ME 690-001 **Final Examination** **Spring 2017**

(Take Home: Due May 1, 2017 at 5:30 pm)
(400 pts.)

You may use class notes and whatever reference material is applicable.

Part I. Analysis (250 pts.)

1. Derive a formula for the required number of iterations, n, of a linear, fixed-point iteration in terms of the spectral radius of the iteration matrix. State any asumptions you employ, and discuss their validity (or lack thereof).

   Use this to predict the total arithmetic (as a function of the number N of unknowns) for 3-D SOR to converge to a specified error tolerance. Provide all details of the analysis including statement of any required theorems.

2. Discuss the underlying rationale in constructing multi-grid methods, in particular, casting this in the context of asymptotic convergence rate of linear fixed-point iterations. Then describe each of the main steps of a multi-grid method, explaining what is accomplished by each. Make a diagram of a V-cycle based full multigrid (FMG) method having four (4) levels, and estimate the total arithmetic for one complete cycle in terms of N, the number of unknowns on the finest grid, under the assumption that a linear iterative method is iterated to convergence on the coarsest grid. Discuss advantages and disadvantages of FMG methods.

3. Consider the PDE system for two dependent variables u and v in two space dimensions given as

$$u_t + (u^2)_x + (uv)_y = \big(a(x,y)u_x\big)_x + \big(b(x,y)u_y\big)_y\,, \tag{1a}$$

$$v_t + (uv)_x + (v^2)_y = \big(a(x,y)v_x\big)_x + \big(b(x,y)v_y\big)_y\,, \tag{1b}$$

   solved on the unit square $(0,1)\times(1,0)\equiv\Omega$, with $t\in(0,t_f]$. Assume boundary conditions on $\partial\Omega$ are of Dirichlet type given by

$$u(x,y,t) = g(x,y,t), \quad (x,y)\in\partial\Omega \quad t\in(0,t_f]\,,$$

   and the initial data are

$$u(x,y,0) = u_0(x,y) \quad (x,y)\in\overline{\Omega}\,.$$

   Employ trapezoidal time integration, δ-form quasilinearization, and uniformly second-order accurate centered spatial discretization.

   (a) Give details of temporal and spatial discretizations, and linearization. Note that only one of Eqs. (1) need be treated in detail. The same uniform grid spacing h may be employed in both spatial directions.

   (b) Show that it is possible to maintain formal temporal accuracy in the absence of iterations for quasilinearization, and indicate circumstances (with regard to time-step sizes, and other issues) when this might fail.

   (c) Cast the linearized equations into the form of a general 2-level difference equation—in particular, provide the contents of the matrices occurring in this form, and employ δ-form Douglas–Gunn time splitting to advance the solution from time t^n to t^{n+1}. Note any assumptions you employ in this construction.

(d) Give the form of the block matrices occurring in the first split step of the D–G procedure, and provide details, including total floating-point arithmetic per time step, of how this linear system would be solved. Include in this description the definitions of various elements appearing in these matrices.

(e) Briefly describe an alternative to this block-coupled solution procedure, and estimate total arithmetic per time step as done in part (d). Include such issues as iteration convergence rate and effects of problem size as you compare required arithmetic of these two approaches.

4. For a steady, linearized Burgers' equation, employ a centered discretization, define the cell Reynolds number, and then show that the roots of the corresponding characteristic equation are:

$$z_+ = \frac{1 + \frac{1}{2}Re_h}{1 - \frac{1}{2}Re_h}\,, \qquad z_- = 1\,.$$

Now give the exact solution to the difference equation up to unknown "integration" constants. State what additional information would be needed to determine these constants. Discuss what properties of this exact solution lead to difficulties in approximations to physical problems. Finally, make a plot of the first of these roots, and use this to discuss detailed implications of the "cell-Re restriction" for centered-difference approximations.

5. Consider the 2-D Shuman filter,

$$\widetilde{u}_{i,j} = \frac{u_{i-1,j} + u_{i,j-1} + \beta u_{i,j} + u_{i,j+1} + u_{i+1,j}}{4 + \beta}.$$

By employing the notion of a discrete molifier, analogous to what is done in 1-D, derive this formula. (Hint: how does the triangle of 1-D generalize to 2-D?)

6. Derive the formula for a second-order accurate approximation to the first derivative, u_x, on a non-uniform grid. Then show that the three-point approximation to the second derivative is only first-order accurate. Discuss implications of these results with respect to use of unstructured grids, especially in two and three space dimensions.

7. Derive the elements of the metric tensor $\boldsymbol{g}$ associated with a 2-D basis change $(x, y) \rightarrow (\xi, \eta)$. Calculate the determinant of this tensor to demonstrate the origin of the notation $\sqrt{g}$ employed in grid generation.

8. Suppose it is desired to compute a solution to

$$u_t + u_x + u_y = \Delta u\,, \qquad (x, y) \in (0, L] \times (S(x), H] \equiv \Omega_{xy}\,,$$

with initial conditions

$$u(x, y, 0) = u_0(x, y)\,,$$

and boundary conditions

$$\begin{aligned} u(0, t) &= U\,, \qquad & u_x(L, t) &= 0\,, \\ u(S, t) &= 0\,, \qquad & u_x(H, t) &= 0\,. \end{aligned}$$

Here $S(x)$ is a prescribed function in $C^2(\Omega_{xy})$, and $H > \max_x S(x)$ holds. Develop body-fitted coordinates for this calculation by carrying out the following steps.

(a) Sketch (hypothetical—and, non-trivial) physical and computational domains.

(b) Derive the required transformation of coordinates and the associated metric information.

(c) Transform the differential equation and boundary conditions so that the new equation can be solved on the domain $(0,1] \times (0,1] \equiv \Omega_{\xi\eta}$ using uniform grid spacing. Note: this result should be put in a form that requires input of only physical-domain grid-point coordinates permitting accurate centered approximations of all derivatives associated with metric information.

Part II. Computer Simulations (150 pts.)

1. Consider the non-trival PDE boundary-value problem

$$a(x,y)u_{xx} + b(x,y)u_{xy} + c(x,y)u_{yy} = f(x,y), \quad (x,y) \in \Omega \equiv [0,1] \times (0,1) \tag{2}$$

with boundary conditions

$$\begin{aligned} u_x(0,y) &= g_1(y) \\ u(x,0) &= g_2(x) \\ u_x + \alpha(y)u &= g_3(y) \\ u(x,1) &= g_4(x)\ . \end{aligned}$$

Here,

$$a(x,y) \equiv e^{x+y}\,, \quad b(x,y) \equiv \frac{xy}{1+x+y}\,, \quad c(x,y) \equiv e^{-(x+y)}\,;$$

also

$$f(x,y) = -8\pi^2\left[\big(5a(x,y) + 2c(x,y)\big)\cos(20\pi x)\sin(4\pi y) + 10b(x,y)\sin(20\pi x)\cos(4\pi y)\right],$$

and

$$\alpha(y) \equiv \log_{10}(1+y)\,.$$

Finally, the boundary condition right-hand-side functions are:

$$\begin{aligned} g_1(y) &= 0 \\ g_2(x) &= 0 \\ g_3(y) &= \alpha(y)\sin(4\pi y) \\ g_4(x) &= 0\ . \end{aligned}$$

The exact solution to this problem is

$$u(x,y) = \cos(20\pi x)\sin(4\pi y)\,. \tag{5}$$

Note that all of this information is already coded in the Fortran 77/90 program ellptcslvr-stdnt-fnlexm.f, and to conduct the required numerical experiments you need only run the code as you did for Homework #1.

(a) Determine the type of PDE given in Eq. (2).

(b) Estimate the number of grid points in each direction needed to minimally resolve the solution; describe how you arrive at this estimate. Note that points will be deducted from your score if your estimate is too conservative. Now conduct grid-function convergence tests by successively doubling the number of points in each direction until the average error per grid point (part of the output to the screen) is less than single-precision machine ϵ ($\sim 10^{-7}$). Demonstrate, graphically (plot L^2 error vs. grid spacing), the order of accuracy of the method for this problem. Employ point SOR with the iteration parameter automatically produced by the code, and an iteration error tolerance of 10^{-10} for these runs.

(c) Explain why it would be impossible to analytically predict exact values of the SOR optimal parameter, ω_b, for this problem. Support your explanation by deriving elements of the corresponding Jacobi iteration matrix—say, for one or two rows of the matrix, and discuss why the approach used for the Laplace–Dirichlet problem cannot be used. Now, for each of the grids employed for your grid-function convergence tests of part (b), numerically find ω_b accurate to <u>three</u> decimal places. Provide a table of these results.

(d) Having found ω_b for each of your grids, test whether SOR theory still holds for this quite complicated problem. Note that in doing this, because the number of grid points is different in the two directions, you will now want to make appropriate plots in terms of $\sqrt{N} \equiv \sqrt{N_x N_y}$.

(e) Finally, for your finest grid (on which the solution is accurate to single-precision machine ϵ), compare run times for all SOR methods (employing the same value of ω_b, found in your numerical experiments) and the BiCGStab procedure. In addition, make a run with the fastest of the SOR methods using the default Dirichlet problem ω_b. Make a table of these results showing number of iterations and run time for each method, and discuss the results.

2. Use the code provided for 2-D parabolic problems to solve the following problem.

$$u_t - a(x,y)u_{xx} - c(x,y)u_{yy} = f(x,y,t), \quad (x,y) \in (0,1)\times(0,1) \ \text{ and } \ t \in (0,t_f]$$

with Dirichlet boundary conditions

$$\begin{aligned} u(0,y,t) &= \sin(\pi^2 t)\cos(\sqrt{e}\pi y) \\ u(x,0,t) &= \sin(\pi^2 t)\cos(8\pi x) \\ u(1,y,t) &= \sin(\pi^2 t)\cos(\sqrt{e}\pi y) \\ u(x,1,t) &= \cos(\sqrt{e}\pi)\sin(\pi^2 t)\cos(8\pi x)\,, \end{aligned}$$

and initial conditions

$$u(x,y,0) \equiv 0\,.$$

Here,

$$a(x,y) \equiv \frac{xy}{1+e^{x+y}}\,, \quad c(x,y) \equiv \frac{1}{1+\log_{10}(1+xy)}\,,$$

and

$$f(x,y,t) = \pi^2\left[\cos\pi^2 t + (64a(x,y) + ec(x,y))\sin\pi^2 t\right]\cos 8\pi x \cos\sqrt{e}\pi y\,.$$

The exact solution is

$$u(x,y,t) = \sin(\pi^2 t)\cos(8\pi x)\cos(\sqrt{e}\pi y)\,.$$

All of these functions are already coded in the available Fortran 77/90 code, and the user need only run the problems as was done in Homework #2.

The purpose of this problem is to demonstrate the effects of variable coefficients and right-hand sides in the differential equation and boundary conditions. To do this, consider $t \in (0, 0.5]$ with the coarsest resolution being $h = k = 0.02$ with refinement of discretizations until the L^2 error is less than 10^{-2} measured at times 0.1, 0.2, 0.3, 0.4, 0.5. Carry out the following steps.

(a) For the Douglas–Gunn method conduct grid-function convergence tests at selected spatial points (you decide which ones, and provide rationale for your choices) keeping the Courant number fixed at 1.0. Make plots of the time series associated with each chosen point. Discuss your observations, in particular, comparing performance—both accuracy and run time—with what you observed in Homework #2 for constant-coefficient cases.

(b) Repeat part (a) using locally one-dimensional time splitting. Again, compare these results with those of Homework #2 and with the current D–G results.

(c) Repeat part (a) using optimal SOR with temporal discretization corresponding to trapezoidal integration. Again, compare these results with those of Homework #2 and with the current D–G results.

(d) Discuss reasons for the large differences in run time for the time-split methods, and why the unsplit (SOR) times seem to differ less from the split times in this variable-coefficient case.