Please remember to register for the final examination in eCampus no later than January 23, 2026.

Fourier Spectral Method for PDEs

File `pdeSpectral.py` contains a program to solve the diffusion equation $\partial_t f = \kappa \partial_{xx} f$ using the Fourier spectral method as discussed in the lecture.

a) Try it out and extend it towards the convection-diffusion equation $\partial_t f = -c\,\partial_x f + \kappa \partial_{xx} f$ with constant c.

b) Can you, in a similar way, integrate the time-dependent, free-space Schrödinger equation,

$$i\hbar \partial_t \psi(x,t) = -\frac{\hbar^2}{2m} \partial_{xx} \psi(x,t)$$

in this one-dimensional setup ? Try, e.g., a wave packet

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

with $x_c = 3$, $L = 10$, $k_0 = 20\,\frac{2\pi}{L}$, $\sigma = 1/4$ as initial condition, and choose $\kappa = \frac{\hbar}{2m} = 1/20$. Hints: Start a new program file for this problem. Plot $\mathrm{Re}(\psi)$ and $|\psi|$ versus x.

Bonus question I: If you were to introduce an additional potential $V(x)$ in Schrödinger's equation – could you still treat the problem using the Fourier method ?

Bonus question II: Which other methods could you envisage to use instead of the Fourier spectral approach ?

juergen.dreher@rub.de kevin.schoeffler@rub.de