06-611 Mathematical Modeling of Chemical Engineering Processes

06-611: Special Topics: Comp. Math

Homework Assignment #6

Due by 5:00pm on Tuesday November 20, 2012

Optimization

1) See the file `HW6.pdf` and files on blackboard.

Boundary Value Problems – Shooting Method

2) For linear boundary value problems of the form $y'' = p(x)y' + q(x)y + r(x)$ there is a simple procedure that makes the shooting method very effective. The function $y(x) = y_1(x) + cy_2(x)$ will be an exact solution to the problem where $y_1(x)$ is the solution to to the IVP that corresponds to the nonhomogeneous BVP and $y_2(x)$ is the solution to the corresponding homogeneous IVP (i.e., with $r(x) = 0$). For the following problem:

$$-u'' + \pi^2 u = 2\pi^2 \sin(\pi x)$$
$$u(0) = u(1) = 0$$

a) Convert this problem into two first order initial value problems to solve for $u_1(x)$ and $u_2(x)$. Show the systems that you plan to solve and the relevant initial value conditions.

b) Use an RK4 method to estimate $u_1(x)$ and $u_2(x)$ at $x_i = 0, 0.25, 0.50, 0.75, 1.00$. Is the prediction for the Dirichlet condition at $x = 1$ correct?

c) Determine the value of c that will give the approximate solution for $y(x)$. Use this to pointwise calculate $w(x) = y_1(x) + cy_2(x)$ given the values calculated in part (b).

d) Since the analytical solution is $u(x) = \sin(\pi x)$ calculate the exact error at each point.

3) Solving nonlinear problems using the shooting method generally comes down to generating solutions for the unknown boundary given different guesses of initial conditions and then using a root finding routine to find the best solution. For the following problem with Robin boundary conditions:

$$y'' = 2y^3$$
$$3y(0) - 9y'(0) = 2,\; y(1) = 1/4$$

a) First do a transformation of the independent variable such that $z = 1 - x$ and comment on the impact on the differential equation and the boundary conditions.

b) To solve this problem, we will determine the value of *p* for which *F(p) = 2 – 3y(1;p) + 9 y'(1;p)* is equal to zero where *y(z;p)* is the solution to the IVP:

$$y'' = 2y^3$$
$$y(0) = 1/4, y'(0) = p$$

Generate a table of values of *y(**1**;p)* for different values of *p* using an ode solver of your choice. Determine the value of p that gives *F(p) = 0* and describe your method.

c) Plot y(x) over the region $x \in [0,1]$ for the value of p found in part (b).

Boundary Value Problems – Finite Difference Methods

4) The code `BVP_2D_Poisson_FD` solves the Poisson equation with Dirichlet-type boundary conditions. You are interested in solving the problem for a microfluidic device. The channel has a rectangular cross section of 100 μm by 150 μm. The fluid flowing in the channel is Newtonian oil with viscosity, μ, and is driven by a pressure drop of ΔP/Δz of 1 Pa/mm.
   a) For a fluid of μ=1 cP, plot the velocity profile in the z direction of the channel, v_z across the channel (as in Fig 6.3). Determine the flow rate in the channel.
   b) Repeat part (a) for a fluid that is 50 times more viscous.

5) Beers **6.B.2**

6) For the second order differential equation $u'' - u = 1$, solve using finite differences using five internal nodes and plot the approximate solution as $w_i(x_i)$ for each of the following boundary conditions:
   a) $u(0) = 0; u(1) = 1$
   b) $u(0) = 0; u(1) + u'(1) = 1$
   c) $u(0) = 0; u'(1) = 1$