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Mathematical and Numerical Physics
Numerical Assignments part 1

VERY IMPORTANT:
Submit your solutions on Canvas before **December 8^{th}, 2020 17:00h**. You have to submit your solutions individually and submit your codes. Use ProblemX_Y_LastName_FirstName, where X and Y indicate the number and subpart of the question as name. For example, "Problem1_a_Stevens_Richard.m". If you use a script to run your codes, this should be called "main", e.g. "Problem1_Stevens_Richard_main.m". You should always briefly discuss what you have done.

Problem 1: One-dimensional parabolic equation (14 points, distribution indicated below)
In the lecture we discussed several methods to solve the following parabolic equation

$$\dot{\phi} = M\nabla^2\phi \tag{1}$$

We will perform the simulation on a domain $x = [0 : 1]$ using the initial condition $\phi(x) = \sin(\pi x)$. Use $M = 0.5$ and calculate the results at $t = 0.6$.

For the boundary conditions use $\phi(0) = \phi(1) = 0$.

VERY IMPORTANT: You do not need to derive the numerical schemes for the different methods. You can directly implement them based on the material provided in the reader. As discussed, the Euler backward and the Crank-Nicholson method are unconditionally stable. However, you must ensure that the time step is small enough to get a converged solution. The analytical solution for this problem is given by:

$$\phi(x) = \exp(-M\pi^2 t)\sin(\pi x) \tag{2}$$

Show your results on grids with $n_x = 8, 16$ and 32.

(a) Implement the Euler forward method (1 point). Show that the solution converges to the analytical result by computing the L_1, L_2, and L_∞ norms. (2 points)

IMPORTANT: In the following problems you can show the convergence to analytical results without using the norms.

(b) Implement the DuFort Frankel method (2 points) and show that the solution converges to the analytical result. (1 point)
Hint: Make sure $\Delta t/\Delta x \to 0$ as you decrease Δx.

(c) Show that the Euler backward method is unconditionally stable (analytical derivation) (1 point).

(d) By using the Euler backwards scheme, bring equation (1) into the form $A\phi^{n+1} = \phi^n$ and solve the matrix system using:

- (d1) matrix inversion (1 point)
- (d2) LU decomposition (1 point)
- (d3) tridiagonal solver (2 points)

IMPORTANT: For this exercise you can use the example files used during the tutorial. Note that after this problem you can use the algorithm of your choice to solve the matrix systems. We picked small problem sizes so that the efficiency of the method is not crucial. In these assignments the focus is on the numerical schemes not the most efficient implementation.

- (d4) Show that the solution converges to the analytical result. (1 point)

(e) Implement the Crank-Nicholson method (1 point) and show that the solution converges to the analytical result. (1 point)

Problem 2: Two-dimensional parabolic equation(11 points, distribution indicated below)
We will again analyze the equation

$$\dot{\phi} = M\nabla^2\phi \tag{3}$$

but now in two dimensions. We will perform the simulation on a domain $[x, y] = [0 : 1][0 : 1]$ using the initial condition $\phi(x, y) = \sin(\pi x)\sin(\pi y)$. Use $M = 0.37$ and calculate the results at $t = 0.4$. Compare your results to the analytical solution $\phi(x, y) = \exp(-2M\pi^2 t)\sin(\pi x)\sin(\pi y)$.

Use the boundary condition: $\phi = 0$ on all boundaries.

(a) Derive the Euler forward method for the two-dimensional case (2 points)
Hint: Use

$$\Delta t = \frac{(\Delta x)^2(\Delta y)^2}{2M((\Delta x)^2 + (\Delta y)^2)} \tag{4}$$

(b) Write a code that implements the Euler forward method. (2 points)
Show that the solution of your code converges to the analytical solution $\phi(x, y) = \exp(-2M\pi^2 t)\sin(\pi x)\sin(\pi y)$. Use the grids (i) $n_x = 16; n_y = 16$, (1 point) (ii) $n_x = 16; n_y = 32$ (1 point)

Challenging problem:
(c) Write a code to solve equation (3) using the two-dimensional Crank-Nicholson method.You can directly use the material from the reader and the lecture and show that the solution agrees with the analytical solution for (i) $n_x = 16; n_y = 16$, and (ii) $n_x = 16; n_y = 32$. (5 points)

Problem 3: Phase separation in one-dimension (17 points, distribution indicated below)

We first consider phase separation on a unity domain $x = [0..1]$ using the partial differential equation derived in the analytical part of the course

$$\dot{\phi} = M\nabla^2(\phi^3 - \phi - \kappa\nabla^2\phi) \tag{5}$$

We first consider the initial condition

$$\phi(x \leq 0.5) = -1 \qquad \phi(x > 0.5) = 1 \tag{6}$$

and use $M = 0.3$ and $\kappa = 1/768$. We investigate the solution in the statistical stationary state. *Hint: Make sure* $\Delta t/\Delta x \to 0$ *as you decrease* Δx.

(a) Derive the Euler forward scheme to discretize equation (5) in a one-dimensional domain using a central second-order finite difference method for the spatial terms. (3 points)

(b) Implement the scheme (3 points) you derived in (a) and show that your code converges to the analytical solution. Use $N_x = 12, 24, 48$. (1 point)
Hint: The analytical solution for the steady state profile is $\phi(x) = \tanh\left(\frac{x-0.5}{\sqrt{2\kappa}}\right)$*; you do NOT have to derive this.*
Hint: Use

$$\Delta t \leq \frac{(\Delta x)^2}{M\left(4 + 8\frac{\kappa}{(\Delta x)^2}\right)} \tag{7}$$

(c) Show that your method conserves mass. (1 point)

(d) Verify that the free energy $F = \int_V [-\frac{\phi^2}{2} + \frac{\phi^4}{4} + \frac{1}{4} + \frac{\kappa}{2}(\nabla\phi)^2]$ is monotonically decreasing (2 points) and discuss the evolution of the different contributions to the total free energy. (2 points)

Challenging problem:
(e) Convert the solver you made in (b) to one that considers a periodic domain (3 points) and show the solution you obtain convergences. (2 points) Use $M = 0.01$ and $\kappa = 1/4096$ and the initial condition $\phi(x) = \sin(\pi x)$.