MATH 405/607E, HWK 4, Due 4 December 2009

1. In the modeling of a semiconductor device the electric potential u satisfies the nonlinear Poisson equation:

$$\begin{aligned} -\lambda^2 u'' &= b(x) - \phi(u), \text{for } 0 < x < L \\ u(0) &= V_a = 0 \text{ and } u(L) = V_b = 10. \end{aligned}$$

   where $\phi(u) = 2K\sinh(u), b(x)$ is known as the doping profile defined to be

$$b(x) = \begin{cases} -1 \text{ if } 0 < x < \frac{L}{2} \\ 1 \text{ if } \frac{L}{2} < x < L \end{cases}$$

   and $\lambda = 1.67 \cdot 10^{-4}$ and $K = 6.77 \cdot 10^{-6}$ are positive constants and assume that $L = 0.1$. Write a finite difference program that uses Newton's method to solve the nonlinear system. As an initial guess use the approximate solution for the small λ limit :

$$u^{(0)} = \begin{cases} -\sinh^{-1}(\frac{1}{2K}) \text{ if } 0 < x < \frac{L}{2} \\ +\sinh^{-1}(\frac{1}{2K}) \text{ if } \frac{L}{2} < x < L \end{cases}$$

   Plot the convergence rate of Newton's method .

2. Spatial finite difference discretizations to partial differential equations (PDE) lead to stiff systems of ODE. To illustrate this point consider the heat equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

   where $(x, t) \in [0, 1]x[0, \infty)$ and u is subject to the boundary conditions $u(0, t) = 0 = u(1, t)$ and the initial condition $u(x, 0) = u_0(x)$. First we discretize in space and think of time as a parameter. Introduce meshpoints $x_n = nh$ where $h = 1/N$ and denote by $U_n(t) \approx u(x_n, t)$. Then using the central difference approximation to the second derivative:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{n+1}(t) - 2u_n(t) + u_{n-1}(t)}{h^2} + O\left(h^2\right) \tag{2}$$

   we obtain the following system of ODE:

$$\frac{dU_n(t)}{dt} = \frac{U_{n+1}(t) - 2U_n(t) + U_{n-1}(t)}{h^2} = A.u_n \quad n = 1, ..., N-1 \tag{3}$$

   where $A. := \frac{E-2I+E^{-1}}{h^2}$ and E is the shift operator.

   (a) Show that the eigenvalues of A are $\lambda_k = -4N^2 \sin^2(k\pi/2N)$

   (b) Determine the stiffness ratio for the system (3) i.e. λ_{N-1}/λ_1

(c) Now regarding (3) as a system of ODE what is the maximum stepsize Δt that can be used to solve (3) by Euler's method? What is the largest time step that can be used if the Implicit Euler method is used? Can the leapfrog method be used for this system?

(d) Use your Euler routine to solve this system with initial condition $u_0(x) = 2x$, for $x \in \left[0, \frac{1}{2}\right]$, $u_0(x) = 2 - 2x$, for $x \in \left(\frac{1}{2}, 1\right]$, $h = 0.1$ and time steps

$$\Delta t = 0.001,\ 0.0025,\ 0.005,\ 0.0075 \tag{4}$$

Integrate out to $t = 0.015$. Compare this numerical solution to the analytic solution

$$u(x,t) = \frac{8}{\pi^2} \sum_{n=1}^{\infty} \frac{\sin(n\pi/2)\sin(n\pi x)\, e^{-(n\pi)^2 t}}{n^2} \tag{5}$$

3. Consider the one dimensional wave equation:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \tag{6}$$

Assume that the central difference approximation is used to obtain a spatial discretization of (6):

$$\frac{dU_n(t)}{dt} = -c\frac{U_{n+1}(t) - U_{n-1}(t)}{2h} = C.u_n \qquad n = 1, \ldots, N \tag{7}$$

where $C. := -c\frac{E-E^{-1}}{2h}$, $x_n = nh$ and $U_n(t) \approx u(x_n, t)$. Also assume that the forward and backward difference operators

$$\dot{U}_n(t) = -c\left(\frac{U_{n+1}(t) - U_n(t)}{h}\right) = F.u_n \tag{8}$$

where $F. := -c\frac{E-1}{h}$ and

$$\dot{U}_n(t) = -c\left(\frac{U_n(t) - U_{n-1}(t)}{h}\right) = B.u_n \tag{9}$$

where $B. := -c\frac{1-E^{-1}}{h}$ are being considered.

(a) Given that $\left\{e^{i\xi x_n}\right\}$ are the eigenfunctions of each of these operators $C.$, $F.$, and $B.$, obtain their eigenvalues by applying each of the operators to $e^{i\xi x_n}$. Discuss which of these spatial discretizations is likely to be stable, unstable, and dissipative.

(b) Which of the following time stepping methods will be stable for (7): Explicit Euler, Backward Euler, RK-2, RK-3, RK-4, Leapfrog?

(c) Use the Trapezoidal Method and the central difference spatial semi-discretization operator C.to solve the following initial-boundary value problem with $c = 0.5$:

$$u(0,t) = 0, \quad u(x,0) = u_0(x) = \begin{cases} 1 & \text{if } x \in [30, 32] \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

on the region $x \in [0, 60]$ and $h = 0.1$. Compare your results with the exact solution $u(x,t) = u_0(x - ct)$. Integrate the solution out to $t = 30$.

4. Consider the following boundary value problem

$$\mathcal{L}u = u'' + k^2 u(x) = f(x), \quad u(0) = \alpha, \quad u'(1) = \beta \tag{11}$$

(a) Use integration by parts to obtain the weak statement of the BVP.

(b) If f is sufficiently differentiable show that the strong and weak formulations of the BVP are equivalent.

(c) Write down the Galerkin formulation of this BVP.

(d) Use piecewise linear basis functions and the weak formulation to obtain a Finite Element discretization of the BVP.

(e) Solve the BVP with $f(x) = x^3$, $k = 10$, $\alpha = 0$, and $\beta = 1$ and $N = 10, 20, 30$ and compare with the exact solution.

(f) In the case $f(x) = 0$, $\alpha = 0$, and $\beta = 0$ we have an eigenvalue problem. By considering the minimization of the appropriate Rayleigh quotient or the appropriate weak formulation, use Finite Elements to discretize the problem and to reduce it to a corresponding generalized matrix eigenvalue problem of the form $Ax = \lambda Bx$. Use the MATLAB function [V,D] = EIG(A,B) to determine the eigenvalues and corresponding eigenvectors for $N = 10$. Discretize the same problem using finite differences, determine an explicit expression for the approximate eigenvalues of the finite difference equations, and determine the order of the error. Compare the results of the FEM and FD solutions by providing the following plots: k_j vs mode number j, and the first three eigenfunctions.