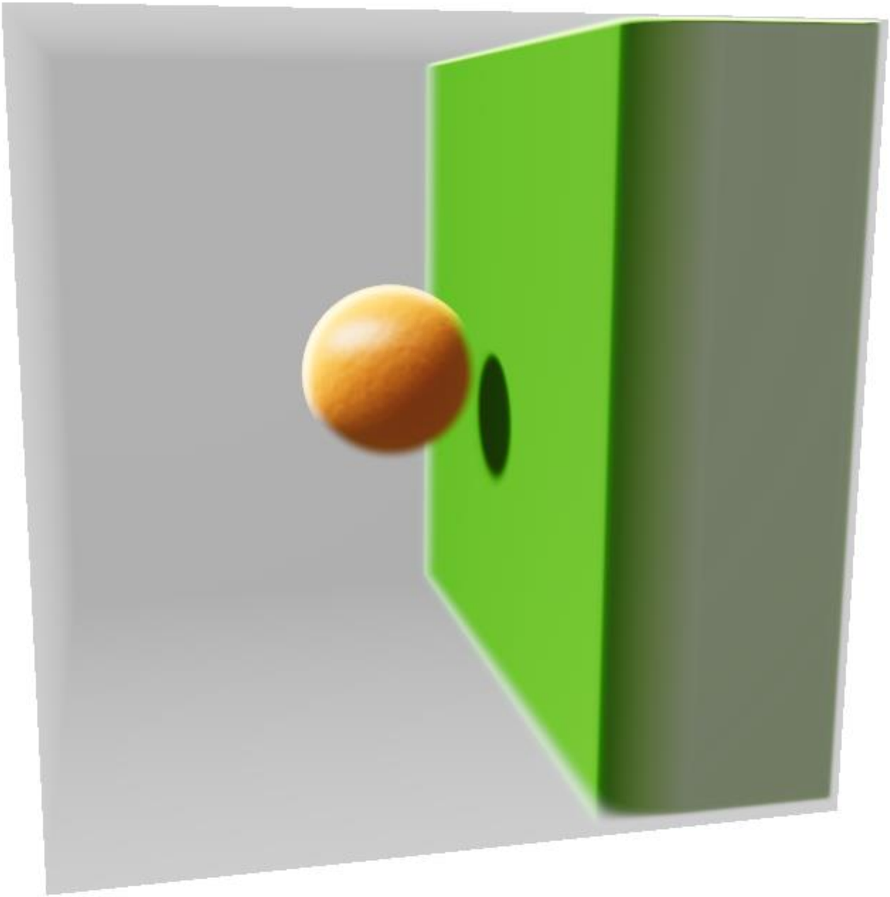
Elapsed time = 12.90 ħ/Hartree = 0.31 fs



Further development

- Experimenting with other simulation methods
- Simulation of multiple 3D particles





Thank you for your attention!

Extra slides

Schrödinger equation

$$i\hbar \frac{d}{dt}\psi(\vec{r},t) = \hat{H}\psi(\vec{r},t)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(\vec{r})$$

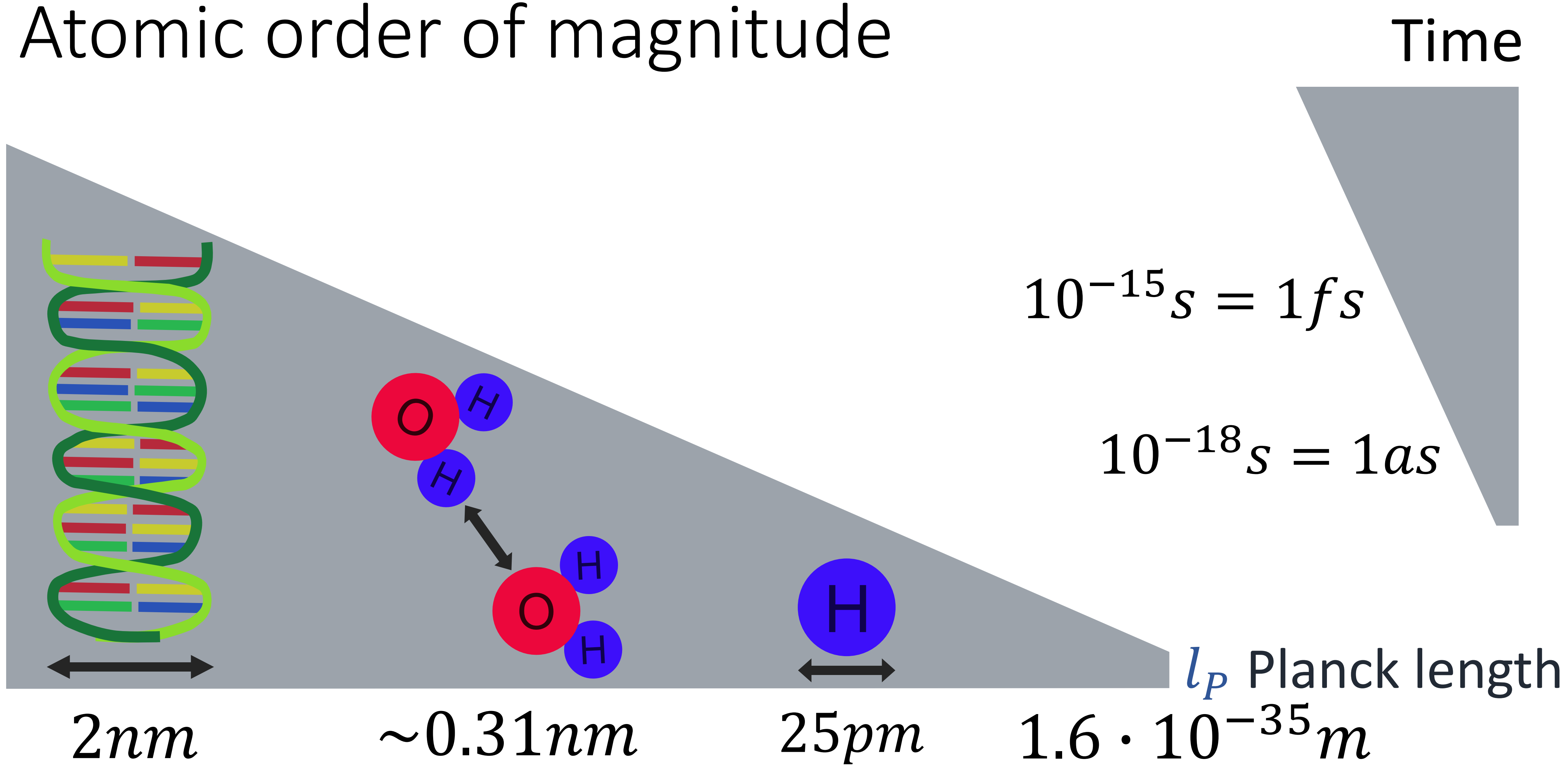
Hamiltonian Kinetic Potential

Erwin Schrödinger 1926

$\rho(\vec{r},t) = |\psi(\vec{r},t)|^2$… probability density of measurement

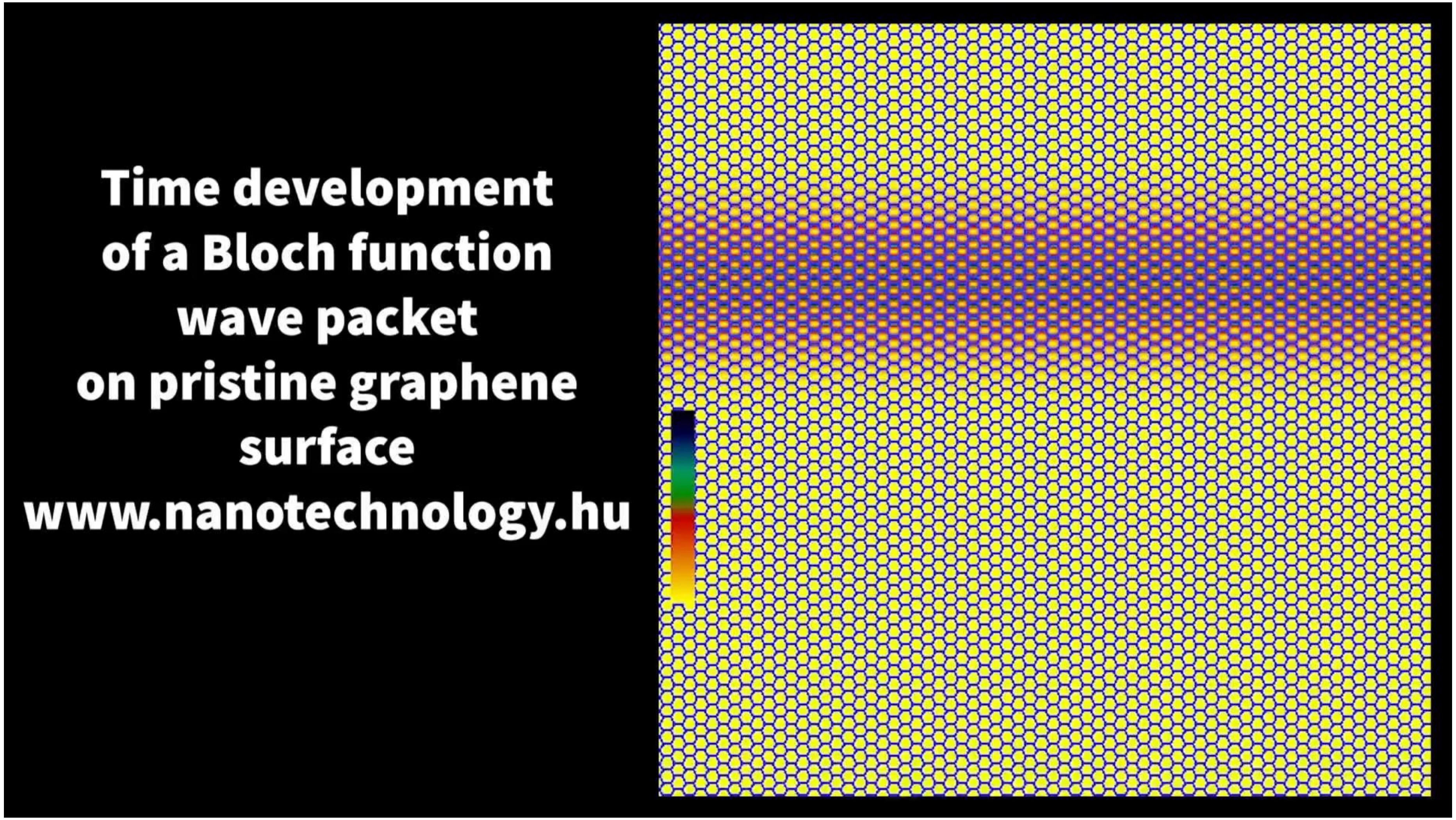
$\hbar \doteq 1.05\times10^{-34} Js$… reduced Planck's constant

Atomic order of magnitude



Double-slit experiment

Wave packet scattering in defected graphene



Mark, G.I.; Vancso, P. Ab-initio wave packet dynamical simulation of defects in 2D materials

This Certificate is awarded to

Geza I. Mark
Peter Vancso

for the paper judged as making the most significant contribution to the conference

18/12/2020

Prof. Dr. Takayoshi Kobayashi
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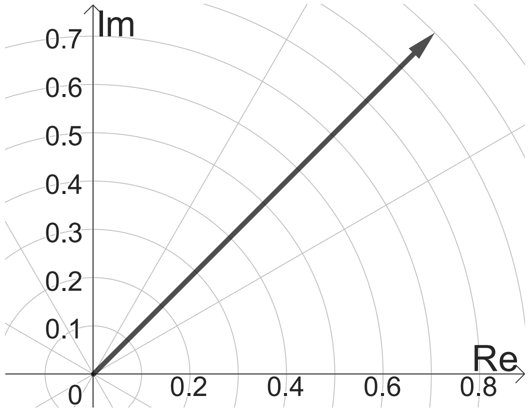
Memory requirement



$512 \times 512 \times 512$ voxel

8 byte / voxel (**4** byte real and **4** byte imaginary part)

- $\psi(\vec{r},t) \in \mathbb{C}$
- $e^{-\frac{ik^2\hbar\delta t}{4m}} \in \mathbb{C}$
- $e^{-\frac{i}{\hbar}V(\vec{r})\delta t} \in \mathbb{C}$
- $\rho(\vec{r},t) \in \mathbb{R}$

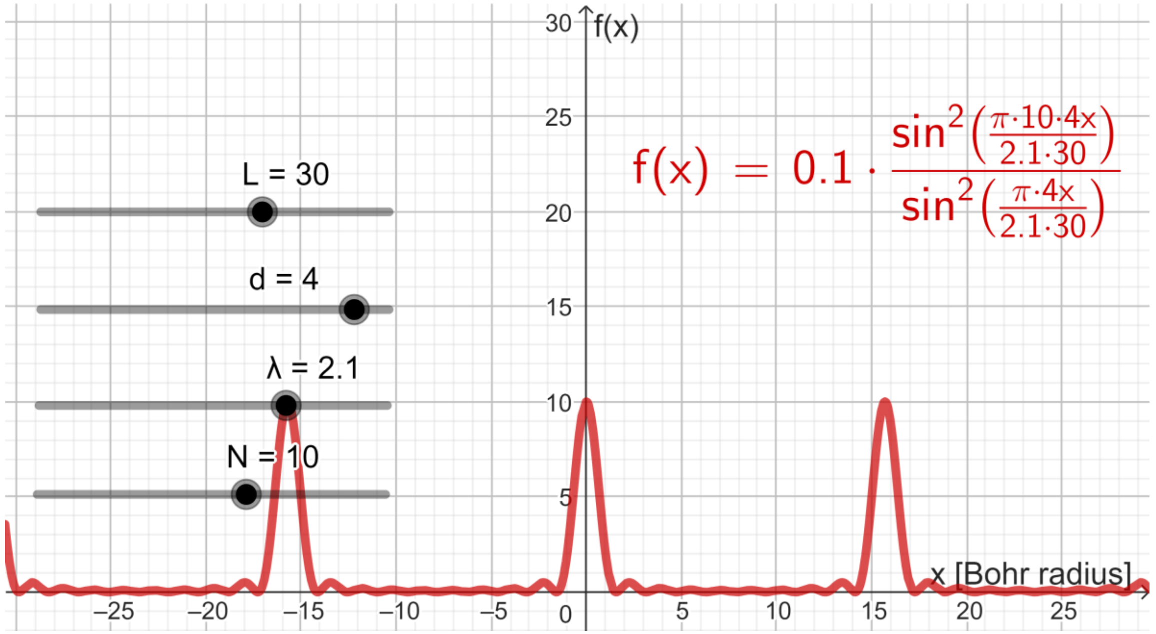
3,5 GB

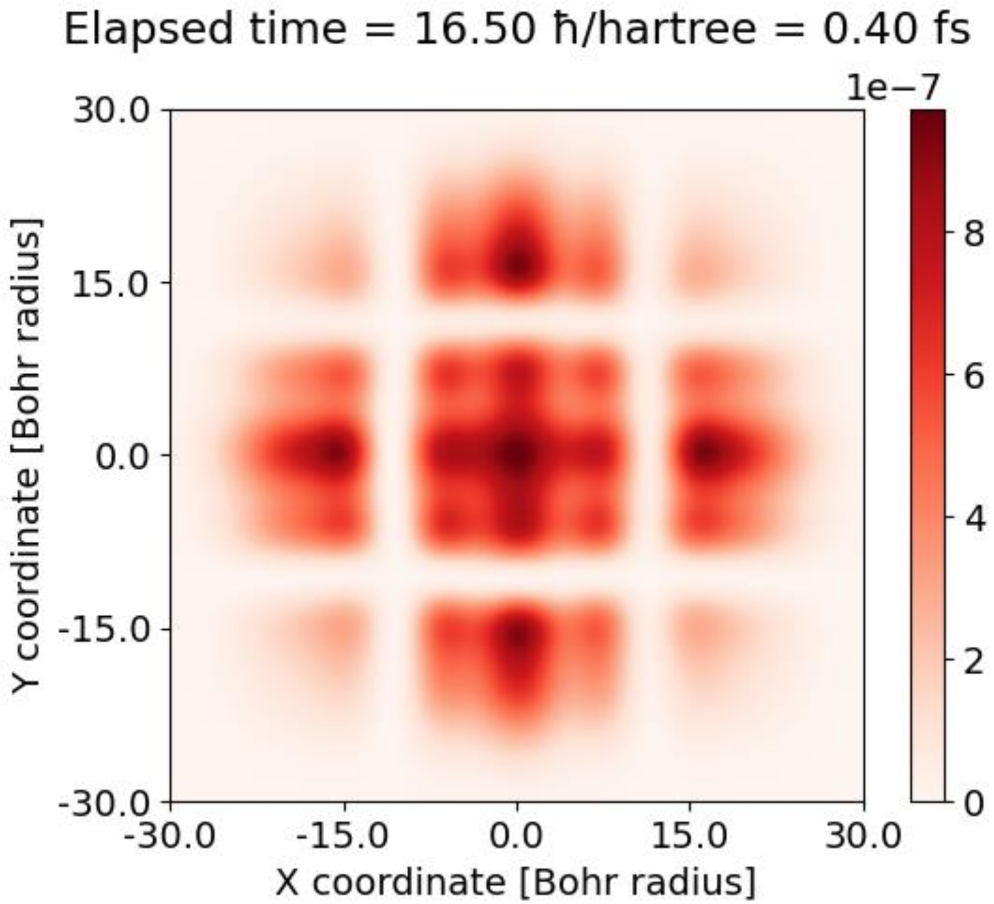
Simulation time

- FFT algorithm $\epsilon\ \mathcal{O}(n\sqrt{n})$
- $\leq 512^3$ voxels are doable
- 1024^3 voxels are already 8 GB

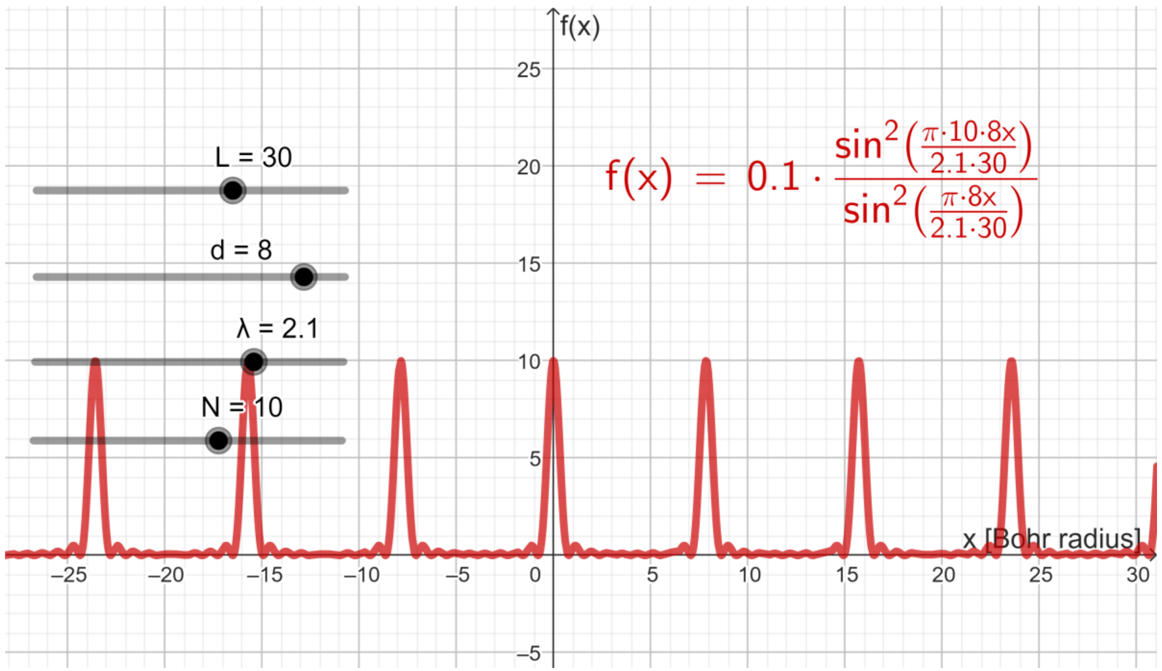
Input size	CPU-only Avg. [iter/s]	GPU accelerated Avg. [iter/s]	Avg. speed up
$128 \times 128 \times 128$	1.1	11.5	$\times 10.45$
$256 \times 256 \times 256$	0.09	6.5	$\times 72.22$
$512 \times 512 \times 512$	0.01	0.5	$\times 50.00$

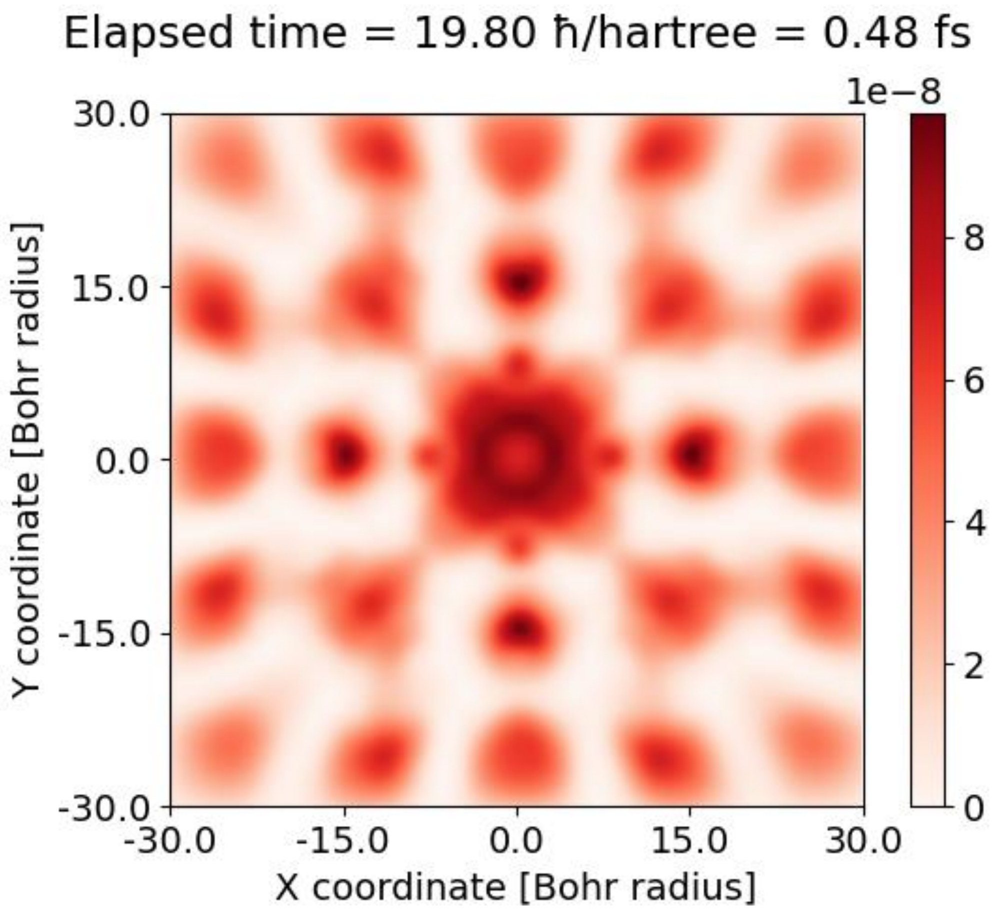
Scattering in diffraction grating (verification)





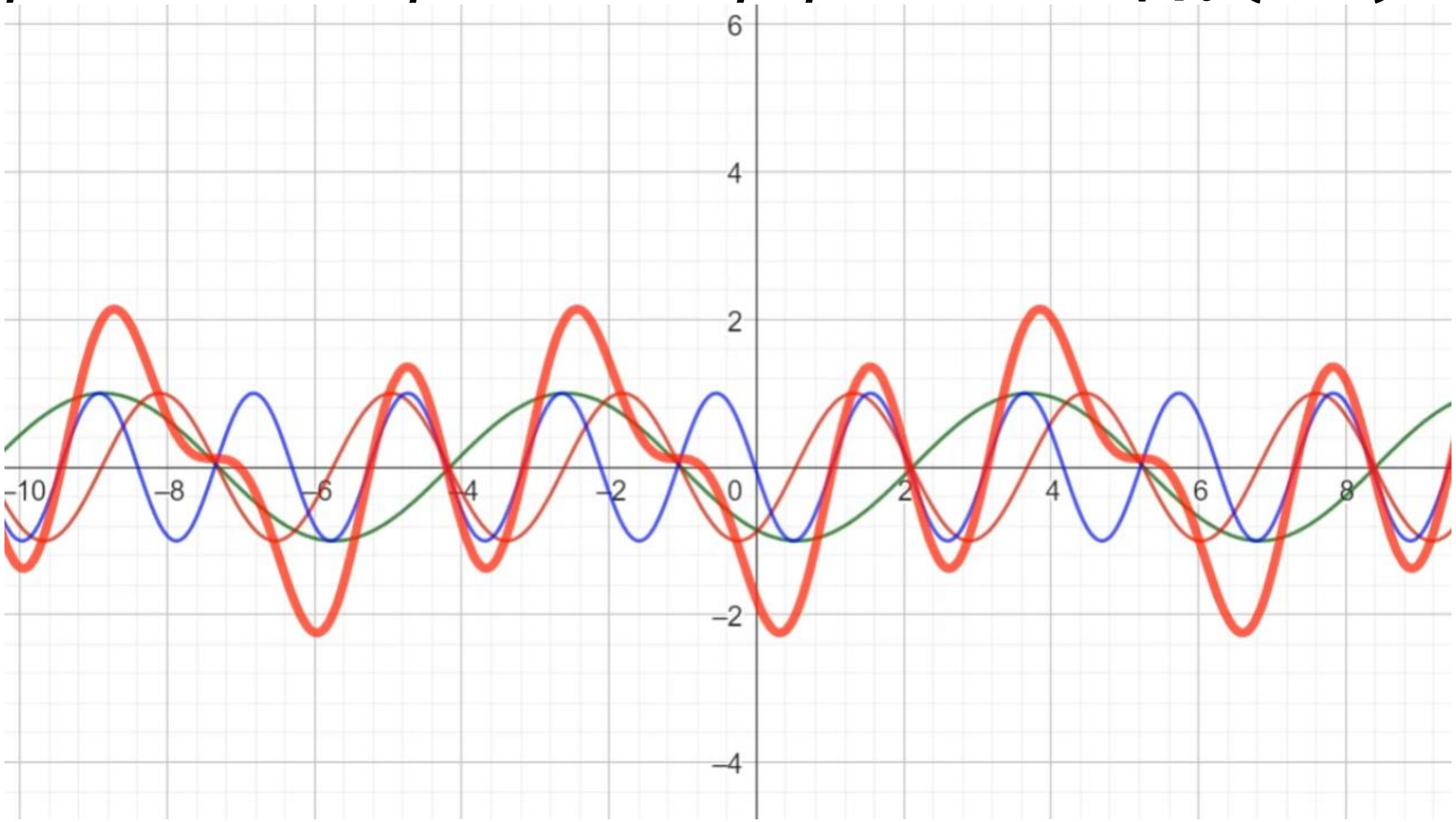
Scattering in diffraction grating (verification)



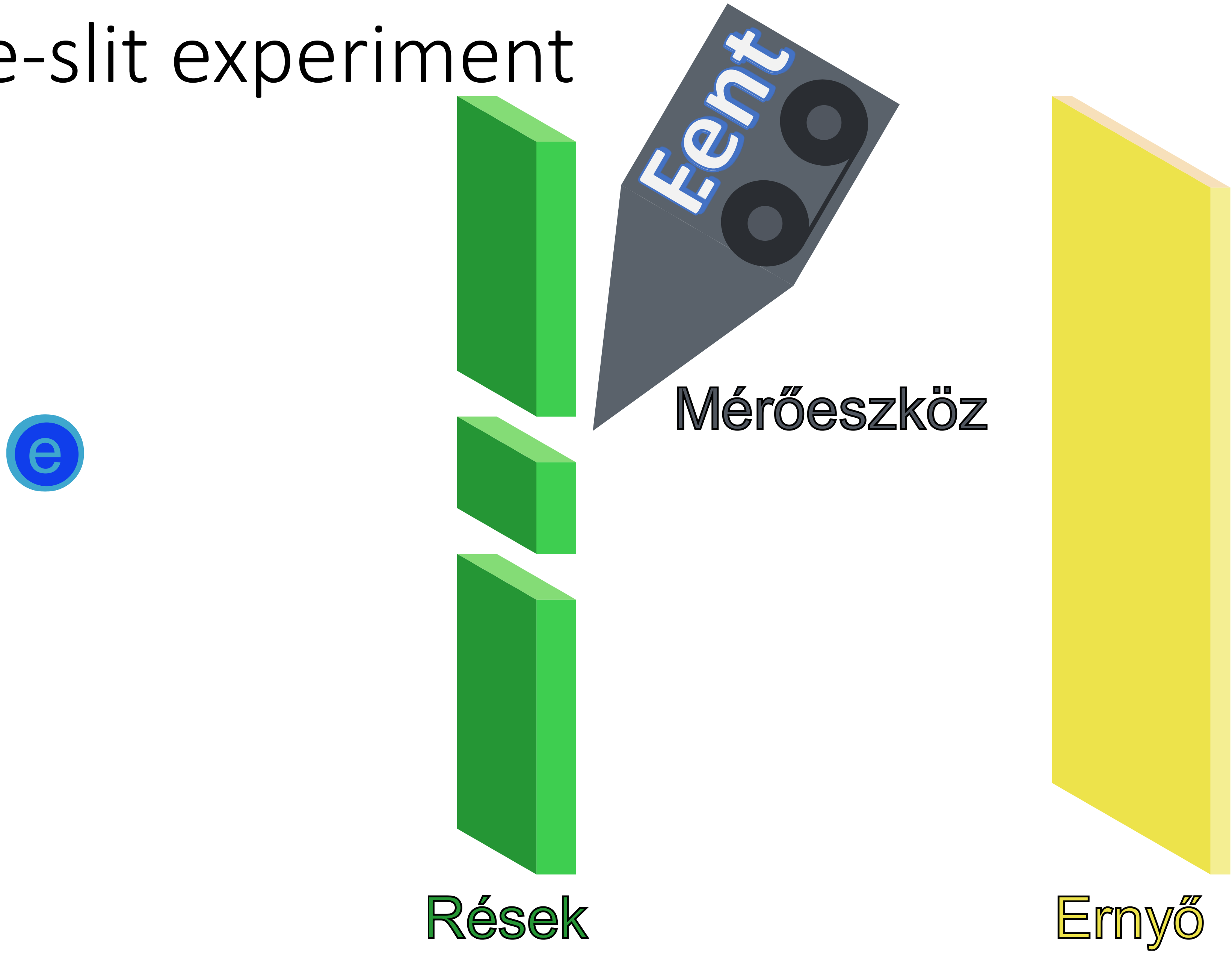


Principle of superposition

$$\psi(\vec{r},t) = \alpha\varphi(\vec{r},t) + \beta\phi(\vec{r},t) + \gamma\chi(\vec{r},t)$$



Double-slit experiment



Newton vs Schrödinger

Newton: $$\frac{d^2}{dt^2}\vec{r} = \frac{1}{m}\vec{F}$$

!

Schrödinger: $$i\hbar\frac{d}{dt}\psi(\vec{r},t) = \hat{H}\psi(\vec{r},t)$$

Hartree atomic units

- Reduced Planck constant … $\hbar = 1$
- Elementary charge … $e = 1$
- Electron rest mass … $m_e = 1$
- Bohr radius … $a_0 = 1$