University of Science Faculity of Mathematics and Computer Science

Worksheet #2

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Course: PUF - High Performance Computing
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Let A be the

- a) matrix defined in worksheet 1
- b) The 1D Finite Difference Matrix
- c) Matrices defined in Matrix Market.

1. Exercise 1

In the restarting **gmres.m** you received, add the missing lines that transform the **Hessenberg** matrix into an upper matrix by applying Givens rotation and which also provides the error at iteration j + 1.

Check that your restarting **gmres.m** is correct using manufactured solutions.

- First, use a restart parameter that is greater than the matrix dimension. What does this imply?
- Analyse in terms of computing and memory storage , the effect of the restarting parameter.

Comment the efficiency of gmres compared to the previous iterative methods worksheet 1).

GMRES.m:

```
, %*******************************
 function [x,error,iter] = GMRES(A,b,x,m,itmax,epsi)
4 % gmres.m solves the linear system Ax=b
_5 % using the Generalized Minimal residual ( GMRESm ) method with restarts
                    REAL nonsymmetric positive definite matrix
6 % input
           Α
7 %
                    REAL initial guess vector
8 %
                   REAL right hand side vector
           m
9 %
                   INTEGER number of iterations between restarts
                 INTEGER maximum number of iterations
           itmax
11 %
                     REAL error tolerance
           epsi
12 %
13 % output x
                    REAL solution vector
14 %
           error
                    REAL error norm
15 %
           iter
                    INTEGER number of iterations performed
16
```

```
17 % initialization
19 normb = norm(b);
20 if ( normb == 0.0 )
      normb = 1.0;
22 end
23 % residual
_{24} r = b - A*x;
25 error(1) = norm(r)/normb;
26 if ( error(1) < epsi )
      return;
28 end
[n,n] = size(A);
V(1:n,1:m+1) = zeros(n,m+1); % Vm+1=[Vm|qm+1]
31 H(1:m+1,1:m) = zeros(m+1,m); % Hessenberg matrix
32 cs(1:m) = zeros(m,1);
sn(1:m) = zeros(m,1);
35 e1
     = zeros(n,1);
                                 % basic vector
36 e1(1) = 1.0;
37 iter = 1;
                                  % step of iterator
38 itt = 1;
39 while iter <= itmax</pre>
                                  % begin iteration
40
      r = b - A * x;
      V(:,1) = r/norm(r);
      s = norm(r)*e1;
42
      for j = 1:m
                                  % construct orthonormal
43
                                 % basis using Gram-Schmidt
          itt = itt+1;
          w = A*V(:,j);
          for i = 1:j
46
              H(i,j) = w'*V(:,i);
47
              w = w - H(i,j) * V(:,i);
          end
49
          % size(H)
50
          H(j+1,j) = norm(w);
51
          V(:,j+1) = w/H(j+1,j);
  % We tranform the Hessenberg matrix H into a triangular matrix by
     applying Givens rotation
54
          for k = 1:j-1
                                  % apply Givens rotation
              temp = cs(k)*H(k,j) + sn(k)*H(k+1,j);
              H(k+1,j) = -sn(k)*H(k,j) + cs(k)*H(k+1,j);
56
                      = temp;
              H(k,j)
          end
          cs(j) = H(j,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
          sn(j) = H(j+1,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
60
          temp = cs(j)*s(j);
                                  % approximate residual norm
61
          s(j+1) = -sn(j)*s(j);
62
          s(j)
                 = temp;
          H(j,j) = cs(j)*H(j,j) + sn(j)*H(j+1,j);
64
          H(j+1,j) = 0.0;
          \% Which also provides the error at iteration j+1
67
          error(itt+1) = abs(s(j+1)) / normb;
68
          69
              y = H(1:j,1:j) \setminus s(1:j);
                                                      % and exit
70
71
              x = x + V(:,1:j)*y;
              % error(i+1) = abs(s(i+1)) / bnrm2;
72
              break;
73
```

```
74
           end
75
       \verb"end"
76
       if ( error(itt+1) <= epsi ), break, end</pre>
77
       y = H(1:m,1:m) \setminus s(1:m);
       % update approximation
       x = x + V(:,1:m)*y;
80
       \% update approximation
81
       % compute residual
       r = b - A*x;
83
       s(j+1) = norm(r);
       error(itt+1) = s(j+1) / normb;
                                             % check convergence
       if ( error(itt+1) <= epsi )</pre>
           break;
87
       end
88
       iter = iter+1;
89
90 end
91 iter = itt;
```

Matrix define in worksheet 1

Compare difference method:

Method	Number of iterations	Error	Time
GS Lower	42	3.1723e-08	0.012816
GS Upper	44	5.0821e-09	0.012816
Steepest Descent	1001	0.40714	0.053916
SOR	25	4.1048e-08	0.013954
CG	136	4.2446e-12	0.013785
GMRES	102	4.411e-14	0.045432

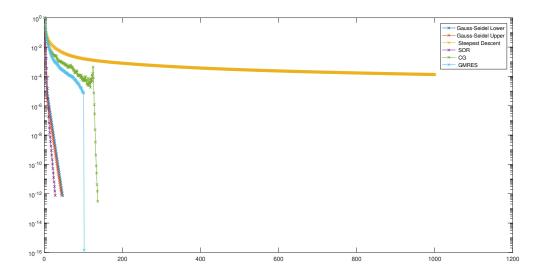


Figure 1: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

Matrix define Laplace 1D

Compare difference method:

Method	Number of iterations	Error	Time
GS Lower	1001	4.8297	0.022161
GS Upper	1001	4.841	0.022161
Steepest Descent	1001	4.8702	0.070996
SOR	1001	4.8091	0.046463
CG	405	2.4533e-09	0.029979
GMRES	102	2.4673e-10	0.064383

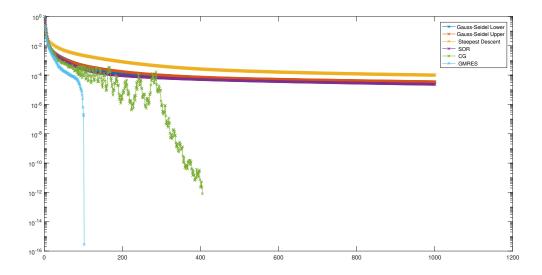


Figure 2: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

Using matrix from Matrix Market

1 **FILE**: 'hor131.mtx'

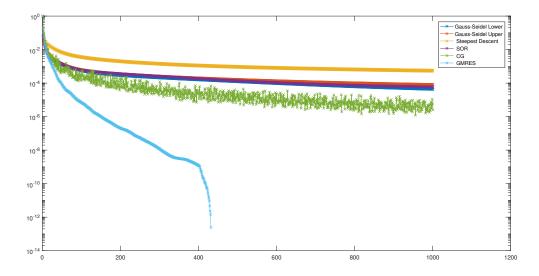


Figure 3: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

2 FILE: 'pde225.mtx'

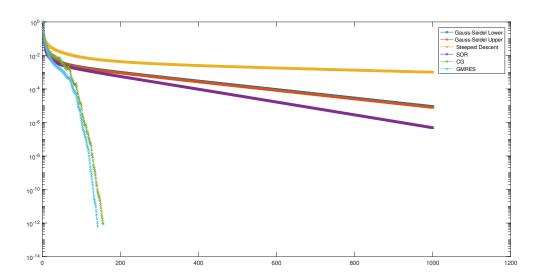


Figure 4: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

3 FILE: 'saylr4.mtx'

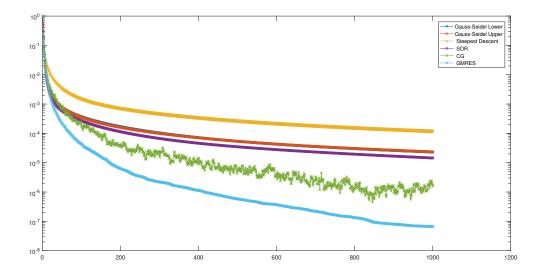


Figure 5: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

4 FILE: 'sherman4.mtx'

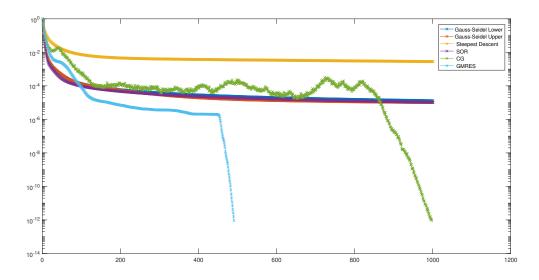


Figure 6: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

5 FILE: 'tub1000.mtx'

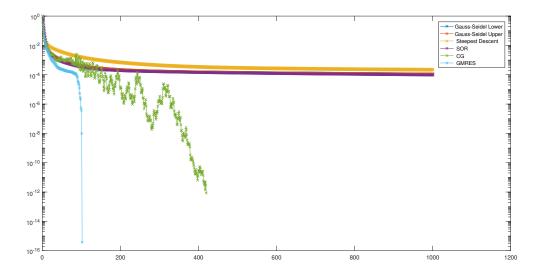


Figure 7: Comparison of value of $||x_{aprox} - x_{exact}||$ of different method with semilogy

Commend: For different case of matrix above, GMRES method show the best result among all method.

2. Exercise 2

```
Left preconditioner: Solve MAx = Mb.

Right preconditioner: Solve AMy = b, and then x = My.

Using the above gmres.m, modify it to precgmres.m so as to be able to use a right preconditioner M that can be changed at each restart of gmres.

Validate your precgmres.m defining M = \text{diag}(A)
```

Left preconditioner:

```
function [x, error, iter] = Left_PRECGMRES( A,b,x,M,m,itmax,epsi)
2 % PRECGMRES.m solves the preconditioner linear system
 % The left preconditioner solve MAx = b
   The right preconditioner solve AMy = b, then x = My
_{5} % Using the above gmres.m, modify it to precgmres.m so as to be able to
_6 % a right preconditioner M that can be changed at each restart of gmres.
                     REAL nonsymmetric positive definite matrix
            Α
8 %
                     REAL initial guess vector
            x
9 %
            b
                     REAL right hand side vector
                     REAL preconditioner matrix
11 %
                     INTEGER number of iterations between restarts
            numb m
12 %
                     INTEGER maximum number of iterations
            max_it
13 %
            tol
                     REAL error tolerance
15 % output x
                     REAL solution vector
16 %
                     REAL error norm
            error
17 %
                     INTEGER number of iterations performed
            iter
 % initialization
normb = norm(b);
```

```
_{21} if ( normb == 0.0 )
      normb = 1.0;
23 end
24
25 % residual
r = M*(b - A*x);
27 error(1) = norm(r)/normb;
28 if ( error(1) < epsi )
      return;
30 end
[n,n] = size(A);
V(1:n,1:m+1) = zeros(n,m+1); % Vm+1=[Vm|qm+1] H(1:m+1,1:m) = zeros(m+1,m); % Hessenberg matrix
34 cs(1:m) = zeros(m,1);
sn(1:m) = zeros(m,1);
37 e1
       = zeros(n,1);
                                    % basic vector
38 e1(1) = 1.0;
39 iter = 1;
                                    % step of iterator
40 itt = 1;
41 while iter <= itmax
                                    % begin iteration
      r = M*(b - A*x);
42
      V(:,1) = r/norm(r);
43
44
      s = norm(r)*e1;
      for j = 1:m
                                     % construct orthonormal
           itt = itt + 1;
                                     % basis using Gram-Schmidt
46
           w = M*A*V(:,j);
47
           for i = 1:j
               H(i,j) = w'*V(:,i);
               w = w - H(i,j)*V(:,i);
50
           end
51
                size(H)
           %
53
           H(j+1,j) = norm(w);
           V(:,j+1) = w/H(j+1,j);
54
           \% We tranform the Hessenberg matrix H into a triangular matrix
      by applying Givens rotation
           for k = 1:j-1
                                                           % apply Givens
      rotation
                       = cs(k)*H(k,j) + sn(k)*H(k+1,j);
57
               temp
               H(k+1,j) = -sn(k)*H(k,j) + cs(k)*H(k+1,j);
                       = temp;
               H(k,j)
59
           end
60
           cs(j) = H(j,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
61
           sn(j) = H(j+1,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
           temp
                = cs(j)*s(j);
                                                            % approximate
63
      residual norm
           s(j+1) = -sn(j)*s(j);
64
           s(j)
                  = temp;
           H(j,j) = cs(j)*H(j,j) + sn(j)*H(j+1,j);
66
           H(j+1,j) = 0.0;
67
           \% Which also provides the error at iteration j+1
           error(itt+1) = abs(s(j+1)) / normb;
70
71
           if ( error(itt+1) <= epsi )</pre>
                                                               % update
72
      approximation
               y = H(1:j,1:j) \setminus s(1:j);
                                                           % and exit
73
               x = x + V(:,1:j)*y;
74
```

```
% error(i+1) = abs(s(i+1)) / bnrm2;
75
                break;
76
77
           end
       end
78
      if ( error(itt+1) <= epsi ), break, end</pre>
      y = H(1:m,1:m) \setminus s(1:m);
81
           x = x + V*y;
                                                                   % update
82 %
      approximation
      x = x + V(:,1:m)*y;
                                                                   % update
83
      approximation
      % compute residual
84
      r = M*(b - A*x);
      s(j+1) = norm(r);
86
      error(itt+1) = s(j+1) / normb;
                                                                     % check
87
      convergence
      if ( error(itt+1) <= epsi )</pre>
89
           break;
      end
90
      iter = iter+1;
91
92 end
93 iter = itt;
```

Right preconditioner:

```
1 function [x, error, iter] = Right_PRECGMRES( A,b,y,M,m,itmax,epsi)
2 % PRECGMRES.m solves the preconditioner linear system
3 % The left preconditioner solve MAx = b
4 % The right preconditioner solve AMy = b, then x = My
_5 % Using the above gmres.m, modify it to precgmres.m so as to be able to
_{6} % a right preconditioner M that can be changed at each restart of gmres.
7 % input
           Α
                    REAL nonsymmetric positive definite matrix
8 %
                     REAL initial guess vector
            X
9 %
            b
                     REAL right hand side vector
10 %
            M
                     REAL preconditioner matrix
11 %
           numb_m INTEGER number of iterations between restarts
12 %
           max_it INTEGER maximum number of iterations
            tol
                     REAL error tolerance
13 %
14 %
15 % output x
                     REAL solution vector
16 %
            error
                     REAL error norm
                     INTEGER number of iterations performed
17 %
            iter
18 % initialization
normb = norm(b);
_{21} if ( normb == 0.0 )
      normb = 1.0;
23 end
24
25 % residual
r = b - A*M*y;
27 error(1) = norm(r)/normb;
28 if ( error(1) < epsi )
29
     return;
30 end
[n,n] = size(A);
V(1:n,1:m+1) = zeros(n,m+1); % Vm+1=[Vm|qm+1]
H(1:m+1,1:m) = zeros(m+1,m); % Hessenberg matrix
```

```
34 cs(1:m) = zeros(m,1);
sn(1:m) = zeros(m,1);
37 e1
       = zeros(n,1);
                                    % basic vector
38 e1(1) = 1.0;
39 iter = 1;
                                    % step of iterator
40 itt = 1;
41 while iter <= itmax
                                    % begin iteration
      r = b - A*M*y;
      V(:,1) = r/norm(r);
43
      s = norm(r)*e1;
44
      for j = 1:m
                                     % construct orthonormal
           itt = itt + 1;
                                     % basis using Gram-Schmidt
           w = A*M*V(:,j);
47
          for i = 1:j
48
               H(i,j) = w'*V(:,i);
49
               w = w - H(i,j)*V(:,i);
51
           %
                size(H)
           H(j+1,j) = norm(w);
           V(:,j+1) = w/H(j+1,j);
           \% We tranform the Hessenberg matrix H into a triangular matrix
      by applying Givens rotation
          for k = 1:j-1
                                                          % apply Givens
      rotation
                        = cs(k)*H(k,j) + sn(k)*H(k+1,j);
               temp
57
               H(k+1,j) = -sn(k)*H(k,j) + cs(k)*H(k+1,j);
               H(k,j)
                       = temp;
           end
           cs(j) = H(j,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
61
           sn(j) = H(j+1,j)/sqrt(H(j,j)^2 + H(j+1,j)^2);
62
           temp
                 = cs(j)*s(j);
                                                           % approximate
      residual norm
           s(j+1) = -sn(j)*s(j);
64
                  = temp;
           s(j)
65
           H(j,j) = cs(j)*H(j,j) + sn(j)*H(j+1,j);
           H(j+1,j) = 0.0;
67
           \% Which also provides the error at iteration j+1
68
69
           error(itt+1) = abs(s(j+1)) / normb;
71
          if ( error(itt+1) <= epsi )</pre>
                                                              % update
72
      approximation
               z = H(1:j,1:j) \setminus s(1:j);
                                                          % and exit
               y = y + V(:,1:j)*z;
74
               % error(i+1) = abs(s(i+1)) / bnrm2;
75
               break;
76
           end
77
      end
78
79
      if ( error(itt+1) <= epsi ), break, end</pre>
      z = H(1:m,1:m) \setminus s(1:m);
81
           x = x + V*y;
                                                               % update
82 %
      approximation
      y = y + V(:,1:m)*z;
                                                               % update
      approximation
      % compute residual
84
      r = b - A*M*y;
85
```

We using **right preconditioner** to apply equation Ax = b become AMy = b and x = My.

Where $M = \operatorname{diag}(\operatorname{diag}(A))$

Method	error	iter	Time (seconds)
GMRES	1.006e-14	101	0.047792
Right preconditioner	2.3357e-13	101	0.060019

Table 1: Compare 2 method method

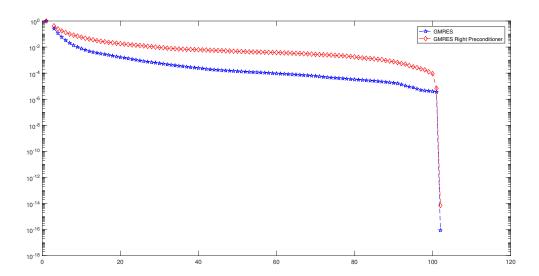


Figure 8: Comparison of GMRES and PRECGMRES

Commend: Although GMRES convergence faster, but PRECGMRES show us a better result (the approx is more close to exact solution)

3. Exercise 3

Look into the matlab function **ILU** that performs an ILU(0) approximation of A. [L0, U0] = ILU(A) Use this ILU(0) as a right preconditioner in precgmres.m to solve Ax = b as in TP1

Answer

Using **ILU** function, we have:

$$[L, U] = ilu(A)$$
$$M = inv(L * U)$$

Matrix in worksheet 1:

Method	error	iter	Time (seconds)
GMRES	2.4282e-14	101	0.040265
Right preconditioner	8.4696 e-15	2	0.03

Table 2: Compare 2 method method

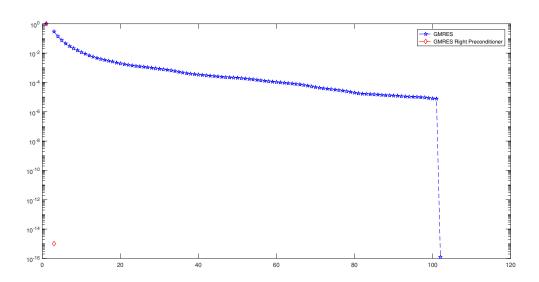


Figure 9: Comparison of GMRES and PRECGMRES

Matrix Market File 'hor131.mtx'

Method	error	iter	Time (seconds)
GMRES Right preconditioner	3.2943e-06 2.4151e-07	427 44	0.35305 0.59493

Table 3: Compare 2 method method

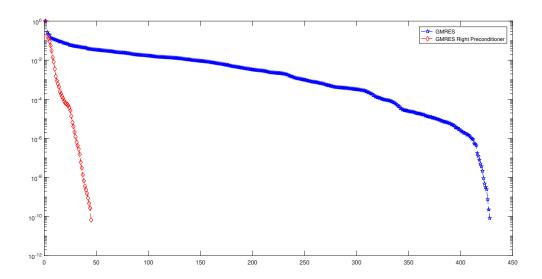


Figure 10: Comparison of GMRES and PRECGMRES

File 'pde225.mtx'

Method	error	iter	Time (seconds)
GMRES Right preconditioner	1.0984e-09 7.9933e-10	76 21	0.033946 0.068774

Table 4: Compare 2 method method

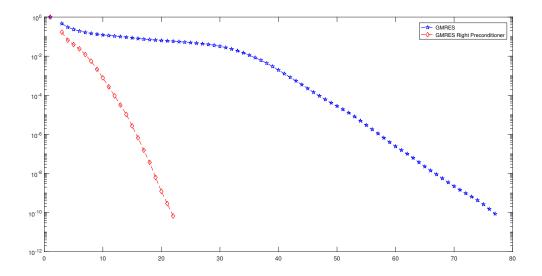


Figure 11: Comparison of GMRES and PRECGMRES

File 'saylr4.mtx'

Method	error	iter	Time (seconds)
GMRES	2.5793e-05	1684	41.2416
Right preconditioner	8.3633e-05	52	38.0274

Table 5: Compare 2 method method

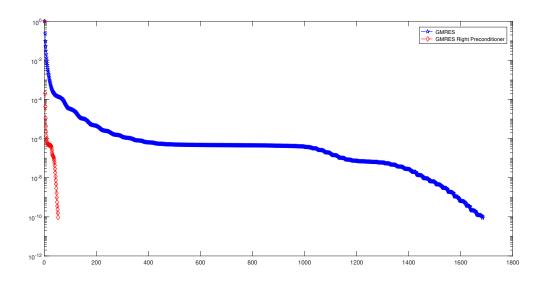


Figure 12: Comparison of GMRES and PRECGMRES

File 'sherman4.mtx'

Method	error	iter	Time (seconds)
GMRES	7.8963e-09	137	0.11605
Right preconditioner	4.3628e-09	38	0.61389

Table 6: Compare 2 method method

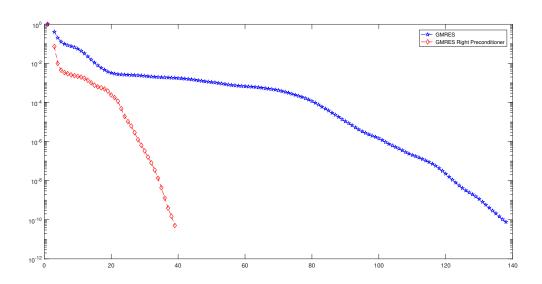


Figure 13: Comparison of GMRES and PRECGMRES

File 'tub100.mtx'

Method	error	iter	Time (seconds)
GMRES	4.4087e-13	101	0.046172
Right preconditioner	3.4059e-11	17	0.035

Table 7: Compare 2 method method

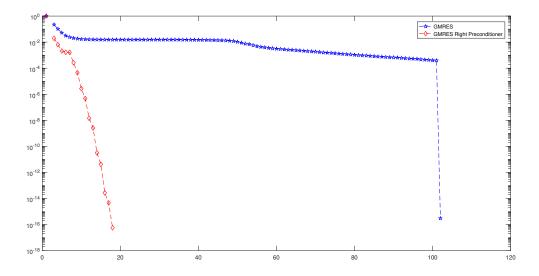


Figure 14: Comparison of GMRES and PRECGMRES