**Numerical Methods for Differential Equations FMNN10/NUMN12**
**Final exam 2018-01-10** V16.4 **Results to be announced 2018-01-19**
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Exam duration 08:00 – 12:00. A minimum of 16 points out of 32 are required to pass. Your grade is determined by the sum of your exam and project scores, in accordance with the rules published on the course home page.

No computers, pocket calculators, cell phones, browsing tablets or any other electronic devices, and no textbooks, lecture notes or written material, may be used during the exam.

1. **(4p)** The special second order initial value problem $\ddot{y} = f(y)$ with initial conditions $y(0) = y_0$ and $\dot{y}(0) = \dot{y}_0$ models many problems in mechanics, e.g. planetary or satellite orbits. We are going to construct a method of the form

$$y_n - 2y_{n+1} + y_{n+2} = h^2 \left(\beta_0 f(y_n) + \beta_1 f(y_{n+1}) + \beta_2 f(y_{n+2})\right).$$

Because we want the method to be symmetric (in order to be able to solve the problem in forward and reverse time without producing different results), we prescribe $\beta_0 = \beta_2$.

(a) Determine the coefficients $\beta_0$ and $\beta_1$ so that the order of consistency is maximal. What is the maximal order? (3p)

(b) Is the method explicit or implicit? (1p)

**Solution**

We try the formula for polynomials $P(t) = t^m$. For simplicity, take $t_n = -h$; $t_{n+1} = 0$; $t_{n+2} = h$. Note that if $y(t) = t^m$, then $\ddot{y} = f(y) = m(m-1)t^{m-2}$, for $m \geq 2$. Moreover, the left hand side is always zero for $m$ odd.

The formula obviously holds for $m = 0$ (because the sum of the coefficients in the left hand side is zero), and for $m = 1$. For $m = 2$ we get

$$(-h)^2 - 2 \cdot 0 + h^2 = h^2 \cdot (2\beta_0 + 2\beta_1 + 2\beta_0)$$

which requires $4\beta_0 + 2\beta_1 = 2$. For $m \geq 3$ we get

$$(-h)^m - 2 \cdot 0 + h^m = h^2 \cdot m(m-1)\left(\beta_0(-h)^{m-2} + \beta_1 \cdot 0 + \beta_0 h^{m-2}\right).$$

This formula holds for all odd $m$. Then, for $m \geq 4$ even, we must require

$$2 = m(m-1)(\beta_0 + \beta_0).$$

Thus for $m = 4$ we get $2 = 12(\beta_0 + \beta_0)$ which implies

$$\beta_0 = 1/12.$$

The formula doesn't hold for $m = 6$, though. Hence the order of consistency is $p = 4$. As the sum of the $\beta_j$ is one, it follows that $\beta_1 = 10/12$. The method is obviously *implicit*.

2. **(6p)** An implicit Runge–Kutta method for the initial value problem $\dot{y} = f(t, y)$ is given by its Butcher tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$

   (a) Introduce suitable notations and write down all formulas for computing stage derivatives and updating the solution (1p)

   (b) Apply the method to the linear test equation $\dot{y} = \lambda y$ and determine the method's stability function $R(h\lambda)$. (3p)

   (c) Show that the method is A-stable. (1p)

   (d) What is the order of this method? (1p)

**Solution**

The method can be written

$$\begin{aligned} hY_1' &= hf(y_n) \\ hY_2' &= hf(y_n + hY_1'/2 + hY_2'/2) \end{aligned}$$

with updating formula

$$y_{n+1} = y_n + \frac{hY_1'}{2} + \frac{hY_2'}{2}.$$

Note that the second stage derivative equation is $hY_2' = hf(y_{n+1})$.

When we apply this method to the test equation $y' = \lambda y$ with $y(0) = 1$, we get

$$\begin{aligned} hY_1' &= h\lambda \\ hY_2' &= h\lambda(1 + h\lambda/2 + hY_2'/2) \end{aligned}$$

Because the method is implicit, we have to solve for the stage derivative $hY_2'$. But we also note that, by the updating formula, $hY_2' = h\lambda y_1$. Thus

$$(1 - h\lambda/2)hY_2' = h\lambda(1 + h\lambda/2),$$

so

$$y_1 = \frac{1 + h\lambda/2}{1 - h\lambda/2} = R(h\lambda).$$

To check whether the method is A-stable, we note that the pole of $R(h\lambda)$ is $h\lambda = 2$, hence in the right half plane. The modulus of $R(h\lambda)$ on the imaginary axis is

$$|R(hi\omega)|^2 = \frac{1 + h^2\omega^2/4}{1 + h^2\omega^2/4} = 1,$$

so the method is indeed A-stable. The method is obviously the Trapezoidal Rule, and the order of the method is $p = 2$.

3. **(6p)** Consider the following nonlinear two-point boundary value problem:

$$\begin{aligned} -u'' + 2uu' + u &= f(x) \\ u(0) = \alpha, \qquad u'(1) &= \beta. \end{aligned}$$

   (a) Introduce a suitable grid and discretize with a standard second order method. Give all details about the grid (number of grid points and their location, as well as mesh width $\Delta x$) and formulate the discretization. Include the boundary conditions in the equation system. (4p)

   (b) Construct the last row of the Jacobian matrix associated with the system. (2p)

**Solution**

We solve this problem by using the standard 2nd order approximation where we introduce an equidistant grid with $N$ interior points $x_j = j\Delta x$ and $\Delta x = 1/(N + 1/2)$ to be able to deal with the Neumann condition on the right. The discretization is

$$\begin{aligned} \frac{-\alpha + 2u_1 - u_2}{\Delta x^2} + u_1 \frac{-\alpha + u_2}{\Delta x} + u_1 &= f(x_1) \\ \frac{-u_{j-1} + 2u_j - u_{j+1}}{\Delta x^2} + u_j \frac{-u_{j-1} + u_{j+1}}{\Delta x} + u_j &= f(x_j) \\ \frac{-u_{N-1} + 2u_N - u_{N+1}}{\Delta x^2} + u_N \frac{-u_{N-1} + u_{N+1}}{\Delta x} + u_N &= f(x_N), \end{aligned}$$

where the right boundary condition is approximated by

$$\frac{u_{N+1} - u_N}{\Delta x} = \beta.$$

This yields $u_{N+1} = \beta\Delta x + u_N$, which is substituted into the last equation, to get the system

$$\begin{aligned}
\frac{2u_1 - u_2}{\Delta x^2} + u_1 \frac{-\alpha + u_2}{\Delta x} + u_1 &= f(x_1) + \alpha/\Delta x^2 \\
\frac{-u_{j-1} + 2u_j - u_{j+1}}{\Delta x^2} + u_j \frac{-u_{j-1} + u_{j+1}}{\Delta x} + y_j &= f(x_j) \\
\frac{-u_{N-1} + u_N}{\Delta x^2} + u_N \frac{-u_{N-1} + u_N + \beta\Delta x}{\Delta x} + u_N &= f(x_N) + \beta/\Delta x.
\end{aligned}$$

The last row of the Jacobian matrix becomes

$$J_{N,\cdot}(y) = \frac{1}{\Delta x^2} \begin{pmatrix} \dots & -1 - u_N\Delta x & 1 + \beta + (2u_N - u_{N-1})\Delta x \end{pmatrix}.$$

4. **(4p)** In the course we have worked with numerical methods for Sturm–Liouville eigenvalue problems. A particular case was the stationary Schrödinger equation

$$\psi'' + V(x)\psi = E\psi$$

with boundary conditions $\psi(0) = \psi(1) = 0$, and where the potential $V(x) > 0$ on $[0, 1]$. Construct a 2nd order discretization of this problem, formulating this equation as an algebraic eigenvalue problem

$$Au = \lambda u.$$

Take care to define your grid, and to introduce the potential $V(x)$ properly, and give the matrix $A$.

**Solution**

We use $N$ internal points $x_j = j \cdot \Delta x$ and $\Delta x = 1/(N + 1)$. Standard second order discretization yields the tridiagonal $N \times N$ Toeplitz matrix

$$T_{\Delta x} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}$$

which approximates $\mathrm{d}^2/\mathrm{d}x^2$ on the grid. Our discrete eigenvalue problem is now

$$\frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} + V(x_j)u_j = \lambda u_j,$$

where $u_j \approx \psi(x_j)$ approximates the wave function $\psi$. Introduce the diagonal matrix $D = \mathrm{diag}(V(x_1)\ \ V(x_2)\ \ \dots\ \ V(x_N))$. The algebraic eigenvalue problem can then be written

$$(T_{\Delta x} + D)u = \lambda u,$$

so the matrix $A = T_{\Delta x} + D$. This is a simple diagonal modification of the usual Toeplitz matrix. In the discretization, $\lambda$ represents a numerical approximation to the energy levels $E$ in the original Schrödinger equation.

5. **(2p)** Consider the nonlinear conservation law $u_t + (f(u))_x = 0$, together with periodic boundary conditions, $u(t, 0) = u(t, 1)$, and where $f$ is assumed to be an integrable function. Using integration by parts, show that $\|u(t, \cdot)\|_2$ remains constant for all $t$.

   **Solution.** Multiply the equation by $u$ and integrate over $[0, 1]$ to get

$$\langle u, u_t \rangle = \langle u, (f(u))_x \rangle = -\langle u_x, f(u) \rangle = -\int_0^1 u' \cdot f(u) \, \mathrm{d}x = -\int_{u(t,0)}^{u(t,1)} f(u) \, \mathrm{d}u = 0,$$

   since $u(0) = u(1)$. Now,

$$\frac{\mathrm{d}}{\mathrm{d}t} \|u(t, \cdot)\|_2^2 = \frac{\mathrm{d}}{\mathrm{d}t} \langle u, u \rangle = 2\langle u, u_t \rangle = 0,$$

   so $\|u(t, \cdot)\|_2 = \text{Const.}$, independent of $t$.

6. **(5p)** Consider the following PDEs for $t \geq 0$ and $x, y \in [0, 1]$:

   (a) $u_{xx} + u_{yy} = f(x, y)$

   (b) $u_{tt} = c^2 u_{xx}$

   (c) $u_t = u_{xx} + u_x + f(u)$

   (d) $u_t + uu_x = -u_{xxx}$

   (e) $u_t = d \cdot u_{xx}$

   For each equation, classify the problem as *elliptic, parabolic or hyperbolic*. In addition, give the *name* of each equation, or, in case it has no name, name it based on the terms that enter the equation.

   **Solution.** The first is the elliptic *Poisson equation* in 2D; the second is the hyperbolic *wave equation*; the third is the parabolic *convection-diffusion-reaction equation*; the fourth is the hyperbolic *Korteweg–de Vries equation* (generating soliton waves); and the fifth is the parabolic *diffusion equation.*

7. **(5p)** Consider the linear convection–diffusion equation

$$u_t = \frac{1}{\mathrm{Pe}}\, u_{xx} + u_x,$$

where Pe is the Péclet number. Consider further homogeneous Dirichlet boundary conditions $u(t,0) = u(t,1) = 0$, and let $u(0,x) = g(x)$ represent the initial condition.

(a) Introduce a suitable notation and write down a standard symmetric (central) 2nd order method-of-lines discretization in space combined with the *trapezoidal rule* for time-stepping (Crank–Nicolson method). (3p)

(b) Motivate the choice of an implicit time–stepping method, and write down the linear system of equations that has to be solved on each time step in matrix–vector form. Is the resulting method unconditionally stable? (2p)

**Solution**

We introduce a grid with $N$ internal points $x_j = j \cdot \Delta x$ on $[0,1]$ with $\Delta x = 1/(N+1)$, and let the usual Toeplitz matrix

$$T_{\Delta x} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{pmatrix}$$

represent a finite difference approximation to $\mathrm{d}^2/\mathrm{d}x^2$. Further, let the skew-symmetric Toeplitz matrix

$$S_{\Delta x} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & & \\ -1 & 0 & 1 & \\ & & \ddots & \\ & & -1 & 0 \end{pmatrix}$$

approximate $\mathrm{d}/\mathrm{d}x$ on the grid. With $u_j(t) \approx u(x_j, t)$ we get the MOL equation

$$\dot{u} = Au = \left( \frac{T_{\Delta x}}{\mathrm{Pe}} + S_{\Delta x} \right) u.$$

with initial condition $u_j(0) = g(x_j)$. Applying the trapezoidal rule to this ODE gives

$$u^{n+1} = u^n + \frac{\Delta t}{2} \left( Au^n + Au^{n+1} \right),$$

where the superscript denotes the time-stepping index, and where $u_j^0 = g(x_j)$. As the method is implicit, we have to solve a linear system on each step. The equation is

$$\left(I - \frac{\Delta t\, A}{2}\right) u^{n+1} = \left(I + \frac{\Delta t\, A}{2}\right) u^n.$$

The system is tridiagonal and can be solved quickly.

The choice of using the trapezoidal rule for the problem is because of the diffusion term, i.e., $T_{\Delta x}$ makes the problem **stiff**, even when the Péclet number is large. Note that on a uniform grid, we also need to have the mesh Péclet number $\Delta x \cdot \mathrm{Pe} < 2$, so a large Péclet number calls for a fine mesh width, which further aggravates stiffness. For this reason we choose an **unconditionally stable** time stepping method. As the trapezoidal rule is **A-stable**, there is no restriction on $\Delta t$, since the convection–diffusion operator has negative real eigenvalues.

Lycka till!
G.S.