Karlsruher Institut für Technologie

Department of Mathematics
Institute for Applied and
Numerical Mathematics

JProf. Dr. Katharina Schratz
Dr. Patrick Krämer

Highly Oscillatory Problems — Exercise Sheet 03 July 12, 2018

In view of constructing numerical integrators for the Klein–Gordon equation

$$\partial_{tt} z(t,x) = -\underbrace{c^2(-\Delta + c^2)}_{=(c\langle\nabla\rangle_c)^2,\ \text{cf. (2)}} z(t,x) + c^2\lambda f(z(t,x)), \quad z(0,x) = \varphi(x), \quad \partial_t z(0,x) = c^2\gamma(x), \tag{1}$$

for $t \in [0,T]$ and $x \in [-\pi,\pi] =: \mathbb{T}$, equipped with periodic boundary conditions, i.e.

$$z(t,-\pi) = z(t,+\pi), \quad \partial_x^m z(t,-\pi) = \partial_x^m z(t,+\pi), \quad \text{for } m \in \mathbb{N} \qquad \text{for all } t \in [0,T],$$

the aim of this exercise sheet is to discuss the discretization of the spatial operators ∂_x^m and in particular

$$\langle\nabla\rangle_c := \sqrt{-\Delta + c^2} \tag{2}$$

with so-called Fourier pseudospectral (FP) methods. We look for solutions $z(t,\cdot)$ of (1) in Sobolev spaces $H^r(\mathbb{T})$, $r \geq 0$ equipped with the norm

$$\|u\|_{H^r} = \sum_{k\in\mathbb{Z}} \left(1 + |k|^2\right)^r |\widehat{u_k}|^2, \quad \text{for all } u \in H^r(\mathbb{T}), \quad \text{(the coefficients } \widehat{u_k} \text{ are defined below)}.$$

Note that all $u \in H^r(\mathbb{T})$ satisfy periodic boundary conditions on $\mathbb{T}$. It is well known that the set $\{e^{ikx}, k \in \mathbb{Z}\}$ forms an infinite basis in the spaces $H^r(\mathbb{T})$, $r \geq 0$, such that all $u \in H^r(\mathbb{T})$ have the Fourier series representation

$$u(x) = \sum_{k\in\mathbb{Z}} \widehat{u_k} e^{ikx}, \qquad \widehat{u_k} = \int_{\mathbb{T}} u(x) e^{-ikx} dx = \int_{-\pi}^{\pi} u(x) e^{-ikx} dx. \tag{3}$$

Exercise 6: (Klein–Gordon in Fourier space)

In the following, assume that for all $t \in [0,T]$ the function

$$z(t,x) := \sum_{k\in\mathbb{Z}} \widehat{z_k}(t) e^{ikx} \tag{4}$$

solves the Klein–Gordon equation (1) for fixed $c \geq 1$, i.e. we set $f(z) = z$.

a) From the ansatz (4), derive an ordinary differential equation for each Fourier coefficient $\widehat{z_k}(t)$ depending on time t for all $k \in \mathbb{Z}$.

b) Exploit the results from part a) in order to motivate the definition of $\langle\nabla\rangle_c = \sqrt{-\Delta + c^2}$ via its Fourier representation

$$\langle\nabla\rangle_c u(x) := \sum_{k\in\mathbb{Z}} \langle k\rangle_c \widehat{u_k} e^{ikx}, \quad \langle k\rangle_c = \sqrt{|k|^2 + c^2}, \qquad u \in H^1(\mathbb{T}).$$

c) *Advanced:* Now let $f(z) = |z|^2 z$ be a cubic nonlinearity. Exploit ansatz (4) and determine the k-th Fourier coefficient $\widehat{f_k}(t)$ of $f(z(t,x))$ by considering

$$f(z(t,x)) = f\left(\sum_{k\in\mathbb{Z}} \widehat{z_k}(t) e^{ikx}\right) \stackrel{!}{=} \sum_{k\in\mathbb{Z}} \widehat{f_k}(t) e^{ikx}.$$

Note that for $k \in \mathbb{Z}$ the coefficient $\widehat{f_k}(t)$ depends on the coefficients $\widehat{z_\ell}(t)$, $\ell \in \mathbb{Z}$, of $z(t,x)$.

next page →

The Fourier Pseudospectral (FP) Space Discretization (based on [Faou2012, Tref2000])

In the following, let u be smooth and periodic on the interval $[-\pi, \pi]$. Furthermore let $N \in \mathbb{N}$ be even and let a discretization of the interval $[-\pi, \pi]$ be defined through

$$x_j = jh, \; j = -N/2, \dots, N/2, \qquad \text{with} \qquad h = (2\pi)/N.$$

In order to discretize spatial differential operators, the idea is to use a **trigonometric interpolation polynomial** $t_N(x)$ to approximate $u(x)$ with interpolation property in the grid points x_j, i.e.

$$t_N(x_j) = u(x_j), \qquad j = -N/2, \dots, N/2.$$

Let $U \in \mathbb{C}^N$ with $U_j = u(x_j), j = -N/2+1, \dots, N/2$. We define the following trigonometric polynomial

$$t_N(x) = \frac{1}{2N}\left(\widehat{U}_{-N/2}e^{-ixN/2} + \widehat{U}_{N/2}e^{ixN/2}\right) + \frac{1}{N}\sum_{k=-N/2+1}^{N/2-1} \widehat{U}_k e^{ikx} \quad \text{for all } x \in [-\pi, \pi]$$

where $\widehat{U} = \mathcal{F}_N U = \left(\widehat{U}_k\right)_{k=-N/2+1}^{N/2}$ is the **discrete Fourier transform** of U, defined via

$$\widehat{U}_k := \sum_{j=-N/2+1}^{N/2} U_j e^{-ijx_k} \quad \text{for all } k = -N/2+1, \dots, N/2.$$

Remark: *Note that $\widehat{U}_k$ can also be interpreted as an approximation to the Fourier coefficient $\widehat{u_k}$ via the application of the trapezoidal quadrature rule with nodes x_j to the integral in* (3).

Exercise 7: (Trigonometric Interpolation Polynomial)

a) Show that for all $k = -N/2, \dots, N/2$ we have that
$$\hat{U}_{-N/2}e^{-ix_kN/2} = \hat{U}_{N/2}e^{ix_kN/2}.$$

b) Exploiting part a), show that t_N satisfies the interpolation property, i.e. show that
$$t_N(x_j) = u(x_j) \qquad \text{for all } j = -N/2, \dots, N/2.$$

In particular, with the aid of Exercise 7, we define the **inverse discrete Fourier transform** $\mathcal{F}_N^{-1}\hat{U}$ of $\hat{U}$ through

$$\left(\mathcal{F}_N^{-1}\hat{U}\right)_j := \frac{1}{N}\sum_{k=-N/2+1}^{N/2} \hat{U}_k e^{ikx_j} = t_N(x_j), \qquad j = -N/2+1, \dots, N/2.$$

Based on the trigonometric polynomial t_N and the discrete Fourier transform above, we numerically approximate the m-th spatial derivative of u, i.e. $\partial_x^m u(x_j)$, in the grid points $x_j, j = -N/2+1, \dots, N/2$ by

$$\partial_x^m t_N(x_j) = t_N^{(m)}(x_j) = \mathcal{F}_N^{-1}\left((i\tilde{k})^m \cdot \mathcal{F}_N U\right)_j, \quad j = -N/2+1, \dots, N/2,$$

where (see remark in the footnote on the ordering in MATLAB and Python)

$$\tilde{k} = [-N/2+1, \dots, N/2-1, \chi], \quad \chi = \begin{cases} N/2, & m \text{ even}, \\ 0, & m \text{ odd}. \end{cases}$$

Note that the theory on spectral derivatives also works for periodic functions on arbitrary intervals $[a, b] \subset \mathbb{R}$.

c) Determine a linear transformation of the interval $[-\pi, \pi]$ to the interval $[a, b] \subset \mathbb{R}$. Which **additional factor** in the coefficients $\tilde{k}$ is then necessary in order to correctly apply the spectral scheme as described?

Remark: *Note that also for higher spatial dimensions $d \geq 1$, i.e. $x \in \mathbb{T}^d$, this scheme satisfies error bounds which only depend on the regularity of u and on the number of grid points $N \in \mathbb{N}$, i.e. for $s' - s > d/2$ we have*

$$\|\partial_x^m u - \partial_x^m t_N\|_{H^r} \leq \|u - t_N\|_{H^{r+m}} \leq K \cdot N^{-s}\|u\|_{H^{r+m+s'}}, \qquad u \in H^{r+m+s'}(\mathbb{T}^d).$$

next page →

Note that the Fourier numbers are order differently in MATLAB and Python as follows $\tilde{k} = [0, \dots, N/2-1, \chi, -N/2+1, \dots, -1]$.

[Faou2012] - E. Faou, *Geometric numerical integration and Schrödinger equations*, EMS 2012
[Tref2000] - L. Trefethen, *Spectral methods in MATLAB*, SIAM 2000

Programming Exercise 3: (Implementation of the FP Discretization Scheme)

Consider $u(x) := \exp(\sin(x))$ on the interval $x \in [-\pi, \pi]$ and consider $N_x = 16$ grid points at first.

a) Implement the spectral space discretization scheme to compute an approximation to the second derivative $u''(x)$. Plot the numerical result together with the exact derivative.

   Hint: Use the MATLAB built-in functions `fft` and `ifft`, and the Python functions `numpy.fft.fft`, `numpy.fft.ifft` respectively. Note that MATLAB and also Python orders the Fourier numbers as follows

$$\tilde{k} = [0, \ldots, N_x/2 - 1, \chi, -N_x/2 + 1, \ldots, -1] \qquad \text{(see also [Tref2000]).}$$

b) Add a finite difference (FD) approximation to u'' to your plot. What do you observe?
   Recall *that, a FD approximation to u'' in the grid points $x_j, j = -N_x/2 + 1, \ldots, N_x/2$ is obtained by computing the matrix vector product AU, where the matrix A is defined via $A := \frac{1}{h^2}\text{tridiag}(1, -2, 1)$, with additional nonzero entries $A_{N_x,1} = \frac{1}{h^2} = A_{1,N_x}$ due to p.b.c., and where the vector U is a vector with entries $U_j := u(x_j)$, $j = -N_x/2 + 1, \ldots, N_x/2$.*

c) Create an order plot for the spatial accuracy of the FP and the FD method using $N_x^\ell = 8 \cdot 2^\ell$, $\ell = 0, \ldots, 9$ grid points. Compute the corresponding errors in the approximate L^2 norm, i.e.

$$\text{err}_\ell = \sqrt{h_\ell}\, \|u''_{num} - u''_{exact}\|_2 .$$

d) Repeat all the steps for the function $g(x) = 1/\cosh(x)$ on the interval $x \in [-\pi, \pi]$. What can you observe?

   How do your results change if we consider g on $x \in [-4\pi, 4\pi]$ instead? Can you give an explanation?

   Hint: $\cosh(x) = (e^x + e^{-x})/2$, $\frac{d}{dx}\cosh(x) = \sinh(x)$, $\cosh(x)^2 = 1 + \sinh(x)^2$.

Programming Exercise 4: (Implementation of an Exponential-type FP Time Integration Scheme for KG)

In this programming exercise, we construct an exponential integrator for the linear Klein–Gordon equation

$$\partial_{tt} z(t,x) = -c^2 \langle\nabla\rangle_c^2 z(t,x) + c^2 \lambda z(t,x), \quad z(0,x) = \varphi(x), \quad \partial_t z(0,x) = c\,\langle\nabla\rangle_c\,\gamma(x), \tag{6}$$

with $\lambda = \frac{1}{2}$ on the torus $\mathbb{T} = [-\pi, \pi]$ (i.e. periodic boundary conditions) and for $t \in [0, T]$.
In the following let $T = 1$ and let

$$\varphi(x) := \frac{\cos(x) - 2\sin(2x)}{2 - \sin(x)} \qquad \text{and} \qquad \gamma(x) =:= \frac{\sin(x) - 2\cos(2x)}{2 - \cos(x)}.$$

For practical implementation issues we consider the discretization of time $t_n = n\tau$, $n = 0, 1, 2, \ldots \lfloor T/\tau \rfloor =: N_T$ and of space $x_j = jh$, $j = -\frac{N_x}{2} + 1, \ldots \frac{N_x}{2}$ with $N_x = 128$ and for

$$\tau = \tau_m = \frac{T}{N_T^m}, \quad N_T^m := 2^m, \qquad m = 1, 2, \ldots, 8 \qquad \text{and} \qquad h = \frac{2\pi}{N_x}.$$

(a) Building up on your code from Programming Exercise 2, combine and implement the exponential integrator Φ_{exp}^τ from Exercise Sheet 2 with the FP space discretization scheme from Programming Exercise 3 in order to approximate the solution of the linear KG equation (6).

(b) Analogously to the previous exercise sheets, the exact solution of (6) is given as

$$z(t,x) = \cos(t\Omega_c)\,\varphi(x) + \frac{\sin(t\Omega_c)}{\Omega_c} c\,\langle\nabla\rangle_c\,\gamma(x), \quad \Omega_c = c\sqrt{\langle\nabla\rangle_c^2 - \lambda}$$

   Animate the numerical solution and the exact solution together in one plot for all times t_n corresponding to the time step τ_6 and for $c = 1$ and $c = 8$.

(c) Proceed according to Programming Exercise 2b) and for $c_\ell = 1.7^\ell$, $\ell = 0, 1, \ldots, 10$ create order plots for both the convergence in the time step size τ and in the parameter c of the scheme Φ_{exp}^τ corresponding to the time step sizes τ_m, $m = 1, \ldots, 8$ considering the maximal error in the discrete L^2 norm (cf. Programming Exercise 3c)), i.e.

$$\text{err}_{\max} = \max_{t_n \in [0,T]} \|z(t_n, \cdot) - z^n\|_{L^2} .$$

   Hint: For each combination of time step τ_m and parameter c_ℓ save the corresponding $\text{err}_{\max}^{\ell,m}$ in a two-dim. array.

Discussion in the problem class friday 11:30 am, in room 2.058 in the Kollegiengebäude Mathematik 20.30.