PHYS 410/555: Computational Physics Fall 2000 Homework 4
DUE: Tuesday, October 31, 10:30 AM Report bugs to choptuik@physics.ubc.ca

The following assignment involves writing and testing three Fortran 77 programs which use LAPACK routines to solve various linear systems. You must also prepare a short `Maple` *worksheet for Problem 3. Follow the instructions carefully and do all program development on* `sgi1`*. All files required by the assignment must reside in the correct places on your* `sgi1` *account for the homework to be considered complete. In addition, for Problem 1, you must "port" your code to the* `vn` *cluster front-end machine,* `vnfe1.physics.ubc.ca`*, and successfully compile and execute it there. Note that you are free—and in fact encouraged—to work from the relevant examples covered in class.*

Note: *This assignment is identical for both 410 and 555 students; i.e. all students must complete all three problems.*

Problem 1a: In directory `~/hw4/a1` on your `sgi1` account, create a source file `lsolve.f` and corresponding executable `lsolve` which solves a general linear system. `lsolve` is to accept exactly two arguments:

```
usage: lsolve <matrix file> <rhs file>
```

where `<matrix file>` is the name of a file which contains an $n \times n$ matrix (A) and `<rhs file>` is the name of a file which contains an n–element column vector (b). `lsolve` is to read the matrix and the right-hand-side vector, then compute the solution, x of the linear system

$$A\,x = b$$

using the `LAPACK` routine `DGESV`. If the solution is successful, the solution vector x is to be written to standard output, one number per line. Use the routines `dvfrom` and `dvto` (see Course Notes, Sep. 28) to read and write the vectors and `dmfrom` (Course Notes, Oct. 5) to read the matrix. It is probably best to include these routines in your `lsolve.f` source file. Recall that all source code covered in class is available in the `phys410` account on `sgi1`. Also note that `dmfrom` reads array entries in standard Fortran order; i.e. column-by-column. Your implementation of `lsolve` should do a reasonable amount of error checking, including:

- verification that the input arguments refer to existing files
- verification that the input matrix, A, is square (i.e. $n \times n$ for some n)
- verification that the length of the rhs vector, b, is n, given that A is $n \times n$
- verification that sufficient storage exists to store A

If any of these error conditions are encountered, `lsolve` should print an error-message to standard error, then exit. Note that you need not test for file-existence in the main program since both `dvfrom` and `dmfrom` return information which can be used to deduce that the specified file did not exist. Test your program using, for example, a small–n problem such as that covered in the October 10–12 lectures, as well as various types of *invalid* input. I will further test your implementation with my own input.

Problem 1b: Once you are satisfied that your program is working, transfer it to the directory `~/hw4/a1` on your account on `vnfe1.physics.ubc.ca`. Note that you can (and should be able to!) accomplish this transfer with a single `scp` command. Build and test your application on the Linux machine (`vnfe1`). (*Hint:* Use an appropriate `Makefile`—see the Oct. 10–12 Course Notes for an example.) I will test your "port" with my own input.

Problem 2: Consider the following boundary value problem (BVP)

$$u''(x) + a(x)\,u'(x) + b(x)\,u(x) = f(x) \qquad 0 \le x \le 1 \qquad u(0), u(1) \ \text{ specified}$$

where $'$ denotes differentiation with respect to x, and $a(x)$, $b(x)$ and $f(x)$ are given functions. In directory `~/hw4/a2` on your `sgi1` account, create a source file `gbvp1d.f` and corresponding executable `gbvp1d` which

approximately solves this problem using second-order ($O(h^2)$) finite-difference methods. Specifically, discretize the continuum domain using a uniform mesh, $x_i, i = 1, \ldots, N$ with mesh spacing $h = 1/(N-1)$ (as discussed in class) and use the following approximations for the first and second derivatives;

$$\frac{u_{i+1} - u_{i-1}}{2h} = u'(x_i) + O(h^2)$$

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u''(x_i) + O(h^2)$$

Your program needs to first set up the tridiagonal system which results from discretizing the BVP using the above approximations and then solve the system using the `LAPACK` routine `DGTSV`. Test your implementation by taking:

$$u(x) \equiv u_{\text{exact}}(x) = \sin(4\pi x) \qquad a(x) = 16x^2 \qquad b(x) = 8x^3$$

then computing what $f(x)$ must be to satisfy the ODE. Your code should thus probably include a routine which calculates the appropriate values for a, b, f and u_{exact} on the finite-difference mesh x_i. Your program should have precisely the same usage and output behaviour as the example `bvp1d` covered in class. In particular, usage for `gbvp1d` should be

```
usage: gbvp1d <level> [<option>]

       Specify option .ne. 0 for output
       of error instead of solution
```

where the required integer argument, `<level>`, specifies the discretization level, l, such that $h = 1/2^l$ and $N = 2^l + 1$. If `<option>` is 0, or not specified, the standard output of `gbvp1d` is (x_i, u_i) (two numbers per line), $i = 1, \ldots n$, where u_i are the components of the computed solution. If `<option>` is non-zero, the standard output of `gbvp1d` is (x_i, e_i) (two numbers per line), $i = 1, \ldots n$, where $e = u_{\text{exact}} - u$ is the error in the computed solution. In all cases, the program should also compute the RMS error of the computed solution and output it to standard error. Using `gnuplot`, make postscript plots showing (A) the level 6 solution and the exact solution as a function of x (`soln6.ps`) and (B) the error for level 5, 6 and 7 solutions, also as a function of x (`err567.ps`). (The postscript files should, of course, be located in the directory `~/hw4/a2`.)

Problem 3: Consider the BVP problem defined in the previous question and, in `~/hw4/a3` on your `sgi1` account, create a source file `gbvp1d4.f` and executable `gbvp1d4` which approximately solves the ODE using a combination of $O(h^4)$ and $O(h^2)$ finite-difference approximations of the first and second derivatives. Specifically, use

$$\frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12h} = u'(x_i) + O(h^4)$$

$$\frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12h^2} = u''(x_i) + O(h^4)$$

for $i = 3, \ldots, N-2$, and the second-order approximations given previously for $i = 2$ and $i = N-1$. Before implementing the program, use `xmaple` to verify that the above difference formulae really *do* provide $O(h^4)$ approximations to $u'(x)$ and $u''(x)$. *Hint:* Consider `maple` expressions such as

```
> convert(taylor(u(x+h),h,8),polynom);
> convert(taylor(u(x+2*h),h,8),polynom);
```

Document your work in a `maple` worksheet called `~/hw4/a3/fd4.mws`. Your implementation of `gbvp1d4` must first set up the pentadiagonal system for the u_i, and then solve the linear system using the `LAPACK` banded-solver `DGBSV`. Use the same $a(x), b(x)$ and $u_{\text{exact}}(x)$ to test your program as you used in Problem 2. `gbvp1d4` *should accept precisely the same arguments and have precisely the same output behaviour as* `gbvp1d`. Using `gnuplot`, make postscript plots showing (A) the level 6 solution and the exact solution, as a function of x (`soln6.ps`) and (B) the error for level 5, 6 and 7 solutions, also as a function of x (`err567.ps`).

Note: You may find this problem significantly more difficult to complete than the other two. Don't leave it until the last minute and don't be afraid to ask for help and/or advice.