Norwegian University of Science and Technology Department of Mathematical Sciences	TMA4212 Finite Difference Method Spring 2021 **Semester Project Part 2**

For the second part of the project, the aim is to study one of the PDEs below. You can either ask a question on Piazza, or to Abdullah Abdulhaque (abdullah.abdulhaque@ntnu.no) or Yuya Suzuki (yuya.suzuki@ntnu.no).

$\boxed{1}$ **Biharmonic equation (Abdulhaque)**

Consider the inhomogeneous Biharmonic equation with clamped boundary conditions on the unit square $\Omega = [0,1]^2$:

$$\nabla^4 u = f \quad , \quad (x,y) \in \Omega \tag{1a}$$

$$u = 0 \ , \ \nabla^2 u = 0 \quad , \quad (x,y) \in \partial\Omega \tag{1b}$$

In this setting, we have two partial differential operators:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \qquad , \qquad \nabla^4 = \frac{\partial^4}{\partial x^4} + 2\frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial y^4}$$

a) Justify that the solution of this BVP can be represented by a double Fourier sine series on the form

$$u(x,y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} F_{mn} \sin(m\pi x) \sin(n\pi y) \tag{2}$$

Calculate the coefficient F_{mn}. How can you choose f such that the infinite series collapse into a single expression? (Hint: Euler's orthogonality relations.)

b) Transform (1) into a system of Poisson equations.

c) Consider the 5-point stencil ($\nabla_5^2 u$) and 9-point stencil ($\nabla_9^2 u$) for $\nabla^2 u = f$:

$$u_{i-1,j} + u_{i+1,j} - 4u_{ij} + u_{i,j-1} + u_{i,j+1} = h^2 f_{ij} \tag{3}$$

$$\begin{aligned} &\frac{1}{6}\left(u_{i+1,j+1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i-1,j-1}\right) \\ &+ \frac{2}{3}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) - \frac{10}{3} u_{ij} \\ &= h^2 \left[\frac{2}{3} f_{ij} + \frac{1}{12}\left(f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1}\right)\right] \end{aligned} \tag{4}$$

Describe in full detail what the system matrix, consisting of several blocks, will look like. What are the eigenvalues of the TST-matrices in this system?
(Hint: TST is an abbreviation for Toeplitz, Symmetric and Tridiagonal. They have many special properties you can take advantage of in the later numerical computation process.)

d) Prove that the 5-point stencil is stable and of order 2. Follow this procedure:

1. Discrete maximum principle: If $\nabla_5^2 v \geq 0$ on Ω, then the maximum value of v on $\overline{\Omega}$ attains its value on $\partial\Omega$.
2. If v_h is a discrete function that equals 0 on $\partial\Omega$, then

$$\|v\|_\infty \leq \frac{1}{8}\|\nabla_5^2 v\|_\infty$$

3. If $\nabla^2 u = f$ and $\nabla_5^2 v = f$, then

$$\|u - v\|_\infty \leq Ch^2 |D^4 v|_\infty$$

e) Prove that the 9-point stencil is stable and of order 4. Follow this procedure:

1. Discrete maximum principle: If $\nabla_9^2 v \geq 0$ on Ω, then the maximum value of v on $\overline{\Omega}$ attains its value on $\partial\Omega$.
2. If v_h is a discrete function that equals 0 on $\partial\Omega$, then

$$\|v\|_\infty \leq \frac{3}{40}\|\nabla_9^2 v\|_\infty$$

3. If $\nabla^2 u = f$ and $\nabla_9^2 v = f$, then

$$\|u - v\|_\infty \leq Ch^4 |D^6 v|_\infty$$

f) Describe how the Fast Poisson Solver method can be used, and give a concise explanation of how it works. (Hint: Fast Fourier Sine Transform.)

g) Perform uniform mesh refinement with $M = \{8, 16, 32, 64, 128, 256\}$ in order to verify the order of the 5-point and 9-point stencils. Apply 1a) to choose an analytical solution, and use the same number of grid points in both directions.

h) Consider the following BVP:

$$\begin{aligned} &\nabla^4 u = f(x,y) && (x,y) \in \Omega \\ &u = 0\,,\ \nabla^2 u = 0 && (x,y) \in \partial\Omega \end{aligned}$$

where $f(x,y) = (\sin(\pi x)\sin(\pi y))^4 e^{-(x-0.5)^2-(y-0.5)^2}$. Solve the given problem as good as you can and report the results in the following loglog-graphs:

- x-axis with degrees of freedom, y-axis for relative l^2-error.
- x-axis with degrees of freedom, y-axis for computational time.

$\boxed{2}$ Sine-Gordon equation (Abdulhaque)

Consider the Sine-Gordon equation on $\Omega \times I$, where $\Omega = [a, b]$ and $I = [0, T]$:

$$
\begin{aligned}
&u_{tt} - u_{xx} + \sin(u) = 0 \quad , \quad (x,t) \in \Omega \times I && \text{(5a)}\\
&u(a,t) = f_1(t)\ ,\ u(b,t) = f_2(t) \quad , \quad (x,t) \in \partial\Omega \times I && \text{(5b)}\\
&u(x,0) = u_0(x)\ ,\ u_t(x,0) = u_1(x) \quad , \quad x \in \Omega \times \{t = 0\} && \text{(5c)}
\end{aligned}
$$

a) Find the analytical solution with the following procedure:

1. Introduce $s = x - ct$ and express the equation in terms of s.
2. Use the chain rule to integrate.
3. Choose 1 and 0 as the constants of integration.
4. Apply the following identities:

$$\frac{1+\cos(x)}{2} = \sin^2\left(\frac{x}{2}\right) \quad , \quad \int \frac{1}{\sin(x)}\,dx = \ln\tan\left(\frac{x}{2}\right) + C$$

b) Show that the energy is conserved when $u_x(a,t), u_x(b,t) = 0$, i.e. $E(t) = E(0)$. (Hint: Multiply the equation with u_t and integrate with respect to x and t)

c) Use semi-discretization (2nd order stencil on u_{xx}) on the equation. Show that we have two systems of equations (1st and 2nd order in time).

d) Implement the following explicit Runge-Kutta schemes:

$$
\begin{array}{c|cc}
0 & 0 & 0\\
1 & 1 & 0\\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{2} & 0 & 0\\
1 & -1 & 2 & 0\\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
\qquad
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0\\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0\\
1 & 0 & 0 & 1 & 0\\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

Table 1: RK2 (order 2), RK3 (order 3), RK4 (order 4).

Perform h- and t-refinement for each integrator (use analytical solution).

e) Implement the following explicit and symplectic Runge-Kutta-Nyström schemes:

$$
\begin{array}{c|c}
0 & 0\\
\hline
\bar{b}_i & \frac{1}{2}\\
\hline
b_i & 1
\end{array}
\qquad
\begin{array}{c|ccc}
\frac{1}{2} - \delta & 0 & 0 & 0\\
\frac{1}{2} & \frac{1}{24\delta} & 0 & 0\\
\frac{1}{2} + \delta & \frac{1}{12\delta} & \delta - \frac{1}{12\delta} & 0\\
\hline
\bar{b}_i & b_1(1-c_1) & b_2(1-c_2) & b_3(1-c_3)\\
\hline
b_i & \frac{1}{24\delta^2} & 1 - \frac{1}{12\delta^2} & \frac{1}{24\delta^2}
\end{array}
$$

Table 2: RKN-12 (order 2), RKN-34 (order 4).

where the generating coefficient is $\delta = \frac{1}{12}(2 - \sqrt[3]{4} - \sqrt[3]{16})$.
Perform h- and t-refinement for each integrator (use analytical solution).

f) Consider the following BVP, where $\Omega = [-2, 2]$ and $I = [0, 4]$:

$$
\begin{aligned}
&u_{tt} - u_{xx} + \sin(u) = 0 && , && (x,t) \in \Omega \times I && \text{(6a)}\\
&u(-2,t) = 0 \ , \ u(2,t) = 0 && , && (x,t) \in \partial\Omega \times I && \text{(6b)}\\
&u(x,0) = \sin(\pi x)^2 e^{-x^2} && , && x \in \Omega \times \{t = 0\} && \text{(6c)}\\
&u_t(x,0) = \sin(\pi x)^4 e^{-x^2} && , && x \in \Omega \times \{t = 0\} && \text{(6d)}
\end{aligned}
$$

Apply the RK4 and RKN-34 integrators, solve the problem as best as you can and report the results in the following two loglog-graphs:

- x-axis with degrees of freedom, y-axis for normalized energy difference, $\Delta E = |E(4) - E(0)|/E(0)$.
- x-axis with degrees of freedom, y-axis for computational time.

Which integrator yields the best result, and what is the reason for this?

3 Advection-Diffusion equation (Suzuki)

Consider the following convection-diffusion equation on $x \in \mathbb{R}$, $t > 0$

$$u_t = cu_x + du_{xx}, \quad u(x,0) = g(x),$$

where c and d are positive constants, with a periodic boundary condition

$$u(x+1,t) = u(x,t),$$

for all $x \in \mathbb{R}$ and $t > 0$. Note that due to this periodic boundary condition, we only need to consider one period $[0,1]$ for the spatial domain.

Consider equidistant points

$$x_0 = 0,\ x_1 = \frac{1}{M+1}, ...,\ x_M = \frac{M}{M+1},\ x_{M+1} = 1,$$

and let $h = 1/(M+1)$.

a) By using the central differences in x direction, and by making use of the periodic boundary condition, construct a linear approximation

$$c\boldsymbol{U}_x + d\boldsymbol{U}_{xx} \approx A\boldsymbol{U},$$

where A is a ***circulant matrix*** which is of the following form:

$$A = \begin{pmatrix} a_0 & a_1 & \cdots & a_{M-1} & a_M \\ a_M & a_0 & \cdots & a_{M-2} & a_{M-1} \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ a_2 & a_3 & \cdots & a_0 & a_1 \\ a_1 & a_2 & \cdots & a_M & a_0 \end{pmatrix}.$$

We are going to denote this circulant matrix by $Cir(\boldsymbol{a})$ where $\boldsymbol{a} = (a_0, a_1, \cdots, a_M)$. Now, consider the general θ method ($\theta \in [0,1]$) to solve the original equation

$$\boldsymbol{U}^{n+1} - \theta k A \boldsymbol{U}^{n+1} = \boldsymbol{U}^n + (1-\theta) k A \boldsymbol{U}^n,$$

where k is the time step size. Rewrite this equation by $\boldsymbol{U}^{n+1} = B\boldsymbol{U}^n$. Fix $r = k/h^2$ and consider specifically three cases of $\theta = 0, \theta = 1/2, \theta = 1$. By analyzing the eigenvalues of B. derive the stability condition depending on r, θ, c and d.

You can make use of the following facts without proof:

[***Fact 1***] The eigenvalues of the circulant matrix $Cir(\boldsymbol{a})$ is given by

$$\lambda_j = a_0 + a_1\omega^j + ... a_M\omega^{Mj},$$

where $\omega = \exp(2\pi \mathrm{i}/(M+1))$ with i being the imaginary unit, $j = 0, ..., M$, with the right eigenvectors:

$$\boldsymbol{p}_j = \frac{1}{\sqrt{M+1}}(1, \omega^j, ..., \omega^{Mj})^\top.$$

[***Fact 2***] Circulant matrices are normal, this means that the spectral radius is same as the l_2 matrix norm:

$$\rho(Cir(\boldsymbol{a})) = \|Cir(\boldsymbol{a})\|_2.$$

b) Implement a stable method of your own choice for $c = 20, d = 1$ and the initial condition $g(x) = \sin(4\pi x)$. For this problem, the analytical solution is given by

$$u(x,t) = \exp(-d(4\pi)^2 t)\ \sin(4\pi(x + ct)).$$

Make a convergence plot in terms of h where $r = k/h^2$ being fixed for the solution at time $t = 0.01$. Further, when the time t is sufficiently big, how does the solution look like? First discuss from your analytical solution and then try to observe numerically (make the plot from your numerical solution).

c) For the above problem, to compare with other groups, submit a code which produces two graphs: x axis for the number of degree of freedom (M/k) and y axis for the relative l_2 error; and x axis for the number of degree of freedom (M/k) and y axis for computational time.

d) Explore the problem in different settings of your own choice: different boundary conditions such as Dirichlet or Neumann (then you only need to consider closed interval $[0, 1]$ for x), or construct your own finite difference scheme. Describe your findings theoretically (such as stability analysis, convergence ,etc) and numerically. This problem is the most important part of this project, so make substantial amount of effort.

4 **Wave equation (Suzuki)**

Consider the following wave equation on $x \in \mathbb{R}$, $t > 0$

$$u_{tt} = c^2 u_{xx}, \quad u(x, 0) = g(x), \quad u_t(x, 0) = h(x),$$

where c is a positive constant, with a periodic boundary condition

$$u(x + 1, t) = u(x, t),$$

for all $x \in \mathbb{R}$ and $t > 0$. Note that due to this periodic boundary condition, we only need to consider one period $[0, 1]$ for the spatial domain.

Consider equidistant points

$$x_0 = 0, \ x_1 = \frac{1}{M+1}, ..., \ x_M = \frac{M}{M+1}, \ x_{M+1} = 1,$$

and let $h = 1/(M + 1)$.

a) By using central differences on both directions x and t, we have

$$\frac{U_j^{n+1} - 2U_j^n + U_j^{n-1}}{k^2} = c^2 \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{h^2}, \tag{7}$$

where k is the time step size, for $(n + 1)$th time step and $j = 0, 1, ..., M$. When $n = 0$, we need to know U_j^{-1}. Express U_j^{-1} from the initial condition $u_t(x, 0) = h(x)$ by using central difference in time, then rewrite (7) for $n = 0$ without using U_j^{-1}.

b) Now, by fixing $r = ck/h$ and by substituting in (7)

$$U_j^n = \xi^n \exp\left(2\pi \mathrm{i} \beta \frac{j}{M+1}\right),$$

where i is the imaginary unit and $j = 0, ..., M$, derive the condition for r such that $|\xi| \le 1$ is satisfied for any $\beta \in \mathbb{Z}$.

Implement the difference method for such r with $c = 1$ and initial condition $g(x) = \cos(4\pi x)$, $h(x) = 0$. Derive the analytical solution for this problem by using separation of variables. Then make a convergence plot of the relative l_2 error in terms of h where $r = ck/h$ being fixed for the solution at time $t = 1$.

Change the initial condition to initial condition $g(x) = \exp(-100(x - 1/2)^2)$, $h(x) = 0$. Observe the time development of the solution and describe it. Make some plots of the solution for different time t.

c) Add one more dimension to the problem: consider for $(x, y) \in \mathbb{R}^2$

$$u_{tt} = c^2(u_{xx} + u_{yy}), \quad u(x, y, 0) = g(x, y), \quad u_t(x, y, 0) = h(x, y),$$

with the periodic boundary condition on both spatial direction

$$u(x + 1, y, t) = u(x, y, t), \quad u(x, y + 1, t) = u(x, y, t),$$

for all $(x, y) \in \mathbb{R}^2$ and $t > 0$. Again, due to this periodicity, we only need to consider one unit square $[0, 1]^2$ for the spatial domain. Consider equidistant points for both direction, but they can be different step sizes:

$$x_0 = 0, \ x_1 = \frac{1}{M+1}, ..., \ x_M = \frac{M}{M+1}, \ x_{M+1} = 1,$$

$$y_0 = 0,\ y_1 = \frac{1}{N+1}, ...,\ y_N = \frac{N}{N+1},\ y_{N+1} = 1,$$

and let $h_x = 1/(M+1)$, $h_y = 1/(N+1)$. Generalize the difference method (7) for this 2D setting.

Again, by fixing $r_x = ck/h_x$, $r_y = ck/h_y$ and by substituting the following for the obtained 2D scheme

$$U_{j,l}^n = \xi^n \exp\left(2\pi \mathrm{i} \beta_1 \frac{j}{M+1}\right) \exp\left(2\pi \mathrm{i} \beta_2 \frac{l}{N+1}\right),$$

where $l = 0, ..., N$ and $j = 0, ..., M$, derive the condition for r_x and r_y such that $|\xi| \leq 1$ is satisfied for any $\beta_1, \beta_2 \in \mathbb{Z}$.

Implement the above difference method for $c = 1$ and the initial condition $g(x, y) = \cos(4\pi x)\sin(4\pi y)$, $h(x, y) = 0$. Derive the analytical solution for this problem by using separation of variables. Then make a convergence plot of the relative l_2 error in terms of h_x where $r_x = ck/h_x$ and $h_x = h_y$ being fixed, for the solution at time $t = 1$. Also, make some 3D plots (x, y, u) of the numerical solution for different time t.

d) For the above 2D problem, $c = 1$ and the initial condition $g(x, y) = \cos(4\pi x)\sin(4\pi y)$, $h(x, y) = 0$, and $t = 1$, to compare with other groups, submit a code which produces two graphs: x axis for the number of degree of freedom (MN/k) and y axis for the relative l_2 error; and x axis for the number of degree of freedom (MN/k) and y axis for computational time.

Appendix

Sparse matrices (all tasks)

Defining matrices in sparse format is useful for reducing memory storage and computational running time when dealing with linear systems of equations. There are two essential Python-modules for this task:

```
import scipy.sparse as sp
import scipy.sparse.linalg as sl
```

Matrices can be converted between full and sparse format:

```
A = sp.csc_matrix(A)     # Sparse format.
A = A.todense()          # Full format.
```

Banded matrices can be defined as follows:

```
A = sp.diags([-1,2,-1],[1,0,-1],shape=[20,20],format='csc')
B = sp.diags([1,-4,10,-4,1],[2,1,0,-1,-2],shape=[20,20],format='csc')
```

Some typical operations with sparse matrices:

```
c = A*b                  # Matrix-vector multiplication, c = A*b
c = sl.spsolve(A,b)      # Linear equation solving, c = A\b
```

Fast Fourier Transform (Task 1)

The Fast Fourier Transform and its variants are included in the Python-module `scipy`:

```
from scipy.fft import fft, ifft, dst, idst
y = fft(x)               # Fast Fourier Transform
x = ifft(y)              # Inverse Fast Fourier Transform
y = dst(x,type=2)        # Fast Fourier Sine Transform
x = idst(y,type=2)       # Inverse Fourier Sine Transform
```

RK- and RKN-integrators (Task 2)

Runge-Kutta (RK) and Runge-Kutta-Nyström (RKN) integrators are defined as

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b} \end{array} \qquad \begin{array}{c|c} \mathbf{c} & \overline{\mathbf{A}} \\ \hline & \overline{\mathbf{b}} \\ \hline & \mathbf{b} \end{array}$$

Applying an RK-method to $y' = f(y)$ yields

$$\begin{aligned} k_i &= f\left(t_n + c_i h, y_n + h\sum_{j=1}^{s} a_{ij}k_j\right) \quad , \quad 1 \le i \le s \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i k_i \end{aligned} \tag{8}$$

Applying an RKN-method to $y'' = f(y)$ yields

$$\begin{aligned} k_i &= f\left(t_n + c_i h, y_n + c_i h y_n' + h^2\sum_{j=1}^{s} \overline{a}_{ij}k_j\right) \quad , \quad 1 \le i \le s \\ y_{n+1}' &= y_n' + h\sum_{i=1}^{s} b_i k_i \\ y_{n+1} &= y_n + h y_n' + h^2\sum_{i=1}^{s} \overline{b}_i k_i \end{aligned} \tag{9}$$