

```

1  !=====!
2  !
3  !   Software Name : HEC-MW Library for PC-cluster   !
4  !           Version : 2.5                           !
5  !
6  !   Last Update : 2006/06/01                       !
7  !           Category : Linear Solver                 !
8  !
9  !           Written by Kengo Nakajima (Univ. of Tokyo) !
10 !
11 !   Contact address : IIS, The University of Tokyo RSS21 project !
12 !
13 !   "Structural Analysis System for General-purpose Coupling   !
14 !   Simulations Using High End Computing Middleware (HEC-MW)" !
15 !
16 !=====!
17
18     module hecmw_solver_33
19     contains
20     !
21     !C***
22     !C*** hecmw_solve_33
23     !C***
24     !
25     subroutine hecmw_solve_33 (hecMESH, hecMAT)
26
27     use hecmw_util
28     use hecmw_solver_CG_33
29     use hecmw_solver_BiCGSTAB_33
30     use hecmw_solver_GMRES_33
31     use hecmw_solver_GPBIG_33
32     use hecmw_solver_BLCG_33
33     use hecmw_solver_BLBIGSTAB_33
34     use hecmw_solver_BLGPBiCG_33
35     use m_hecmw_solve_error
36     use m_hecmw_comm_f

```

```

37      use hecmw_matrix_ass
38      use hecmw_matrix_contact
39
40      implicit none
41
42      type (hecmwST_matrix)      :: hecMAT
43      type (hecmwST_local_mesh) :: hecMESH
44
45      integer(kind=kint) :: ERROR
46      real(kind=kreal), dimension(3,3) :: ALU
47      real(kind=kreal), dimension(3)   :: PW
48
49      integer(kind=kint) :: ITER, METHOD, PRECOND, NSET
50      integer(kind=kint) :: iterPREmax, ii, i, j, k
51
52      real(kind=kreal) :: RESID, SIGMA_DIAG, THRESH, FILTER
53
54      integer(kind=kint) :: ITERlog, TIMElog
55      real(kind=kreal)  :: TIME_setup, TIME_comm, TIME_soltot, TR
56      real(kind=kreal), dimension(1) :: RHS
57      integer (kind=kint), dimension(1) :: IFLAG
58
59      integer(kind=kint) :: NREST, NPLU, iSO, iS, inum, k0
60      real(kind=kreal)   :: SIGMA, S1_time, E1_time, TIME_sol
61
62      !C===
63      !C +-----+
64      !C | PARAMETERS |
65      !C +-----+
66      !C===
67      ITER      = hecMAT%Iarray(1)
68      METHOD     = hecMAT%Iarray(2)
69      PRECOND   = hecMAT%Iarray(3)
70      NSET      = hecMAT%Iarray(4)
71      iterPREmax= hecMAT%Iarray(5)
72      NREST     = hecMAT%Iarray(6)

```

```

73
74     ITERlog= hecMAT%Iarray (21)
75     TIMElog= hecMAT%Iarray (22)
76
77     TIME_setup = 0. d0
78     TIME_comm  = 0. d0
79     TIME_soltot = 0. d0
80
81     RESID      = hecMAT%Rarray(1)
82     SIGMA_DIAG= hecMAT%Rarray(2)
83     SIGMA      = hecMAT%Rarray(3)
84
85     THRESH= hecMAT%Rarray(4)
86     FILTER= hecMAT%Rarray(5)
87
88     if (iterPREmax.lt.1) iterPREmax= 1
89     if (iterPREmax.gt.4) iterPREmax= 4
90
91     !C===
92     !C +-----+
93     !C | ERROR CHECK |
94     !C +-----+
95     !C===
96         ERROR= 0
97
98     !C
99     !C-- ZERO RHS norm
100         RHS(1)= 0. d0
101         do i= 1, hecMAT%N
102             RHS(1)= RHS(1) + hecMAT%B(3*i-2)**2 + hecMAT%B(3*i-1)**2      &
103             &                + hecMAT%B(3*i )**2
104         enddo
105         if (hecMESH%mpc%n_mpc > 0) then
106             do i= 1, hecMESH%mpc%n_mpc
107                 RHS(1)= RHS(1) + hecMESH%mpc%mpc_const(i)**2
108             enddo

```

```

109         endif
110         call hecmw_allreduce_R (hecMESH, RHS, 1, hecmw_sum)
111
112         if (RHS(1).eq.0.d0) then
113             ERROR= 2002
114             call hecmw_solve_error (hecMESH, ERROR)
115         endif
116
117     !C
118     !C-- ZERO DIAGONAL component
119         IFLAG(1)= 0
120         do i= 1, hecMAT%N
121             if (dabs(hecMAT%D(9*i-8)).eq.0.d0) IFLAG(1)= 1
122             if (dabs(hecMAT%D(9*i-4)).eq.0.d0) IFLAG(1)= 1
123             if (dabs(hecMAT%D(9*i  )).eq.0.d0) IFLAG(1)= 1
124         enddo
125
126         call hecmw_allreduce_I (hecMESH, IFLAG, 1, hecmw_sum)
127         if (IFLAG(1).ne.0) then
128             ERROR= 2001
129             call hecmw_solve_error (hecMESH, ERROR)
130         endif
131
132     !C
133     !C-- INCONSISTENT SOLVER/PRECONDITIONING
134         IFLAG(1)= 0
135         if (METHOD.le.0 .or. METHOD.ge.5) IFLAG(1)= 1
136         if (PRECOND.le.0 .or. PRECOND.gt.21) IFLAG(1)= 1
137
138         call hecmw_allreduce_I (hecMESH, IFLAG, 1, hecmw_sum)
139         if (IFLAG(1).ne.0) then
140             ERROR= 1001
141             call hecmw_solve_error (hecMESH, ERROR)
142         endif
143
144         IFLAG(1)= 1

```

```

145     if (METHOD.eq.1) then
146         if (PRECOND.eq.1) IFLAG(1)=0
147         if (PRECOND.eq.2) IFLAG(1)=0
148         if (PRECOND.eq.3) IFLAG(1)=0
149         if (PRECOND.eq.10) IFLAG(1)=0
150         if (PRECOND.eq.11) IFLAG(1)=0
151         if (PRECOND.eq.12) IFLAG(1)=0
152     endif
153
154     if (METHOD.eq.2) then
155         if (PRECOND.eq.1) IFLAG(1)=0
156         if (PRECOND.eq.2) IFLAG(1)=0
157         if (PRECOND.eq.3) IFLAG(1)=0
158         if (PRECOND.eq.10) IFLAG(1)=0
159         if (PRECOND.eq.11) IFLAG(1)=0
160         if (PRECOND.eq.12) IFLAG(1)=0
161     endif
162
163     if (METHOD.eq.3) then
164         if (PRECOND.eq.1) IFLAG(1)=0
165         if (PRECOND.eq.2) IFLAG(1)=0
166         if (PRECOND.eq.3) IFLAG(1)=0
167     endif
168
169     if (METHOD.eq.4) then
170         if (PRECOND.eq.1) IFLAG(1)=0
171         if (PRECOND.eq.2) IFLAG(1)=0
172         if (PRECOND.eq.3) IFLAG(1)=0
173         if (PRECOND.eq.10) IFLAG(1)=0
174         if (PRECOND.eq.11) IFLAG(1)=0
175         if (PRECOND.eq.12) IFLAG(1)=0
176     endif
177
178     if (IFLAG(1).ne.0) then
179         ERROR=1001
180         call hecmw_solve_error (hecMESH, ERROR)

```

```

181         endif
182
183     !C===
184     !C +-----+
185     !C | BLOCK LUs |
186     !C +-----+
187     !C===
188         if (.not. associated(hecMAT%ALU).and. PRECOND.lt.10) NSET= 0
189         if (    associated(hecMAT%ALU).and. PRECOND.lt.10) NSET= -1
190
191         S1_time= HECMW_WTIME()
192         if (NSET.eq.0 .and. PRECOND.lt.10) then
193             allocate (hecMAT%ALU(9*hecMAT%N))
194         endif
195         if (NSET.le.0 .and. PRECOND.lt.10) then
196             hecMAT%ALU = 0.d0
197
198         do ii= 1, hecMAT%N
199             hecMAT%ALU(9*ii-8) = hecMAT%D(9*ii-8)
200             hecMAT%ALU(9*ii-7) = hecMAT%D(9*ii-7)
201             hecMAT%ALU(9*ii-6) = hecMAT%D(9*ii-6)
202             hecMAT%ALU(9*ii-5) = hecMAT%D(9*ii-5)
203             hecMAT%ALU(9*ii-4) = hecMAT%D(9*ii-4)
204             hecMAT%ALU(9*ii-3) = hecMAT%D(9*ii-3)
205             hecMAT%ALU(9*ii-2) = hecMAT%D(9*ii-2)
206             hecMAT%ALU(9*ii-1) = hecMAT%D(9*ii-1)
207             hecMAT%ALU(9*ii ) = hecMAT%D(9*ii )
208         enddo
209
210         if (hecMAT%cmat%n_val.gt.0) then
211             do k= 1, hecMAT%cmat%n_val
212                 if (hecMAT%cmat%pair(k)%i.ne.hecMAT%cmat%pair(k)%j) cycle
213                 ii = hecMAT%cmat%pair(k)%i
214                 hecMAT%ALU(9*ii-8) = hecMAT%ALU(9*ii-8) + hecMAT%cmat%pair(k)%val(1, 1)
215                 hecMAT%ALU(9*ii-7) = hecMAT%ALU(9*ii-7) + hecMAT%cmat%pair(k)%val(1, 2)
216                 hecMAT%ALU(9*ii-6) = hecMAT%ALU(9*ii-6) + hecMAT%cmat%pair(k)%val(1,

```

```

217 3)
218     hecMAT%ALU(9*i i-5) = hecMAT%ALU(9*i i-5) + hecMAT%cmat%pair(k)%val(2,
219 1)
220     hecMAT%ALU(9*i i-4) = hecMAT%ALU(9*i i-4) + hecMAT%cmat%pair(k)%val(2,
221 2)
222     hecMAT%ALU(9*i i-3) = hecMAT%ALU(9*i i-3) + hecMAT%cmat%pair(k)%val(2,
223 3)
224     hecMAT%ALU(9*i i-2) = hecMAT%ALU(9*i i-2) + hecMAT%cmat%pair(k)%val(3,
225 1)
226     hecMAT%ALU(9*i i-1) = hecMAT%ALU(9*i i-1) + hecMAT%cmat%pair(k)%val(3,
227 2)
228     hecMAT%ALU(9*i i ) = hecMAT%ALU(9*i i ) + hecMAT%cmat%pair(k)%val(3,
229 3)
230     enddo
231
232     call hecmw_cmat_LU( hecMAT )
233
234 endif
235
236 do ii= 1, hecMAT%N
237     ALU(1,1)= hecMAT%ALU(9*i i-8)
238     ALU(1,2)= hecMAT%ALU(9*i i-7)
239     ALU(1,3)= hecMAT%ALU(9*i i-6)
240     ALU(2,1)= hecMAT%ALU(9*i i-5)
241     ALU(2,2)= hecMAT%ALU(9*i i-4)
242     ALU(2,3)= hecMAT%ALU(9*i i-3)
243     ALU(3,1)= hecMAT%ALU(9*i i-2)
244     ALU(3,2)= hecMAT%ALU(9*i i-1)
245     ALU(3,3)= hecMAT%ALU(9*i i )
246     do k= 1, 3
247         ALU(k,k)= 1.d0/ALU(k,k)
248         do i= k+1, 3
249             ALU(i,k)= ALU(i,k) * ALU(k,k)
250             do j= k+1, 3
251                 PW(j)= ALU(i,j) - ALU(i,k)*ALU(k,j)
252             enddo

```

```

253         do j= k+1, 3
254             ALU(i, j)= PW(j)
255         enddo
256     enddo
257 enddo
258 hecMAT%ALU(9*ii-8)= ALU(1, 1)
259 hecMAT%ALU(9*ii-7)= ALU(1, 2)
260 hecMAT%ALU(9*ii-6)= ALU(1, 3)
261 hecMAT%ALU(9*ii-5)= ALU(2, 1)
262 hecMAT%ALU(9*ii-4)= ALU(2, 2)
263 hecMAT%ALU(9*ii-3)= ALU(2, 3)
264 hecMAT%ALU(9*ii-2)= ALU(3, 1)
265 hecMAT%ALU(9*ii-1)= ALU(3, 2)
266 hecMAT%ALU(9*ii )= ALU(3, 3)
267     enddo
268 endif
269
270 E1_time= HECMW_WTIME()
271 TIME_setup= TIME_setup + E1_time - S1_time
272
273 !C===
274 !C +-----+
275 !C | ITERATIVE solver |
276 !C +-----+
277 !C===
278
279 !C
280 !C-- CG
281     if (METHOD.eq.1 .and. PRECOND.lt.10) then
282         if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
283             if (PRECOND.eq.1) write (*,'(a,i3)') '### 3x3 B-IC-CG (0)', &
284                 & iterPREmax
285             if (PRECOND.eq.2) write (*,'(a,i3)') '### 3x3 B-SSOR-CG(0)', &
286                 & iterPREmax
287             if (PRECOND.eq.3) write (*,'(a,i3)') '### 3x3 B-scale-CG ', &
288                 & iterPREmax

```



```

289         endif
290
291         call hecmw_solve_CG_33( hecMESH, hecMAT, ITER, RESID, ERROR, &
292 &                               TIME_setup, TIME_sol, TIME_comm )
293     endif
294
295 !C
296 !C-- BiCGSTAB
297     if (METHOD.eq.2 .and. PRECOND.lt.10) then
298         if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
299             if (PRECOND.eq.1) write (*,'(a,i3)') &
300 &           '### 3x3 B-ILU-BiCGSTAB (0)', iterPREmax
301             if (PRECOND.eq.2) write (*,'(a,i3)') &
302 &           '### 3x3 B-SSOR-BiCGSTAB(0)', iterPREmax
303             if (PRECOND.eq.3) write (*,'(a,i3)') &
304 &           '### 3x3 B-scale-BiCGSTAB ', iterPREmax
305         endif
306
307         call hecmw_solve_BiCGSTAB_33( hecMESH, hecMAT, ITER, RESID, ERROR, &
308 &                                     TIME_setup, TIME_sol, TIME_comm )
309     endif
310
311 !C
312 !C-- GMRES
313     if (METHOD.eq.3 .and. PRECOND.lt.10) then
314         ! imposing MPC by penalty
315         call hecmw_mat_ass_equation ( hecMESH, hecMAT )
316
317         if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
318             if (PRECOND.eq.1) write (*,'(a,i3)') &
319 &           '### 3x3 B-ILU-GMRES (0)', iterPREmax
320             if (PRECOND.eq.2) write (*,'(a,i3)') &
321 &           '### 3x3 B-SSOR-GMRES(0)', iterPREmax
322             if (PRECOND.eq.3) write (*,'(a,i3)') &
323 &           '### 3x3 B-scale-GMRES ', iterPREmax
324         endif

```

```

325
326     call hecmw_solve_GMRES_33           &
327     &   ( hecMAT%N, hecMAT%NP, hecMAT%NPL, hecMAT%NPU,           &
328     &     hecMAT%D, hecMAT%AL, hecMAT%indexL, hecMAT%itemL,       &
329     &       hecMAT%AU, hecMAT%indexU, hecMAT%itemU,               &
330     &     hecMAT%B, hecMAT%X, hecMAT%ALU, RESID, ITER,           &
331     &     ERROR, hecMESH%my_rank,                                   &
332     &     hecMESH%n_neighbor_pe, hecMESH%neighbor_pe,             &
333     &     hecMESH%import_index, hecMESH%import_item,             &
334     &     hecMESH%export_index, hecMESH%export_item,             &
335     &     hecMESH%MPI_COMM, PRECOND, iterPREmax, NREST,           &
336     &     TIME_setup, TIME_sol, TIME_comm, ITERlog)
337   endif
338
339   !C
340   !C-- GPBiCG
341     if (METHOD.eq.4 .and. PRECOND.lt.10) then
342       ! imposing MPC by penalty
343       call hecmw_mat_ass_equation ( hecMESH, hecMAT )
344
345       if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
346         if (PRECOND.eq.1) write (*,'(a,i3)')           &
347         &       '### 3x3 B-ILU-GPBiCG (0)', iterPREmax
348         if (PRECOND.eq.2) write (*,'(a,i3)')           &
349         &       '### 3x3 B-SSOR-GPBiCG (0)', iterPREmax
350         if (PRECOND.eq.3) write (*,'(a,i3)')           &
351         &       '### 3x3 B-scale-GPBiCG ', iterPREmax
352       endif
353
354       call hecmw_solve_GPBiCG_33           &
355       &   ( hecMAT%N, hecMAT%NP, hecMAT%NPL, hecMAT%NPU,           &
356       &     hecMAT%D, hecMAT%AL, hecMAT%indexL, hecMAT%itemL,       &
357       &       hecMAT%AU, hecMAT%indexU, hecMAT%itemU,               &
358       &     hecMAT%B, hecMAT%X, hecMAT%ALU, RESID, ITER,           &
359       &     ERROR, hecMESH%my_rank,                                   &
360       &     hecMESH%n_neighbor_pe, hecMESH%neighbor_pe,             &

```

```

361      &      hecMESH%import_index, hecMESH%import_item,      &
362      &      hecMESH%export_index, hecMESH%export_item,      &
363      &      hecMESH%MPI_COMM, PRECOND, iterPREmax,      &
364      &      TIME_setup, TIME_sol, TIME_comm, ITERlog)
365      endif
366
367  !C
368  !C-- CG-1/2
369      if (METHOD.eq.1 .and. (PRECOND.ge.10.and.PRECOND.le.20)) then
370          ! imposing MPC by penalty
371          call hecmw_mat_ass_equation ( hecMESH, hecMAT )
372
373          if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
374              if (PRECOND.eq.10) write (*,'(a)') '### 3x3 B-IC-CG (0)'
375              if (PRECOND.eq.11) write (*,'(a)') '### 3x3 B-IC-CG (1)'
376              if (PRECOND.eq.12) write (*,'(a)') '### 3x3 B-IC-CG (2)'
377          endif
378
379          SIGMA      = 1.d0
380          SIGMA_DIAG= 1.d0
381          call hecmw_solve_BLCG_33      &
382      &      ( hecMAT%N, hecMAT%NP, hecMAT%NPL, hecMAT%NPU,      &
383      &      hecMAT%D, hecMAT%AL, hecMAT%indexL, hecMAT%itemL,      &
384      &      hecMAT%AU, hecMAT%indexU, hecMAT%itemU,      &
385      &      hecMAT%B, hecMAT%X, RESID, SIGMA, SIGMA_DIAG,      &
386      &      ITER, ERROR, hecMESH%my_rank,      &
387      &      hecMESH%n_neighbor_pe, hecMESH%neighbor_pe,      &
388      &      hecMESH%import_index, hecMESH%import_item,      &
389      &      hecMESH%export_index, hecMESH%export_item,      &
390      &      hecMESH%MPI_COMM, PRECOND, iterPREmax,      &
391      &      TIME_setup, TIME_sol, TIME_comm, ITERlog)
392      endif
393
394  !C
395  !C-- BiCGSTAB-1/2
396      if (METHOD.eq.2 .and. (PRECOND.ge.10.and.PRECOND.le.20)) then

```

```

397         ! imposing MPC by penalty
398         call hecmw_mat_ass_equation ( hecMESH, hecMAT )
399
400         if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
401             if (PRECOND.eq.10) write (*,'(a)')                                     &
402             &             '### 3x3 B-IIU-BiCGSTAB (0)'
403             if (PRECOND.eq.11) write (*,'(a)')                                     &
404             &             '### 3x3 B-IIU-BiCGSTAB (1)'
405             if (PRECOND.eq.12) write (*,'(a)')                                     &
406             &             '### 3x3 B-IIU-BiCGSTAB (2)'
407         endif
408
409         SIGMA      = 1.d0
410         SIGMA_DIAG= 1.d0
411         call hecmw_solve_BLBiCGSTAB_33                                           &
412         &         ( hecMAT%N, hecMAT%NP, hecMAT%NPL, hecMAT%NPU,                 &
413         &         hecMAT%D, hecMAT%AL, hecMAT%indexL, hecMAT%itemL,             &
414         &         hecMAT%AU, hecMAT%indexU, hecMAT%itemU,                         &
415         &         hecMAT%B, hecMAT%X, RESID, SIGMA, SIGMA_DIAG,                   &
416         &         ITER, ERROR, hecMESH%my_rank,                                    &
417         &         hecMESH%n_neighbor_pe, hecMESH%neighbor_pe,                       &
418         &         hecMESH%import_index, hecMESH%import_item,                       &
419         &         hecMESH%export_index, hecMESH%export_item,                       &
420         &         hecMESH%MPI_COMM, PRECOND, iterPREmax,                           &
421         &         TIME_setup, TIME_sol, TIME_comm, ITERlog)
422     endif
423
424     !C
425     !C-- GPBiCG-1/2
426     if (METHOD.eq.4 .and. (PRECOND.ge.10.and.PRECOND.le.20)) then
427         ! imposing MPC by penalty
428         call hecmw_mat_ass_equation ( hecMESH, hecMAT )
429
430         if (hecMESH%my_rank.eq.0 .and. (ITERlog.eq.1 .or. TIMElog.eq.1)) then
431             if (PRECOND.eq.10) write (*,'(a)') '### 3x3 B-ILU-GPBiCG (0)'
432             if (PRECOND.eq.11) write (*,'(a)') '### 3x3 B-ILU-GPBiCG (1)'

```

```

433         if (PRECOND.eq.12) write (*,'(a)') '### 3x3 B-ILU-GPBiCG (2)'
434     endif
435
436     SIGMA      = 1.d0
437     SIGMA_DIAG= 1.d0
438     call hecmw_solve_BLGPBiCG_33                                &
439 &     ( hecMAT%N, hecMAT%NP, hecMAT%NPL, hecMAT%NPU,          &
440 &     hecMAT%D, hecMAT%AL, hecMAT%indexL, hecMAT%itemL,      &
441 &     hecMAT%AU, hecMAT%indexU, hecMAT%itemU,                &
442 &     hecMAT%B, hecMAT%X, RESID, SIGMA, SIGMA_DIAG,          &
443 &     ITER, ERROR, hecMESH%my_rank,                           &
444 &     hecMESH%n_neighbor_pe, hecMESH%neighbor_pe,            &
445 &     hecMESH%import_index, hecMESH%import_item,             &
446 &     hecMESH%export_index, hecMESH%export_item,             &
447 &     hecMESH%MPI_COMM, PRECOND, iterPREmax,                  &
448 &     TIME_setup, TIME_sol, TIME_comm, ITERlog)
449     endif
450
451     if (RESID.gt.hecMAT%Rarray(1)) then
452         call hecmw_solve_error (hecMESH, 3001)
453     endif
454
455     if (hecMESH%my_rank.eq.0 .and. TIMElog.eq.1) then
456         TR= (TIME_sol-TIME_comm)/(TIME_sol+1.d-24)*100.d0
457         write (*,'(/a)')          '### summary of linear solver'
458         write (*,'(i10,a,1pe16.6)')  ITER, ' iterations ', RESID
459         write (*,'(a,1pe16.6)') ' set-up time      : ', TIME_setup
460         write (*,'(a,1pe16.6)') ' solver time      : ', TIME_sol
461         write (*,'(a,1pe16.6)') ' solver/comm time : ', TIME_comm
462         write (*,'(a,1pe16.6/)') ' work ratio (%)   : ', TR
463     endif
464
465     if (hecMAT%cmat%n_val.gt.0) then
466         call hecmw_cmat_LU_free( hecMAT )
467     endif
468

```

```
469     end subroutine hecmw_solve_33
470 end module hecmw_solver_33
```