Math*6020 Scientific Computing
Instructor: Prof. H.J.Eberl

Assignment 2
Due: 23 Feb 2016, in class

- First/last name and ID number must be clearly legible
- Submit your assignments in a report cover and/or make sure they are sturdily stapled together.
- Please submit your assignment (i) to me directly (MACN508), or (ii) my mailbox in the Math/Stats mail room, or (iii) to the Mathematics main office, or (iv) bring it to class on TUE Feb 23
- The source code of the program should be emailed to me at `heberl@uoguelph.ca`.

A2.1 **Non-stationary linear solvers.** In Barrett et al, "Templates for the solution of linear systems: Building blocks for iterative methods", SIAM, 1994, section 2.3.8 describes the BiConjugate Gradient Stabilized Method (BiCGSTAB) as an extension of the Conjugate Gradient method that is applicable to non-symmetric problems.

a) Implement this method in Fortran for sparse matrices stored in diagonal format, using the subroutine interface as defined in the file `LSDIAGtest.f90`. You may use the matrix-vector product defined in the same file. Test this method with non-symmetric matrices using the testbed of `LSDIAGtest.f90`. Briefly describe the test that you ran and document the results (including information on error tolerances used).

b) We are now considering the case $Ax = b$ with $A \in \mathbb{R}^{n \times n}$ where $n = 160,000$. The matrix A in diagonal format has the offsets `ioff`$= (-400, -1, 0, 1, 400)$, in the main diagonal everywhere the entry -5 and +1 in the four sub-diagonals, i.e. $A(:, 3) = -5$, $A(:, 1 : 2) = 1$, $A(:, 4 : 5) = 1$. Show that the matrix $-A$ is symmetric, positive definite, and diagonally dominant.

c) Using the CG algorithm that was provided in class, solve for the matrix A defined in b) the problem $Ax = b$ where the vector on the right hand side right hand side is $b = (-1, ..., -1)^T$. In both cases use tolerances $err1 = err2 = 10^{-10}$. Document the convergence of the method by plotting the residual $r_k := b - Ax_k$ and the update $x_k - x_{x-1}$ as functions of the iteration count k.

(*N.B. you can achieve this by either redirecting the output that is normally written to screen into a text file and then edit the text file for plotting, or by writing directly into a text file from within the subroutine of the linear solver*).

d) Repeat c) for the BiCGSTAB algorithm implemented in part a), as well as for the Jacobi and the Gauss-Seidel method. Compare the results obtained with both methods (in your discussion include also the numbers of iterations needed for convergence and the computing time used)

e) Change now A to be non-symmetric, $A(:,3) = -5.5$, $A(:,2) = 1.5$ and leave the other sub-diagonals as before. Solve the problem $Ax = b$ with $b = (1, ..., 1)^T$ with BiCGSTAB and the Conjugate Gradient method and describe and compare the convergence of the methods (if applicable).

A2.2 A very simple stationary solver for linear problems $Ax = b$ is the **Richardson Method with Relaxation**. It is given by

$$(*) \qquad x_{k+1} = x_k + \omega(b - Ax_k)$$

where ω is a scalar parameter that is chosen such that the iteration converges.

a) Find the matrices M and N of the first normal form of the iteration, and the matrix G and vector f of the second normal form.

b) Show that for symmetric positive definite A $(*)$ converges for $0 < \omega < \frac{2}{\lambda_{max}}$, where λ_{max} is the largest eigenvalue.

c) Show that for symmetric positive definite A the spectral radius of the matrix $G = I - \omega A$ is

$$\rho(G) = \max(1 - \omega\lambda_{min}, \omega\lambda_{max} - 1)$$

where $\lambda_{min,max}$ are the smallest and largest eigenvalues of A. Determine the value ω_{opt} for which the convergence rate of $(*)$ is optimal.

A2.3 **Iterative refinement** is an algorithm to improve the accuracy of the numerically computed (i.e. inexact) solution x_c of the linear system $Ax = b$. The algorithm is

[0] initialize: $x_0 := x_c$; let $i := 0$
[1] compute the residual $r_i := b - Ax_i$
[2] solve $Ad_i = r_i$ numerically with a given solver
[3] correct $x_{i+1} := x_i + d_i$
[4] if $\|d_i\| < tol$ terminate, else set $i := i + 1$ and go to [1]

Iterative refinement can be written as

$$(*) \qquad x_{k+1} = x_k + B^{-1}(b - Ax_k), \quad x_0 := x_c$$

where matrix B is such that the given numerical solver for $Ax = b$ produces an exact solution of $Bx = b$ (i.e. $x_c = B^{-1}b$). Thus B^{-1} is an approximation of A^{-1}, i.e $B^{-1}A \approx I$, $\|I - B^{-1}A\| < 1$.

a) Show that $(*)$ converges to the exact solution x of $Ax = b$.

b) Let $e_k := x_k - x$ be defined as the error of the kth iterate. Show that $e_{k+1} = (I - B^{-1}A)^{k+1}e_0$

A2.4 This is the missing piece of the proof that the Gauß-Seidel method converges for symmetric positive definite matrices A: Let L be a strictly lower triangular real matrix and D be a diagonal matrix with positive coefficients. Let $G := (D - L)^{-1}L^T$, $\tilde{G} := D^{1/2}GD^{-1/2}$, $\tilde{L} := D^{-1/2}LD^{-1/2}$. Show: $\tilde{G} = (I - \tilde{L})^{-1}\tilde{L}$.