MASSACHUSETTS INSTITUTE OF TECHNOLOGY
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2.29 NUMERICAL FLUID MECHANICS — SPRING 2015

Problem Set 4

Issued: Wednesday, March 18, 2015 Due: Wednesday, April 8, 2015

Grading Note: Please provide your solutions either as hand-written/hard-copy solutions or by submitting via course website. MATLAB® codes should be submitted via course website. The bulk of the grades will be given to detailed explanations and to algorithms and numerical schemes that capture the essence of the numerical problems. We know that successful coding of numerical schemes can be time consuming and prone to small errors. Such small errors or omissions in a code will not be heavily penalized.

The goals of this Problem Set are to: (i) develop and apply lower-order finite-difference schemes to solve differential equations in idealized fluid mechanics and tracer transport problems; (ii) become familiar with dispersion and stability criteria of time-marching Finite-difference (FD) schemes; (iii) develop and utilize higher-order FD difference schemes in time and space, in one and two spatial dimensions.

Problem 1 (Modified from Chapra and Canale, Problem 30.7)

The following advection-diffusion equation is used to compute the distribution of the concentration of a chemical along the length of a rectangular reactor (assumed one-dimensional):

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} - U \frac{\partial c}{\partial x} - k\, c$$

where c is the concentration (mg/m^3), t time (s), κ the eddy diffusivity coefficient (m^2/s), x the distance along the reactor ($0 \le x \le L$ where L is the length of the reactor), U the mean constant velocity in the x direction and k a reaction rate corresponding to the decay of the chemical to another form (i.e. "$k\, c$" is the reaction-decay term).

a) Develop an explicit scheme to solve this equation numerically.

b) Compute and plot the solution $c(x, t)$ for the following parameter values: κ = 1.7 m^2/s , U = 0.02 m/s , k = 0.0025 s^{-1} and L = 10 m , for the duration t = [0, 6000] s, and assuming:

- a zero initial concentration in the tank, $c(x, 0) = 0$
- a balance of flux boundary condition (advective and eddy diffusive fluxes are equal) at the inflow point x = 0 m, which can be written, $U\, c_{in} = U\, c(0,t) - \kappa \left.\frac{\partial c}{\partial x}\right|_{(0,t)}$, where the incoming concentration of chemical in the reactor is fixed for all times at $c_{in}(0, t)$ = 100 mg/m^3.
- a balance of flux boundary condition at the outflow point assuming no local eddy diffusion, $\kappa \left.\frac{\partial c}{\partial x}\right|_{(L,t)} = 0$. In other words, the outflow concentration is the concentration at the end of the reactor.

c) Repeat b) for an increased eddy diffusivity κ = 10 m^2/s.

d) Repeat b) for an increased reaction rate k = 0.01 s^{-1}.

Problem 2: ***Effective numerical wave numbers and dispersion of a numerical FD scheme***
Consider the example problem shown in lecture for the study of waves on a string, governed by

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2} \qquad 0<x<L, \quad 0<t<\infty \qquad (1)$$

and with initial conditions $u(x,0) = \mathrm{e}^{-(5-x)^2/2}\cos(\pi(x-5))$. In lecture, an explicit central difference scheme (CDS), 2nd order in time and space, was used. To study the modification of the dispersion and wavenumber properties of the analytical solution, consider the application of the second-derivative operator to the function e^{ikx}. The application of a FD operator for the second derivative will give: $\left(\frac{\partial^2 e^{ikx}}{\partial x^2}\right)_j = -k_{\text{eff}}^2\, e^{ikx_j}$. This relation defines the effective wavenumber k_{eff} for a FD representation of a 2nd order spatial derivative. As shown in lecture, an effective wave speed can also be estimated by inserting this spatial FD in the original PDE (1).

a) Using Fourier analysis, find the effective wavenumber and wave speeds for the following schemes: i) 2nd-order CDS, ii) 4th-order CDS (see Tables provided in the lecture notes) and iii) 4th-order compact Pade' Scheme, $\left(\frac{\partial^2 u}{\partial x^2}\right)_{j-1} + 10\left(\frac{\partial^2 u}{\partial x^2}\right)_j + \left(\frac{\partial^2 u}{\partial x^2}\right)_{j+1} = \frac{12}{\Delta x^2}(u_{j-1} - 2u_j + u_{j+1})$

b) Plot the results $\left(k_{\text{eff}}\,\Delta x\right)^2$ versus $k\,\Delta x$ for $0 \le k\,\Delta x \le \pi$. Describe the results and relate to the example given in lecture.

c) Optional, bonus (only if you have time and are interested by this sub-question). Implement the above 4th-order CDS or 4th-order compact Pade' Scheme in space (e.g. in MATLAB), and solve the 2nd order wave equation, using an explicit 2nd order in time FD scheme. Compare your solution to that of the 2nd order in time and space CDS used in Lecture (for the same Δx and Δt). Relate the results you obtain to the above effective wavenumbers.

Problem 3: ***Stability of an idealized Navier-Stokes-like equation.***
Consider the advection-diffusion-reaction equation which was used above to compute the distribution of the concentration of a chemical along the length of a rectangular reactor (assumed one-dimensional):

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} - U\frac{\partial c}{\partial x} - kc$$

where c is the concentration (mg/m^3), t time (s), κ the eddy diffusivity coefficient (m^2/s), x the distance along the reactor ($0 \le x \le L$ where L is the length of the reactor), U the mean constant velocity in the x direction and k a reaction rate corresponding to the decay of the chemical to another form (i.e. "$k\,c$" is the reaction-decay term).

a) Discretize this equation using an explicit FD scheme which is first order forward in time and second order centered in space.
Use the von Neumann stability analysis to show that if the diffusion term dominates the advection term (i.e. $\Delta x \le 2\kappa/U$ or the cell Peclet number is smaller than 2), then a sufficient stability condition is:

$$\Delta t \le \frac{(\Delta x)^2}{2\kappa + k(\Delta x)^2}.$$

Hint: Prove that von-Neumann stability requires the following condition to be satisfied

$$k^2\Delta t^2 - 2k\Delta t + \left(\frac{16\kappa^2\Delta t^2}{\Delta x^4} + \frac{8\kappa k\Delta t^2}{\Delta x^2} - \frac{8\kappa\Delta t}{\Delta x^2}\right)\sin^2\left(\frac{\beta\Delta x}{2}\right) \le 0$$

and then show that from this we can conclude the sufficient stability condition given above. Note that a possible necessary and sufficient condition is: $\Delta t \le \left(2k + \frac{8\kappa}{\Delta x^2}\right) \Big/ \left(k^2 + \frac{16\kappa^2}{\Delta x^4} + \frac{8\kappa k}{\Delta x^2}\right)$.

b) Show that the two conditions $\Delta x \le 2\kappa/U$ and $\Delta t \le (\Delta x)^2/2\kappa + k(\Delta x)^2$ can be obtained from the strict requirement of positive concentrations: *c*(*x*, *t*) for all *x* and *t* > 0. Hint: consider the coefficients a_1, a_2 and a_3 of the nodal values in the RHS of the discretized equation, e.g. $c^{n+1}(i) = a_1\, c^n(i+1) + a_2\, c^n(i) + a_3\, c^n(i-1)$.

c) If the reaction rate (*k*) and the eddy diffusivity coefficient (κ) are zero, then what is the type of the resultant PDE (hyperbolic, parabolic or elliptic)? Carry out the von Neumann stability analysis for the resultant FD equation using the above discretization.

d) What is the type of the resultant PDE if the reaction rate (*k*) and mean velocity (*U*) are set to zero? Derive the stability condition for the resultant FD equation using a von Neumann analysis.

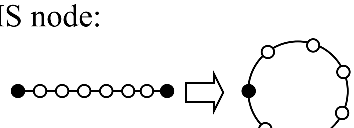
Problem 4: *Higher-order FD schemes applied to the wave equation*.

The 1D Sommerfeld wave radiation equation is governed by $\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$. This linear equation is one of the most studied for the derivation of finite difference schemes. It corresponds to a constant speed advection. Traveling waves in the form of $u(x,t) = f(k\,x - \omega t)$ are solutions of this equation if $\omega = k\,c$ which implies that the waves travel at constant amplitudes at fixed phase speed $\omega / k = c$ (non-dispersive waves). For the following, you may want to check the tables given in lecture (from Lapidus and Pinder, 1982) that give you the stability properties of different schemes for this classic equation.

a) Solve the Sommerfeld equation for: a wave-speed, *c* = 0.5 *m/s*; domain size 1 *m*; and final time = 6 seconds. The initial condition $u(x,0)$ of the wave has the following shape:

$$u(x,0) = \begin{cases} \sin(4\pi x) & 0.0 \le x < 0.25 \\ \sin[4\pi(x-0.25)] & 0.25 \le x \le 0.5 \\ 0 & \textit{elsewhere} \end{cases}$$

The boundary condition is periodic. That is to say, the left-hand side (LHS) node is treated as though it is lying next to the RHS node:



Using MATLAB (or your preferred software), numerically solve for $u(x,t)$ using 601 nodes in time and 51 nodes in space, and:

i) Using a first order explicit forward in time and backward in space FD scheme (as in Problem Set 3)
ii) Using a FD scheme implicit first order backward in time, and second order central in space.
Plot the solution at $t = [0, 2, 4, 6]$ seconds and briefly comment on the results.
Hint: For the implicit scheme you will have to solve a set of simultaneous linear equations. You must form an '**A**' matrix, and a '**b**' matrix. In this case, the '**A**' matrix will be the same for all time, while the '**b**' matrix will change over time. Try to take advantage of this fact.

b) Repeat a) but using 201 nodes in time and 101 nodes in space. Discuss the results in terms of the CFL condition and the stability analysis presented in lecture.

c) First order schemes in time are often not very accurate. The original waveform is quickly lost after only a few integrations. This is unacceptable for a realistic application. In order to improve the solution, the grid can be refined, however this can be expensive computationally. In this part of the question, you will implement a fourth-order accurate implicit compact Padé scheme. The formula for the fourth order accurate Padé scheme is:

$$\frac{1}{4}\left(\frac{\partial \phi}{\partial \xi}\right)_{j+1} + \left(\frac{\partial \phi}{\partial \xi}\right)_{j} + \frac{1}{4}\left(\frac{\partial \phi}{\partial \xi}\right)_{j-1} = \frac{3}{4\Delta\xi}\phi_{j+1} - \frac{3}{4\Delta\xi}\phi_{j-1}$$

i) Write out the Padé scheme for $\frac{\partial u}{\partial x}$ at time "*k+1*." Express your answer in the form

$\mathbf{B}_1(b_{11}, b_{12}, b_{13})\left(\frac{\partial \phi}{\partial \xi}\right)^{k+1} = \mathbf{B}_2(b_{21}, b_{22}, b_{23})\phi^{k+1}$, where $\mathbf{B}(b_1, b_2, b_3)$ is a banded matrix of the form: $\mathbf{B} = \begin{bmatrix} b_2 & b_3 & & & \\ b_1 & b_2 & b_3 & & \\ & \ddots & \ddots & \ddots & \\ & & b_1 & b_2 & b_3 \\ & & & b_1 & b_2 \end{bmatrix}$ and $\left(\frac{\partial \phi}{\partial \xi}\right)^{k+1}, \phi^{k+1}$ are vectors. Note that boundary conditions can be included in the **B** matrices.

ii) Using the results from i) and the PDE $\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$, express the time derivative vector at time *k+1*, i.e. $\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k+1}$, in terms of $\mathbf{B}_1^{-1}, \mathbf{B}_2$, and $\mathbf{u}^{k+1}$. Notice this equation contains two vectors of unknowns.

iii) Write out the Padé scheme for $\frac{\partial \mathbf{u}}{\partial t}$. Notice this equation contains the same two vectors of unknowns as in ii).

iv) Eliminate $\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k+1}$ from the equation found in iii) by substituting for $\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k+1}$ using the results from part ii). Re-arrange the equation to solve for $\mathbf{u}^{k+1}$ and express your solution as $\mathbf{u}^{k+1} = \left[C_1\mathbf{B}_1^{-1}\mathbf{B}_2 + C_2\mathbf{I}\right]^{-1}\left\{C_3\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k-1} + C_4\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k} + C_5\mathbf{u}^{k-1}\right\}$, where C_i are constant scalars.

d) Using MATLAB (or your preferred software), numerically solve for $u(x,t)$ using 601 nodes in time and 51 nodes in space using the Padé scheme developed in c). To start the scheme, you need to estimate values at one time step after the initial condition. You may calculate this time step analytically (using the given boundary conditions) or you may use the first order time schemes developed previously. Plot the solution at t = [0, 2, 4, 6] seconds and briefly compare the results with those obtained in b).

Hints: You need to calculate $\left(\frac{\partial \mathbf{u}}{\partial t}\right)^{k}$ using the Padé scheme from c.ii) before calculating $\mathbf{u}^{k+1}$ using the formula in c.iv). Also, the matrix $\left[C_1\mathbf{B}_1^{-1}\mathbf{B}_2 + C_2\mathbf{I}\right]^{-1}$ does not change over time, so compute it once and use the result.

e) The Padé scheme is compact and of higher-order, but computationally more expensive. To evaluate the computational efficiency of the Padé scheme you can use "cputime" in MATLAB
i) How much CPU time did you need to run the Padé scheme?
ii) Compare the CPU time of the Padé scheme to the CPU time of the implicit "forward in time, centered in space" scheme from a.ii) for a run with 2401 nodes in time and 201 nodes in space.

f) Instead of the scheme employed in c)-d)-e), one could have implemented the Padé scheme in the form of a system to be solved for both function values and derivative values at the FD nodes (a richer representation than just the function values). We refer to this implementation as the Padé system scheme.
i) Discuss the advantages/disadvantages of this system scheme and compare it to the scheme employed in c)-d)-e).
ii) Bonus: implement and utilize this system scheme and compare its results to the results obtained in c)-d)-e).

Problem 5: ***(Modified problem 32.14 from Chapra and Canale)***
Solve the non-dimensional transient heat conduction equation in two-dimensions, which represents the transient temperature distribution in an insulated plate. The governing equation is $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{\partial T}{\partial t}$, where T is temperature, x and y spatial coordinates, and t time. The boundary and initial conditions are given by:

$$\textit{Boundary conditions}: \begin{cases} T(x,0,t)=0 \\ T(x,1,t)=1 \\ T(0,y,t)=0 \\ T(1,y,t)=1 \end{cases} \qquad \textit{Initial conditions}: \begin{cases} T(x,y,0)=0 \\ 0 \le x < 1;\ 0 \le y < 1 \end{cases}$$

a) Develop the FD scheme using a Crank-Nicolson scheme (two-dimension in space case).
b) What is the type of the resultant matrix (**A x** = **b**)?
c) Write a MATLAB code to implement the solution using this Crank-Nicolson scheme. To do this, you can directly utilize the MATLAB codes that have been given to you in problem sets, quiz 1 or lecture, or even in MATLAB itself. Estimate the CPU time required to do this computation: you can use the "cputime" function in MATLAB as follows:

```
t=cputime;
<Run Solution>
Dt=cputime-t;
```

d) Utilize the alternating direction-implicit (ADI) technique to solve the same problem. Estimate the CPU time and compare it to that obtained in part c).

e) Plot the results of part c) and d) using 3-dimensional plots where the horizontal plane is the plate (*x* and *y* axes) and the *z* axis is temperature (*T*). Construct plots of your solution for the following three time instances: initial transition time, approximately half way to steady state and steady-state condition.

f) Repeat part d), but for $T(x,1,t)=0$ and $T(1,y,t)=1+0.5\sin(2\pi ft)$ with $f = 10$ (a time-varying temperature boundary conditions on one edge). Plot your results $T(x,y,t)$ from t=0:0.125:1 (e.g. all plots on a single page) or provide an animation.