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Tentamen i Kursen DN2221
Tillämpade Numeriska Metoder I
Monday 2009-12-14 kl 14–19

No means of help allowed. To pass 13 credits of max 27 is needed. Present your answers in English or Swedish.

1. Assume that the $n \times n$ matrix A is diagonalizable with eigenvalues in the diagonal matrix D and the corresponding eigenvectors as columns in the matris S.

(1) a) What is the definition of the exponential matrix e^{At}?

(2) b) Calculate e^{At} when

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

2. Given an ODE-system $\dot{\mathbf{x}} = A\mathbf{x}$, where A is a real anti-symmetric matrix, i.e. a matrix satisfying $A + A^T = 0$. The eigenvalues of such a matrix are always imaginary, i.e. $\lambda_k = i\mu_k$, where μ_k is real. In this problem we assume that all eigenvalues are simple. Clear motivations with explaining formulas are needed for the questions below.

(1) a) Verify that the analytic solutions of such a system are stable.

(2) b) Will the numerical solution be stable if Euler's explicit method is used?

(3) c) Same question as b) if the explicit midpoint method, $u_{k+1} = u_{k-1} + 2hf(t_k, u_k)$, is used.

(3) 3. Investigate if it is possible to obtain 4th order accuracy using 5 points for a 2nd derivative approximation, i.e. is it possible to determine a, b, c, d, e in

$$y''(0) = \frac{ay(2h) + by(h) + cy(0) + dy(-h) + ey(-2h)}{h^2} + O(h^4)$$

4. Given the advection equation

$$\frac{\partial u}{\partial t} - \frac{\partial u}{\partial x} = 0, \quad 0 \le x \le 1, \quad t > 0$$

(1) a) Which are the characteristics?

(1) b) Given the initial condition $u(x, 0) = u_0(x)$. Where can the boundary condition be given? Motivate!

(1) c) Formulate the downwind (FTFS) discretization method for the PDE-problem.

(3) 5. Given the parabolic problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - u, \quad u(x,0) = f(x), \quad u(0,t) = u(1,t) = 0, \quad 0 \le x \le 1, t > 0$$

Present the Galerkin method with an ansatz $\tilde{u}(x,t) = \sum_{k=1}^{n} a_k(t)\varphi_k(x)$ and describe the elements of the matrices and vectors in the ODE-system for the coefficients $a_k(t)$ for the PDE-problem given above. Also show how the initial condition is formulated.

6. Consider a spherical particle with radius R $[m]$. The particle is surrounded by a liquid containing a substance A with the concentration c_0 $[mol/m^3]$. The substance is transported into the particle by diffusion and disappears in the particle through a reaction $A \rightarrow B$. The concentration $c(r,t)$ of A in the particle is modelled by the PDE:

$$\frac{\partial c}{\partial t} = D(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}) - kc, \quad c(r,0) = 0, \quad 0 \le r \le R, \quad t > 0$$

assuming that the particle at time $t = 0$ contains no substance A. In the PDE D $[m^2/s]$ is the diffusion constant and k $[1/s]$ is the chemical rate constant. The boundary conditions are

$$\frac{\partial c}{\partial r}(0,t) = 0, \qquad c(R,t) = c_0$$

(2) a) Verify that the PDE-problem after scaling of the variables can be formulated as:

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} + \frac{2}{x}\frac{\partial u}{\partial x} - au, \quad u(x,0) = 0, \quad \frac{\partial u}{\partial x}(0,\tau) = 0, \; u(1,\tau) = 1$$

Hint: Let $r = Rx$, $c = c_0 u$, $t = \alpha\tau$, where the scaling factor α is chosen so that the scaled PDE-problem contains only one dimensionless parameter a.

(5) b) Describe carefully the discretization process when the Method of Lines (MoL) is used to discretize the PDE-problem in a). Present the fundamental steps: i) the discretization of the interval [0,1] into a grid with the numbering of the grid points, ii) the discretization of the PDE into a system of ODEs and iii) the discretization of the boundary conditions. - Give your final answer in the form

$$\frac{d\mathbf{u}}{d\tau} = A\mathbf{u} + \mathbf{b}(\tau), \quad \mathbf{u}(0) = \mathbf{u}_0$$

(2) c) If the temperature T $[K]$ in the particle is not constant but increases due to heat release of the reaction the model must be modified:

$$\frac{\partial c}{\partial t} = D(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r}\frac{\partial c}{\partial r}) - kc$$

$$\rho C\frac{\partial T}{\partial t} = \kappa(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}) + \Delta H kc$$

where k is now T-dependent:

$$k = f e^{-\frac{E}{RT}}$$

where ρ, C, D, κ, ΔH, f, E and R are constant parameters. Assume the MoL is used. Describe the structure of the jacobian of this ODE-system. You need not write out the elements of the matrix in detail. It is enough to draw lines showing where you have nonzero diagonals. You need not do any scaling here.