

CO2020 : Computer-Aided Numerical Methods II

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Homework 5

Due Date: 27 April 2023

Topic: Parabolic PDEs

Question 1: Using metric terms, derive the following equations in Cylindrical (r, θ) coordinates.

(a) The continuity equation:

$$\frac{\partial u_r}{\partial r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} = 0$$

(b) The Laplacian operator:

$$\nabla^2 T = \nabla \cdot (\nabla T) = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2}$$

Question 2: The 1D heat conduction equation over the range $x \in [0, 1]$ with the diffusivity $\kappa = 1$ and boundary values $T(0) = -1$ and $T(1) = 1$ has the exact solution $T(x, t) = \text{erf}((x - 0.5)/2\sqrt{t})$ for small times. “Small” here is with respect to the boundaries, i.e. the time until which the exact solution at the boundaries is not significantly different from the imposed conditions ($T(0) = -1$ and $T(1) = 1$).

A code to solve this equation numerically is provided to you. The domain is discretized into nx grid points, with $x[0] = 0$ and $x[nx - 1] = 1$. We have discussed how to use the 2nd-ordered centered-difference approximation for the spatial derivative and the first-order forward Euler time stepping for the temporal derivative in class. The same has been implemented in the code given to you.

(a) Modify the code so as to use the 4th-order centered-difference scheme for spatial discretization, i.e.

$$\left(\frac{\partial^2 T}{\partial x^2} \right)_i = \frac{1}{(\Delta x)^2} \left[\frac{4}{3} (T_{i+1} + T_{i-1}) - \frac{1}{12} (T_{i+2} + T_{i-2}) - \frac{5}{2} T_i \right].$$

Note that the above expression is valid for the interior points, $i = 2, 3, \dots, nx - 4, nx - 3$. At the boundary points, $i = 0$ and $i = nx - 1$, the Dirichlet boundary conditions imply that the solution need not be updated (rhs[i] can be set to zero). At the first point adjacent to the two ends, i.e. at $i = 1$ and $i = nx - 2$, one-sided stencils need to be used. Derive these sided derivative schemes using the method discussed briefly in class.

- (b) Perform von-Neumann stability analysis for this problem and derive the constraint on $r = \kappa(\Delta t) / (\Delta x)^2$ for the simulations to be stable. Use only the expression for the interior nodes. Determine the largest possible value of nx for stable simulation for a given time step Δt . Satisfy yourself that your code is stable when executed with nx smaller than this value and blows up (you get Nan or Inf or grid-to-grid oscillations) when executed with larger values of nx .
- (c) Verify your implementation by numerically reproducing the expected order of accuracy. For this purpose, start your simulation from the exact solution at $t = 0.001$. Modify the code to write out the L_2 norm of the error between the exact solution and the numerical solution at the final time, t_{final} . Determine convergence behaviour (i.e. plot L_2 norm of the error between the exact and numerical solution for different values of nx) and explain your observations. On the same figure, plot the errors for the following conditions:

- (a) $t_{final} = 0.002, \Delta t = 1.25 \times 10^{-7}$
- (b) $t_{final} = 0.002, \Delta t = 3.125 \times 10^{-6}$

Your figure and discussion should demonstrate the following:

- (a) nx should range from around 10 to around 1000 in roughly equal increments.
- (b) starting from small values of nx , the error reduces at 4th-order as nx is increased. On a log-log plot, your error values should be parallel to a straight line with slope of -4.
- (c) the error starts to saturate (becomes constant or grows with nx) beyond a certain nx .

General instructions:

1. Use Matlab or any other postprocessing software to generate line plots and contour plots. Ensure that the font size of the legend and labels is large enough to be easily visible. Ensure that the line thickness is appropriately large. Export your image as a png or eps file and include it in your report.
2. Prepare a short report documenting the results (mainly figures with captions) and brief comments as directed. To reduce your work, do not repeat the problem statement.
3. Please put some thought in preparing the report so that it is easily readable. For example, do not simply dump every png or eps file that you generate into your pdf. Group similar figures together to create a meaningful figure, say Fig. 1 with several sub-panels such as Fig. 1(a), Fig. 1(b), etc. One png file should not span the entire width of the page. Two (or sometimes three) figures can easily fit side-by-side on one page. Please prepare a report you would like to read yourself a few years from now!
4. Please submit your report as one pdf file as per the directions above. In addition, submit a zip or tar file with all codes, any input files or Makefile you may have used.