Computational Fluid Dynamics
Problem Set 3

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Regarding implementations in the following questions, you may use `python` *or another language of your choice. Please submit your code as a separate file or files.*

Problem 1 (Finite difference operators & truncation errors)

Consider the function $u(x) = \sin(x)$. As usual, we will use the following notation: $u^{(k)} \equiv \mathrm{d}^k/\mathrm{d}x^k$.

(*a*) Consider $u^{(1)}(1)$. Implement forward and centred difference approximations to $u^{(1)}(x)$ and compute corresponding approximations to $u^{(1)}(1)$, considering different grid spacings $\Delta x = \{1, 0.1, 0.01, 0.001\}$. Plot the resulting truncation errors as a function of Δx in log-log scale and fit appropriate functions to the 'data' points to verify that the truncation errors are $\mathcal{O}(\Delta x)$ and $\mathcal{O}((\Delta x)^2)$ for forward and centred differences, respectively.

(*b*) Following the general method outlined in the lectures, devise and implement a second-order accurate, one-sided (backward) finite difference approximation to $u^{(2)}(x)$. Following analogous steps as in (*a*), verify that your implementation is indeed $\mathcal{O}((\Delta x)^2)$.

Problem 2 (The heat equation: stability & explicit vs. implicit)

Consider the one-dimensional diffusion or heat equation

$$u_t - \nu_\mathrm{d} u_\mathrm{xx} = 0 \tag{1}$$

in the domain $0 \leq x \leq 1$ with the diffusion coefficient ν_d. The analytical solution to an initial 'heat spike' $u(x, 0) = \delta(x - 0.5)$ 'injected' at the centre of the domain at $t = 0$, subject to the boundary conditions $u(0, t) = u(1, t) = 0$, is given by

$$v(x,t) = 2\sum_{n=1}^{\infty} \sin\left(\frac{\pi}{2}n\right) \sin(\pi n x) \exp(-\pi^2 n^2 \nu_\mathrm{d} t) \tag{2}$$

for $t > 0$.

(*a*) Derive a numerical scheme to solve Eq. (1) using a stencil that is first-order forward in time and second-order centered in space.

(*b*) Implement the scheme in (*a*) and advance the analytical solution $v(x,1)$ at $t = 1$ numerically to $t = 3$, using $\nu_\mathrm{d} = 0.001$. Plot the fractional global error $E_i^n = |u_i^n - v(x_i, t^n)|/|v(x_i, t^n)|$ at $t^n = 3$ as a function of x_i, where u_i^n denotes the numerical solution, for two sets of experiments: (*i*) keep $\Delta x = 0.02$ fixed and vary $\Delta t = 0.2, 0.1, 0.05$ and (*ii*) keep $\Delta t = 0.2$ fixed and vary $\Delta x = 0.02, 0.01, 0.005$. What do you observe? Does this scheme converge?

(*c*) Perform a von Neumann stability analysis of your scheme (*a*) and derive a corresponding stability criterion. Interpret your heuristic findings from (*b*) in light of this stability analysis. According to the Lax theorem, where would you expect the scheme not to converge?

(*d*) The stability restriction of explicit schemes for the heat equation, such as $\Delta t \propto (\Delta x)^2$ found above, often make it very expensive to evolve the heat equation. This motivates implicit schemes, such as the following: Consider the Crank-Nicholson scheme,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \nu_\mathrm{d}\frac{1}{2}\left[\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + \frac{u_{i+1}^{n} - 2u_i^{n} + u_{i-1}^{n}}{(\Delta x)^2}\right] = 0, \tag{3}$$

and prove that it is unconditionally stable (no limitation on Δt and Δx).
Remark: This scheme is second-order centered in time and space, with the stencil centered at $(i, n+1/2)$. The space discretization at the intermediate time level is obtained by averaging those at n and $n+1$: $\frac{1}{2}(D^2 u_i^{n+1} + D^2 u_i^n)$.

(*e*) *(Bonus points, not required)*
Implement the scheme discussed in (*d*) and, in analogy to (*b*), illustrate the stability properties by drastically varying the timestep Δt.
Hint: Start by writing the scheme in matrix form,

$$L\mathbf{u}^{n+1} = Q\mathbf{u}^n, \tag{4}$$

with a tridiagonal matrix L and state vector $\mathbf{u}^n = (u_1^n, \ldots, u_I^n)$.