HW

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Problem 1

(a) In this part we use the fact

$$\int_{-\infty}^{\infty} \exp\big(-ax^2 + bx\big) dx = \left(\frac{\pi}{a}\right)^{1/2} \exp\left[\frac{b^2}{4a}\right]$$

Take the Fourier transform of the PDE in x, using the fact $\widehat{\partial_x^n \psi} = (i\xi)^n \psi$.

$$\hat{\psi}_t = \frac{i}{2}(i\xi)^2 \hat{\psi} = -\frac{i}{2}\xi^2 \hat{\psi} \implies \hat{\psi}(\xi, t) = \hat{\psi}_0(\xi) \exp\left[-\frac{i}{2}\xi^2 t\right]$$

Take the inverse Fourier transform.

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \hat{\psi}_0(\xi) \exp\left[ix\xi - \frac{i}{2}t\xi^2\right] d\xi$$

Take the Fourier transform of the initial condition.

$$\begin{aligned}
\hat{\psi}_0(\xi) &= \frac{1}{(2\pi)^{1/2}} \frac{1}{(2\pi\sigma_0^2)^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{4\sigma_0^2} + ik_0 x - i\xi x\right] dx \\
&= \frac{1}{(2\pi)^{3/4}\sigma_0^{1/2}} \int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{4\sigma_0^2} + i(k_0 - \xi)x\right] dx \\
&= \frac{1}{(2\pi)^{3/4}\sigma_0^{1/2}} \pi^{1/2} 2\sigma_0 \exp\big[-(\xi - k_0)^2 \sigma_0^2\big] \\
&= \frac{2^{1/4}\sigma_0^{1/2}}{\pi^{1/4}} \exp\big[-(\xi - k_0)^2 \sigma_0^2\big]
\end{aligned}$$

Then

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}} \frac{2^{1/4}\sigma_0^{1/2}}{\pi^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\sigma_0^2(\xi - k_0)^2 - \frac{i}{2}t\xi^2 + ix\xi\right] d\xi$$

Rewrite the argument of exp as

$$-\sigma_0^2(\xi - k_0)^2 - \frac{i}{2}t\xi^2 + ix\xi = -\sigma_0^2(\xi^2 + k_0^2 - 2k_0\xi) - \frac{i}{2}t\xi^2 + ix\xi = -\left(\sigma_0^2 + \frac{i}{2}t\right)\xi^2 + (ix + 2\sigma_0^2 k_0)\xi - \sigma_0^2 k_0^2$$

so that

$$\begin{aligned}
\psi(x,t) &= \frac{\sigma_0^{1/2}}{2^{1/4}\pi^{3/4}} \int_{-\infty}^{\infty} \exp\left[-\left(\sigma_0^2 + \frac{i}{2}t\right)\xi^2 + (ix + 2\sigma_0^2 k_0)\xi - \sigma_0^2 k_0^2\right] d\xi \\
&= \frac{\sigma_0^{1/2}}{2^{1/4}\pi^{3/4}} e^{-\sigma_0^2 k_0^2} \left(\frac{\pi}{\sigma_0^2 + \frac{i}{2}t}\right)^{1/2} \exp\left[\frac{-x^2 + 4\sigma_0^4 k_0^2 + 4i\sigma_0^2 k_0 x}{4\left(\sigma_0^2 + \frac{i}{2}t\right)}\right] \\
&= \frac{\sigma_0^{1/2} e^{-\sigma_0^2 k_0^2}}{2^{1/4}\pi^{1/4}} \left(\sigma_0^2 + \frac{i}{2}t\right)^{-1/2} \exp\left[\frac{-x^2 + 4\sigma_0^4 k_0^2 + 4i\sigma_0^2 k_0 x}{4\left(\sigma_0^2 + \frac{i}{2}t\right)}\right]
\end{aligned}$$

(b) Discretize the PDE in space with stepsize h and use central differences.

$$\psi_j'(t) = \frac{i}{2h^2}[\psi_{j+1}(t) + u_{j-1}(t) - 2u_j(t)]$$

Let v be such that $v(x_j, t) = \psi_j(t)$.

$$v_t(x,t) = \frac{i}{2h^2}[v(x+h,t) + v(x-h,t) - 2v(x,t)]$$

Taylor expand.

$$\begin{aligned}
v(x+h,t) &= v + hv_x + \frac{1}{2}h^2 v_{xx} + \frac{1}{6}h^3 v_{xxx} + \frac{1}{24}h^4 v_{xxxx} + \frac{1}{120}h^5 v_{xxxxx} + O(h^6) \\
v(x-h,t) &= v - hv_x + \frac{1}{2}h^2 v_{xx} - \frac{1}{6}h^3 v_{xxx} + \frac{1}{24}h^4 v_{xxxx} - \frac{1}{120}h^5 v_{xxxxx} + O(h^6)
\end{aligned}$$

Plug in the expansions.

$$v_t = \frac{i}{2h^2}\left[h^2 v_{xx} + \frac{1}{12}h^4 v_{xxxx} + O(h^6)\right] = \frac{i}{2}v_{xx} + \frac{i}{24}h^2 v_{xxxx} + O(h^4)$$

We obtain the (third order) modified equation.

$$v_t - \frac{i}{2}v_{xx} = \frac{i}{24}h^2 v_{xxxx}$$

The Fourier transform of the RHS term is

$$\frac{i}{24}h^2 \xi^4 \hat{v}$$

so its corresponding term within the solution $\hat{v}(\xi, t)$ in Fourier space is

$$\exp\left[\frac{i}{24}h^2 \xi^4 t\right]$$

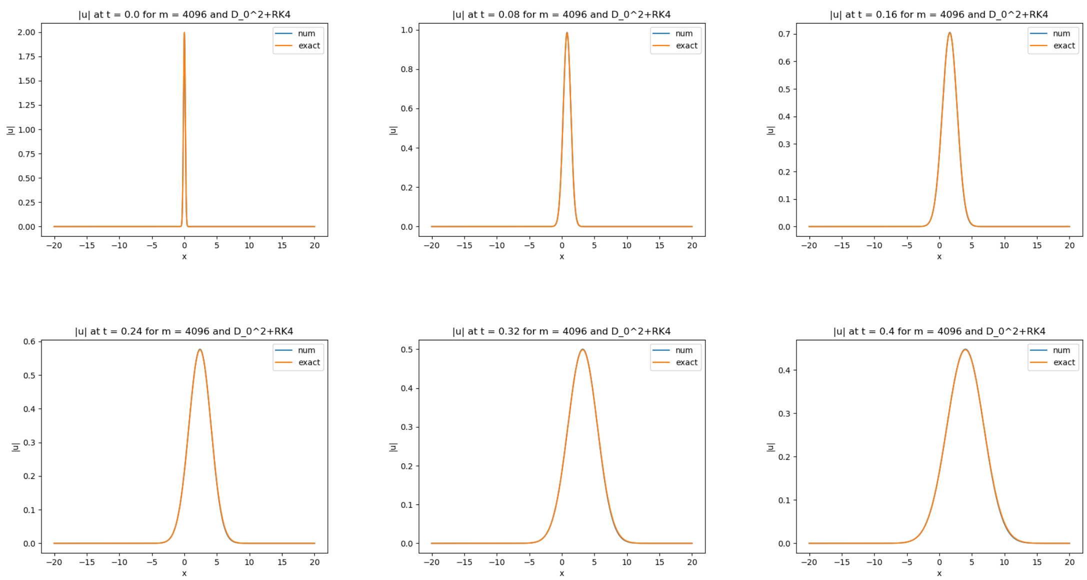
Thus the modified equation introduces artificial Fourier modes which do not decay over time.

(c) pick maximum time T
pick stepsize h and timestep k
set mesh using stepsize h
$N \leftarrow \frac{T}{k}$
set time points between 0 and T using timestep k
set initial condition vector u_0
$\hat{u}_0 \leftarrow$ DFT of u_0
$\xi \leftarrow 2\pi$ times vector of wavenumbers corresponding to mesh
$\hat{u} \leftarrow$ solution of PDE in Fourier space, $\hat{u}_t = -\frac{i}{2}\xi^2\hat{u}$ (use SciPy solver with $\hat{u}_0$ and set of time points)

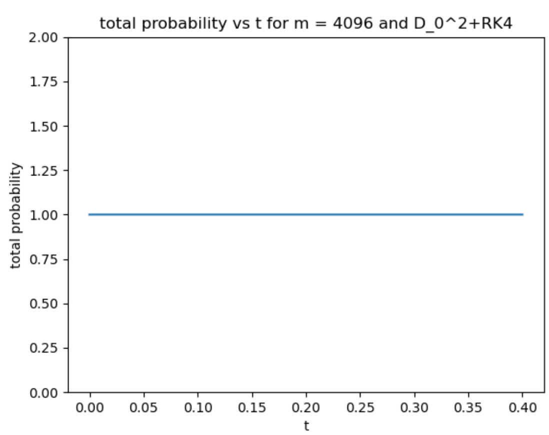
$u \leftarrow$ array of 0s with the same size as $\hat{u}$
for jth row of u **do**
  set the jth row of u as the inverse DFT of the jth row of $\hat{u}$
end for
for $j = 0, \ldots, N$ **do**
  if $jk \in [0, t_1, \ldots, t_M]$ **then**
    print jth row of u
  end if
end for

Problem 2

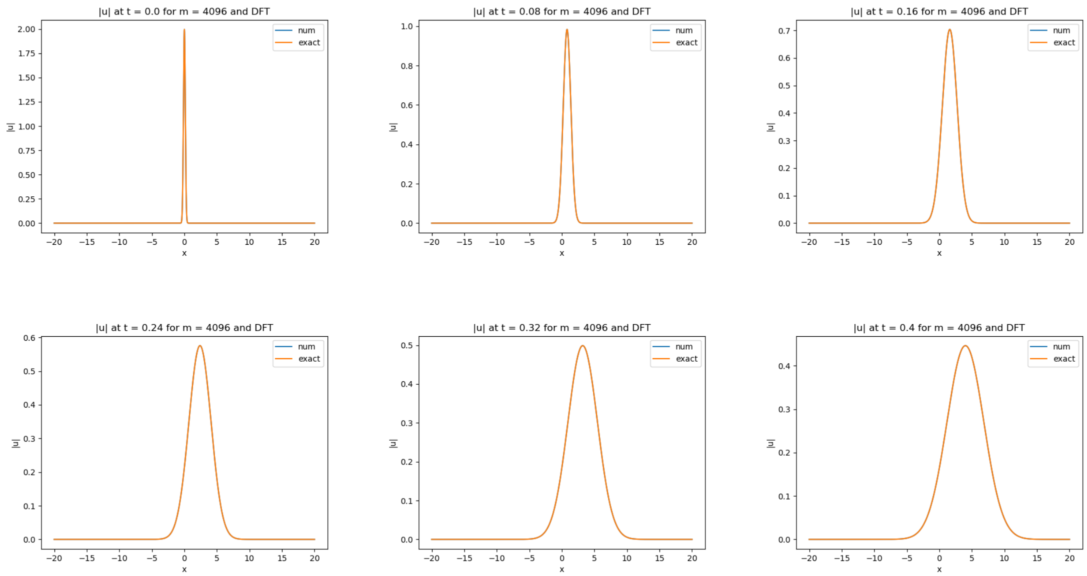
(a) In this part we take 4096 points in space. For D_0^2+RK4:



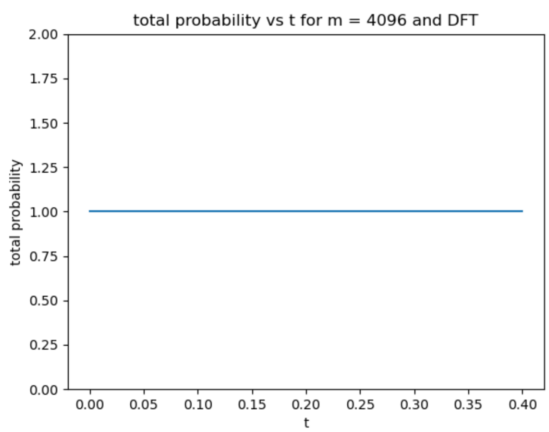
We check the total probability is nearly equal to 1.



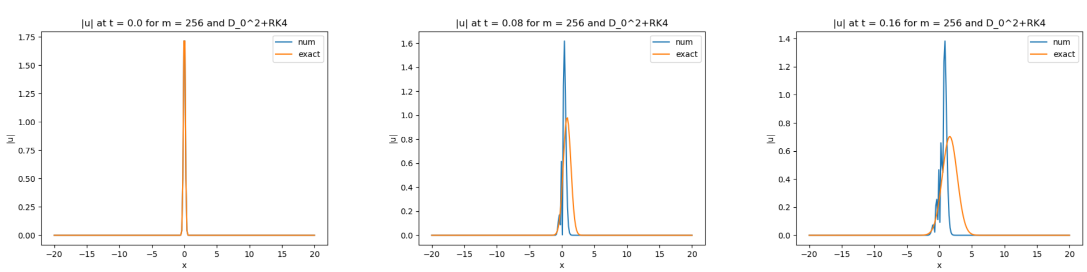
For the method using the discrete Fourier transform (DFT):

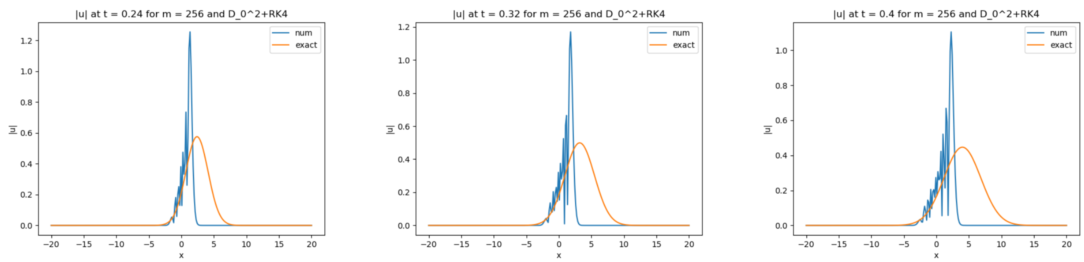


We check the total probability is nearly equal to 1.

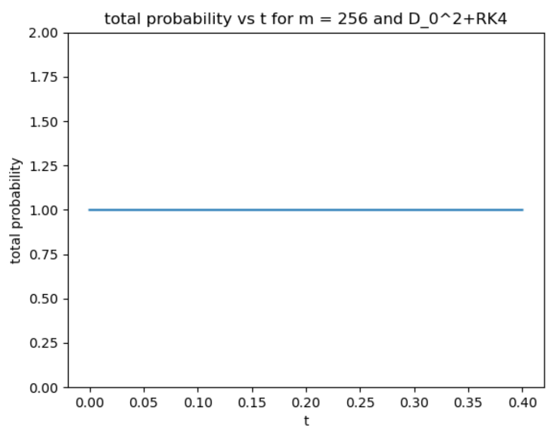


(b) In this part we take 256 points in space. For D_0^2+RK4:

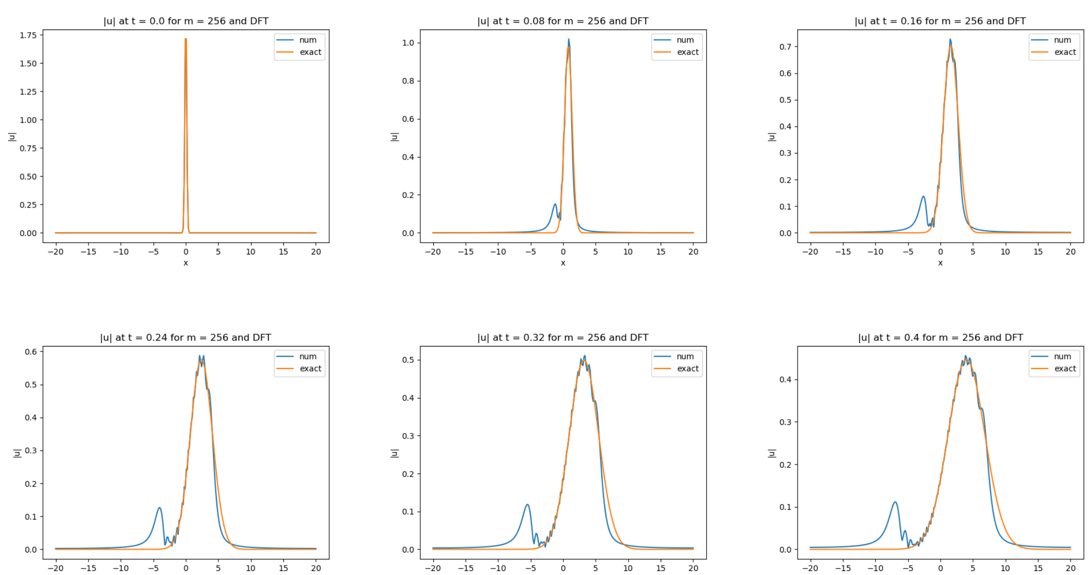




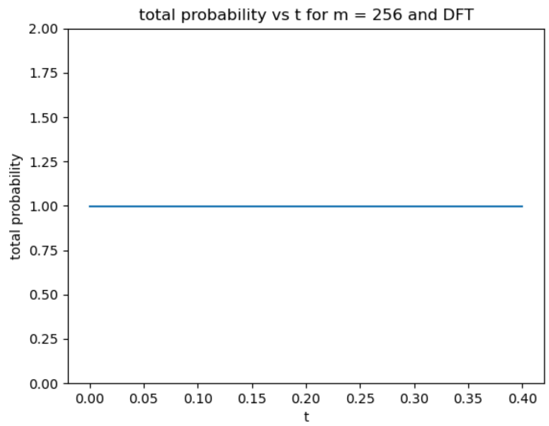
We check the total probability is nearly equal to 1.



For the method using the discrete Fourier transform (DFT):



We check the total probability is nearly equal to 1.



Recalling the modified equation for D_0^2+RK4, the error arises from artificial Fourier modes which do not decay over time. For DFT, the error arises from the splitting of the solution into Fourier modes of different propagation speeds.

Problem 3

(a) Fix a test function $v \in H_0^1(\Omega)$. Multiply the PDE by v and integrate over Ω.

$$\int_\Omega \epsilon v \Delta u dx = \int_\Omega (u^3 - u) v dx$$

Using Green's first identity and the fact $v = 0$ on $\partial\Omega$, the LHS is

$$\int_\Omega \epsilon v \Delta u dx = -\int_\Omega \epsilon \nabla u \cdot \nabla v dx + \int_{\partial\Omega} \epsilon v \frac{\partial u}{\partial n} ds = -\int_\Omega \epsilon \nabla u \cdot \nabla v dx$$

Then we obtain the weak formulation.

$$-\int_\Omega \epsilon \nabla u \cdot \nabla v dx = \int_\Omega (u^3 - u) v dx \implies \int_\Omega \epsilon \nabla u \cdot \nabla v dx - \int_\Omega (u - u^3) v dx = 0$$

(b) Using Newton's iteration

$$y_{n+1} = y_n - J^{-1}(y_n) F(y_n)$$

we obtain

$$J^{-1}(y_n) F(y_n) = y_n - y_{n+1} \implies F(y_n) = J(y_n)(y_n - y_{n+1})$$

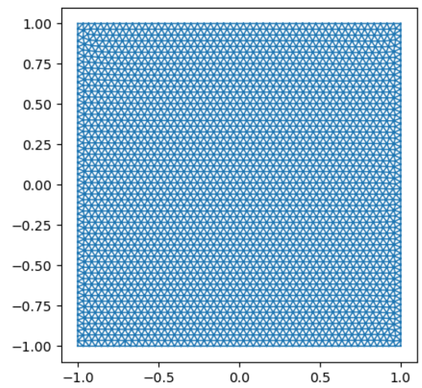
Writing $y_n = (u^n, v)$ and casting $u^n - u^{n+1}$ as a parameter of J,

$$F(u^n, v) = J(u^n, v; u^n - u^{n+1})$$

(c) Code for problem 3:

`https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/FINAL%20q3.ipynb`

Below is a mesh of Ω.


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−1.0
−0.5
0.0
0.5
1.0