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1 program norminv2
2 !
3 ! *****80
4 ! Program NorMinV2 accepts partial extraction chemical analyses and
5 ! calculates a corresponding normative copper-iron sulfide content. This
6 ! program was written in FORTRAN 90 for Minera Escondida Ltda. using the
7 ! GNU Fortran compiler (MinGW.org GCC-8.2.0-3.
8 ! User documentation is provided in the accompanying report
9 !   < NorMinV2 Programming and User Guide >
10 !
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12 !
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22 !
23 ! File:   NorMinV2.f90
24 ! Author: Richard Preece
25 !
26 ! VERSION 1 Created August 16, 2019, NORMINESC to calculate 3-component
27 ! sulfide assemblages. Two different mineral models were available for
28 ! calculation of CP-CC-CV and CP-BN-(CC-CV) mineral models. The program
29 ! reproduced algorithm, capabilities and options previously coded as
30 ! Microsoft EXCEL spreadsheets. Additional capabilities include
31 !   - user selection of sulfide mineral model (with or without bornite)
32 !   - capability to read variably-formatted csv input files
33 !   - capability to write csv output file
34 !   - calculation of volume percent mineral content
35 ! VERSION 2 Created February 2020, NORMINV2 to add capabilities for calculating
36 ! 4-component oxide-sulfide mineral models. Program automatically selects mineral
37 ! model based on the Minera Escondida Mineral Zone coding structure and certain
38 ! analytical criteria.
39 ! VERSION 2.1 Modified February 2021, Corrected bug in get_real subroutine that
40 ! failed to read input data when in the last value field of the line
41 ! VERSION 2.2 Modified June 2021, Revised MinZone codes for Leach Cap and Oxide
42 ! for consistency with standard MEL geological codes
43 !       Leach Cap: Old Code= 1  New Code= 0
44 !       Oxide:     Old Code= 2  New Code= 1
45 ! VERSION 2.3 Modified August 2022, Added TCu, Fe and S2 values to output file
46 !
47 ! Define variable types and values
48 !
49   integer err_flag
50   real (kind = 8), DIMENSION(3,3) :: m_cpcccv, m_cpccbn, m_cpcvbn
51   real (kind = 8), dimension(4,4) :: m_gocbbrxc, m_cpccbrxc, m_cpcccvbr
52   real (kind = 8), dimension(4,4) :: m_min1, m_min2, m_min3, m_min4
53   real (kind = 8) :: d_cpcccv, d_cpccbn, d_cpcvbn
54   real (kind = 8) :: d_gocbbrxc, d_cpccbrxc, d_cpcccvbr

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54 real (kind = 8) :: d_goccbixc, d_epecbixc, d_epeccvbi
55 real (kind = 8) :: d_min1, d_min2, d_min3, d_min4
56 real (kind = 8) :: m33det, m44det
57
58 character (len = 25) :: paramfile, inputcsv, outputcsv
59 character (len = 25) :: dhname, sampid
60 character (len = 1) :: yesno
61 character (len = 80) :: dumline
62 character (len = 256) :: record, rec_out
63
64 ! Current program version number 23 Aug 2022
65 vers = 2.3
66 idebug = 0 ! Debug switch. Set = 1 to print raw & final CSR values
67
68 !=====
69 ! START DATA INPUT SECTION
70 ! To be replaced by direct IO to data base
71 !=====
72 ! Welcome message to screen
73 call timestamp()
74 write (*, '(a)') ' '
75 write (*, '(a, f5.1,/)' ) &
76 'ESCONDIDA NORMATIVE MINERAL CALCULATIONS version:', vers
77
78 ! Ask for parameter file name, stop program if not found
79 write (*, '(a)') ' Enter name of parameter file'
80 read (*, '(a)') paramfile
81 open (52, file = paramfile, status = "old", iostat = ios)
82 if (ios > 0) then
83 write (*, '(2a)') paramfile, ' is not found'
84 stop
85 end if
86
87 ! Read parameter file for mineral definition parameters
88 write (*, '(a)') ' Reading mineral data from parameter file'
89 read (52, '(a)') dumline
90 read (52, 10) cpxcu, cpxfe, cpxs, cpxas, cprfs, cprcn, cpras
91 read (52, 10) ccxcu, ccxfe, ccxs, ccxas, ccrfs, ccrcn, ccras
92 read (52, 10) cvxcu, cvxfe, cvxs, cvxas, cvrfs, cvrcn, cvas
93 read (52, 10) bnxcu, bnxfe, bnx, bnxas, bnrfs, bnrcn, bnras
94 read (52, 10) enxcu, enxfe, enxs, enxas, enrfs, enrcn, enras
95 read (52, 10) brxcu, brxfe, brxs, brxas, brrfs, brrcn, brras
96 read (52, 10) xcxcu, xcxfe, xcxs, xcxcas, xcrfs, xcrcn, xcras
97 read (52, 10) goxcu, goxfe, goxs, goxcas, gorfs, gorcn, goras
9810 format (15x, 7f10.3)
99
100 ! Reading data file structure defined in parameter file
101 write (*, '(a)') ' Now reading data file structure'
102 ! Skip header lines
103 do i = 1, 3
104 read (52, '(a)') dumline
105 end do
106 read (52, 11) nhdr
107 read (52, 11) idh

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108     read (52, 11) ismp
109     read (52, 11) ifrom
110     read (52, 11) ito
111     read (52, 11) itcu
112     read (52, 11) iscu
113     read (52, 11) icncu
114     read (52, 11) ifscu
115     read (52, 11) ife
116     read (52, 11) is2
117     read (52, 11) imz
118     read (52, 12) ias, ind_as
119     read (52, 12) ibn, ndef_bn
120     read (52, 13) idens, dens_def
12111 format (15x,i10)
12212 format (15x, 2i10)
12313 format (15x, i10,f10.0)
124     close (52)
125
126 ! Ask for data input file name, stop program if not found
127     write ( *, '(a)') ' Enter name of input data file'
128     read (*, '(a)') inputcsv
129     open (51, file = inputcsv, status = "old", iostat = ios)
130     if (ios > 0) then
131         write (*, '(2a)') inputcsv, ' is not found'
132         stop
133     end if
134
135 ! Ask for output file name, check if file currently exists
136100 write ( *, '(a)') ' Enter name of output data file'
137     read (*, '(a)') outputcsv
138     open (61, file = outputcsv, status = "new", iostat = ios, &
139         err = 101)
140
141 ! Error recovery if data file currently exists
142101 continue
143     if (ios > 0) then
144         write (*, '(2a)') outputcsv, ' already exists.'
145         write (*, fmt = '(a)', advance = 'NO') &
146             'Enter Y to overwrite current file, N to enter new file name >'
147         read (*, '(a1)') yesno
148         if (yesno == 'Y' .or. yesno == 'y') then
149             open (61, file = outputcsv, status = "unknown", &
150                 iostat = ios, err = 100)
151         else
152             go to 100
153         end if
154     end if
155     if (idebug .eq. 1) open (62, file = "debuglist.dat", status = "unknown")
156
157 ! Write header record for output file
158 !     Version 2.3, Added TCU, Fe, S2 fields to header record
159     write (61, '(6a)') &
160         'dhname,f_int,t_int,sampid,err_flag,minzon,ind_bn,tcu,fe,s2,', &
161         'xxxx xxxx xxxx' &

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161      cspcp,csicc,csicv, &
162      'csrbrn,csrgo,csrbr,csrxc,csppc,cspsc,cspsv,cspsbn,cspsgo,cspsbr,cspxc,', &
163      'cspen,cp_wtpct,cc_wtpct,cv_wtpct,bn_wtpct,go_wtpct,br_wtpct,xc_wtpct,', &
164      'en_wtpct,py_best,xfe,cp_volpct,cc_volpct,cv_volpct,bn_volpct,', &
165      'go_volpct,br_volpct,xc_volpct,en_volpct,py_volpct'
166
167 !=====
168 !      END OF SECTION FOR SETTING UP DATA INPUT FILES
169 !      Begin section for initializing variables and reading data records
170 !=====
171 !      ! Initialize record counter and move to first record of input file
172      ndata = 0
173      do i = 1, nhdr
174          read (51,'(a80)') dumline
175      end do
176 !
177 ! Set matrix for end-member extraction rates of cp-cc-cv, calculate determinant
178      do j = 1, 3
179          m_cpcccv (1,j) = 1.0
180      end do
181      m_cpcccv (2,1) = cprcn
182      m_cpcccv (2,2) = ccrcn
183      m_cpcccv (2,3) = cvrcn
184      m_cpcccv (3,1) = cprfs
185      m_cpcccv (3,2) = ccrfs
186      m_cpcccv (3,3) = cvrfs
187      d_cpcccv = M33DET (m_cpcccv)
188
189 ! Set matrix for end-member extraction rates of cp-cc-bn, calculate determinant
190      do j = 1, 3
191          m_cpccbn (1,j) = 1.0
192      end do
193      m_cpccbn (2,1) = cprcn
194      m_cpccbn (2,2) = ccrcn
195      m_cpccbn (2,3) = bnrcn
196      m_cpccbn (3,1) = cprfs
197      m_cpccbn (3,2) = ccrfs
198      m_cpccbn (3,3) = bnrfs
199      d_cpccbn = M33DET (m_cpccbn)
200
201 ! Set matrix for end-member extraction rates of cp-cv-bn, calculate determinant
202      do j = 1, 3
203          m_cpcvbn (1,j) = 1.0
204      end do
205      m_cpcvbn (2,1) = cprcn
206      m_cpcvbn (2,2) = cvrcn
207      m_cpcvbn (2,3) = bnrcn
208      m_cpcvbn (3,1) = cprfs
209      m_cpcvbn (3,2) = cvrfs
210      m_cpcvbn (3,3) = bnrfs
211      d_cpcvbn = M33DET (m_cpcvbn)
212
213 ! Set matrix for end-member extraction rates of CuGoe-cc-br-chrys, calculate determinant
214      do j = 1, 4

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215     m_goccbrrxc (1,j) = 1.0
216   end do
217   m_goccbrrxc (2,1) = gorcn
218   m_goccbrrxc (2,2) = ccrcn
219   m_goccbrrxc (2,3) = brrcn
220   m_goccbrrxc (2,4) = xcrcn
221   m_goccbrrxc (3,1) = gorfs
222   m_goccbrrxc (3,2) = ccrfs
223   m_goccbrrxc (3,3) = brrfs
224   m_goccbrrxc (3,4) = xcrrfs
225   m_goccbrrxc (4,1) = goras
226   m_goccbrrxc (4,2) = ccras
227   m_goccbrrxc (4,3) = brras
228   m_goccbrrxc (4,4) = xcrras
229   d_goccbrrxc = M44DET (m_goccbrrxc)
230
231 ! Set matrix for end-member extraction rates of cp-cc-br-chrys, calculate determinant
232   do j = 1, 4
233     m_cpccbrxc (1,j) = 1.0
234   end do
235   m_cpccbrxc (2,1) = cprcn
236   m_cpccbrxc (2,2) = ccrcn
237   m_cpccbrxc (2,3) = brrcn
238   m_cpccbrxc (2,4) = xcrcn
239   m_cpccbrxc (3,1) = cprfs
240   m_cpccbrxc (3,2) = ccrfs
241   m_cpccbrxc (3,3) = brrfs
242   m_cpccbrxc (3,4) = xcrrfs
243   m_cpccbrxc (4,1) = cpras
244   m_cpccbrxc (4,2) = ccras
245   m_cpccbrxc (4,3) = brras
246   m_cpccbrxc (4,4) = xcrras
247   d_cpccbrxc = M44DET (m_cpccbrxc)
248
249 ! Set matrix for end-member extraction rates of cp-cc-cv-br, calculate determinant
250   do j = 1, 4
251     m_cpcccvbr (1,j) = 1.0
252   end do
253   m_cpcccvbr (2,1) = cprcn
254   m_cpcccvbr (2,2) = ccrcn
255   m_cpcccvbr (2,3) = cvrcn
256   m_cpcccvbr (2,4) = brrcn
257   m_cpcccvbr (3,1) = cprfs
258   m_cpcccvbr (3,2) = ccrfs
259   m_cpcccvbr (3,3) = cvrfs
260   m_cpcccvbr (3,4) = brrfs
261   m_cpcccvbr (4,1) = cpras
262   m_cpcccvbr (4,2) = ccras
263   m_cpcccvbr (4,3) = cvrras
264   m_cpcccvbr (4,4) = brras
265   d_cpcccvbr = M44DET (m_cpcccvbr)
266 !
267 !-----
268 ! Program reads and processes one data record at a time

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269 ! SECTION FOR READING DATA RECORD FROM CVS FILE
270 ! Replace with code for reading data base record
271 !-----
272 ! Read new record
273 200 ndata = ndata + 1
274 read (51, 201, end = 900) record
275 201 format(a)
276
277 ! Parse record to retrieve data
278 ! Find number of values (n_count) and record length (l_count)
279 call csv_value_count(record, istatus, n_count, l_count)
280 ! Call subroutine to extract data, identified by counting number of values
281 ! Different subroutines used based on data type (real, integer, character)
282 call get_char (dhname,idh,record,n_count,l_count,ios)
283 if (ios .gt. 0) write (*,'(2(a,i6))') &
284 'Error in DH Name on line ', ndata,'Error code = ',ios
285 call get_char (sampid,ism,record,n_count,l_count,ios)
286 if (ios .gt. 0) write (*,'(2(a,i6))') &
287 'Error in Sample ID on line ', ndata,'Error code = ',ios
288 call get_real (f_int,ifrom,record,n_count,l_count,ios)
289 if (ios .gt. 0) write (*,'(2(a,i6))') &
290 'Error in From on line ', ndata,'Error code = ',ios
291 call get_real (t_int,it,record,n_count,l_count,ios)
292 if (ios .gt. 0) write (*,'(2(a,i6))') &
293 'Error in From on line ', ndata,'Error code = ',ios
294 call get_real (tcu,itcu,record,n_count,l_count,ios)
295 if (ios .gt. 0) write (*,'(2(a,i6))') &
296 'Error in TCu on line ', ndata,'Error code = ',ios
297 call get_real (scu,iscu,record,n_count,l_count,ios)
298 if (ios .gt. 0) write (*,'(2(a,i6))') &
299 'Error in SCu on line ', ndata,'Error code = ',ios
300 call get_real (cncu,icncu,record,n_count,l_count,ios)
301 if (ios .gt. 0) write (*,'(2(a,i6))') &
302 'Error in CNCu on line ', ndata,'Error code = ',ios
303 call get_real (fscu,ifscu,record,n_count,l_count,ios)
304 if (ios .gt. 0) write (*,'(2(a,i6))') &
305 'Error in FSCu on line ', ndata,'Error code = ',ios
306 call get_real (fe,ife,record,n_count,l_count,ios)
307 if (ios .gt. 0) write (*,'(2(a,i6))') &
308 'Error in Fe on line ', ndata,'Error code = ',ios
309 call get_real (s2,is2,record,n_count,l_count,ios)
310 if (ios .gt. 0) write (*,'(2(a,i6))') &
311 'Error in S2 on line ', ndata,'Error code = ',ios
312 call get_real (as,ias,record,n_count,l_count,ios)
313 if (ios .gt. 0) write (*,'(2(a,i6))') &
314 'Error in As on line ', ndata,'Error code = ',ios
315 call get_integer (minzon,imz,record,n_count,l_count,ios)
316 if (ios .gt. 0) write (*,'(2(a,i6))') &
317 'Error in MinZone on line ', ndata,'Error code = ',ios
318 call get_integer (ind_bn,ibn,record,n_count,l_count,ios)
319 if (ind_bn .lt. 0) ind_bn = ndef_bn ! Set default flag value
320 if (ios .gt. 0) write (*,'(2(a,i6))') &
321 'Error in Bornite Flag on line ', ndata,'Error code = ',ios

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322     call get_real (density, idens, record, n_count, l_count, ios)
323     if (density .lt. 0) density = dens_def           ! Set default density value
324     if (ios .gt. 0) write (*, '(2(a,i6))') &
325         'Error in Density on line ', ndata, 'Error code = ', ios
326 !-----
327 !     END SECTION FOR READING DATA RECORD
328 !     Begin section for processing PtXt data and calculation of
329 !     normative mineralogy
330 !-----
331 ! Check for complete assay set
332     if (min(tcu, scu, cncu, fscu) .lt. 0.0) then
333         write (*, '(a,i6,/,a)') 'Assay data missing in line number ', ndata, &
334             'Record not processed '
335         go to 200
336     end if
337 ! Check for valid mineral zone
338     if (minzon .lt. 0 .or. minzon .gt. 10) then
339         write (*, '(a,i6,/,a)') 'Invalid mineral zone in line number ', ndata, &
340             'Record not processed '
341         go to 200
342     end if
343
344     if (idebug .eq. 1) &
345         write(62, '(i6,1x,a,2f10.1,i5)') ndata, dhname, f_int, t_int, minzon
346 !-----
347 ! Start normative mineral calculations
348 ! Six potential mineral associations are defined, 3 for sulfide and 3 for oxide/mixed
349 ! Selection of the mineral association depends on:
350 !     - logged mineral zone
351 !         MinZones 0, 1, 5 routed to oxide/mixed 4-component associations
352 !         Minzones 4, 6, 7, 8, 10 routed to sulfide 3-component associations
353 !     - analytical criteria
354 !         Sulfide sulfur <0.15% S or SCu >= CNCu routed to oxide only association
355 !     - normative mineral errors
356 !         Normative mineral CSR <-0.1 or > 1.1 routed to alternative mineral association
357 !-----
358     if (minzon .le. 2 .or. minzon .eq. 5) go to 400
359
360 !-----
361 ! Start Sulfide association
362 !-----
363 ! Adjust assays for As-bearing mineral, depending on ind_as flag setting
364 ! Skip adjustment in oxide mineral zones
365     if (as .lt. 0 .or. ind_as .eq. 0) then           ! ind_as = 0 don't process As values
366         as = 0.0
367         en_wtpct = 0.0
368         go to 210
369     else if (ind_as == 1) then                       ! ind_as = 1 value input as ppm As, convert to wt. %
370         as = as / 10000
371     end if                                           ! ind_as = 2 value as wt. %
372
373 ! Calculate wt % arsenic mineral from As assay
374 ! Adjust As mineral content for those samples with low TCu and elevated As
375     en_wtpct = min(as/enxas, (tcu-0.005)/enxcu) ! Check for samples with

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376 210 cspen = en_wtpct*enxcu      ! Calculate CSPen from mineral and Cu content
377 !
378 ! Adjust PtXt for contribution by As mineral
379   tcumod = tcu - cspen
380   fscumod = max(0.001,fscu - (cspen*enrfs))
381   cncumod = max(0.001,cncu - (cspen*enrcn))
382   fscu_rat = fscumod/tcumod
383   cncu_rat = cncumod/tcumod
384
385 ! Calculation of chalcopyrite-chalcocite-covellite association, executed for
386 ! samples with ind_bn = 0
387 300 continue
388   if (ind_bn == 1) go to 320
389   csrctp_raw = ((ccrcn*cvrfs)-(ccrfs*cvrcn)+(cvrcn-ccrcn)*fscu_rat &
390               + (ccrfs-cvrfs)*cncu_rat)/d_cpcccv
391   csrcc_raw = ((cvrcn*cprfs)-(cvrfs*cprcn)+(cvrfs-cprfs)*cncu_rat &
392               + (cprcn-cvrcn)*fscu_rat)/d_cpcccv
393   csrcv_raw = 1-csrctp_raw-csrcc_raw
394   csrbn_raw = 0.0
395
396 ! Set flags for calculated csr value that exceed tolerances of 10%
397   if (max(csrctp_raw,csrcc_raw,csrcv_raw).le. 1.100 .and. &
398       min(csrctp_raw,csrcc_raw,csrcv_raw).ge. -0.100) then
399     err_flag = 0
400     go to 310
401   end if
402   if (tcu < 0.15 .and. min(csrctp_raw,csrcc_raw,csrcv_raw)< -0.100) then
403     err_flag = 1      ! Low Grade flag, likely round-off errors or high As value
404     if (csrcv_raw < -0.100) then
405       if (idebug .eq. 1) &
406       write(62,'(a,3f7.3)') ' cpcccv raw ->',csrctp_raw,csrcc_raw,csrcv_raw
407       go to 400
408     end if
409   else if (csrcv_raw < -0.100) then
410     err_flag = 2      ! Elevated FSCu relative to CNCu, potentially oxidized
411     if (idebug .eq. 1) &
412     write(62,'(a,3f7.3)') ' cpcccv raw ->',csrctp_raw,csrcc_raw,csrcv_raw
413     go to 400
414   else if (csrctp_raw < -0.100) then
415     err_flag = 3      ! Elevated CNCu relative to FSCu
416   else
417     err_flag = 4      ! Undefined error
418   end if
419 !
420 ! Adjust mineral csr for csrctp < 0 and csrcv < 0
421 310 continue
422   if (csrctp_raw .lt. 0.000) then
423     csrctp1 = 0.0000
424   else if (csrcv_raw .lt. 0.000) then
425     csrctp1 = csrctp_raw/(csrctp_raw + csrcc_raw)
426   else
427     csrctp1 = csrctp_raw
428   end if

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429
430     if (csrcv_raw .lt. 0.000) then
431         csrcc1 = csrcc_raw/(csrcp_raw + csrcc_raw)
432         csrcv1 = 0.0000
433     else
434         csrcc1 = csrcc_raw
435         csrcv1 = csrcv_raw
436     end if
437 !
438 ! Second-stage adjustment, for csrcp1 > 1 and csrcc1 < 0
439     if (csrcp1 .gt. 1.000) then
440         csrcp = csrcp1/(csrcp1 + csrcv1)
441     else
442         csrcp = csrcp1
443     end if
444
445     if (csrcc1 .lt. 0.000) then
446         csrcc = 0.0000
447     else
448         csrcc = csrcc1/(csrcp1 + csrcc1 + csrcv1)
449     end if
450
451     csrcv = 1 - csrcp - csrcc
452     csrbn = 0.0000
453     csrgo = 0.0000
454     csrbr = 0.0000
455     csrxc = 0.0000
456
457     if(idebug .eq. 1) &
458     write(62,'(a,3f7.3,a,3f7.3)') ' cpcccv raw ->',csrcp_raw,csrcc_raw,csrcv_raw, &
459     ' cpcccv final -> ', csrcp, csrcc, csrcv
460     go to 600
461 !
462 ! Calculation of chalcopyrite-bornite-chalcocite association, executed for
463 ! samples with ind_bn = 1
464 320 continue
465     csrcp_raw = ((ccrcn*bnrfs)-(ccrfs*bnrcn)+(bnrcn-ccrcn)*fscu_rat &
466     + (ccrfs-bnrfs)*cncu_rat)/d_cpccbn
467     csrcc_raw = ((bnrcn*cprfs)-(bnrfs*cprcn)+(bnrfs-cprfs)*cncu_rat &
468     + (cprcn-bnrcn)*fscu_rat)/d_cpccbn
469     csrbn_raw = 1-csrcp_raw-csrcc_raw
470     csrcv_raw = 0.0000
471
472 ! Check for consistency with bn-cc assumption, calculate bn-cv if negative cc
473     if (csrcc_raw .le. -0.005) go to 330
474
475 ! Set error flag for calculated csr value that exceed tolerances of +/-10%
476     if (max(csrcp_raw,csrcc_raw,csrbn_raw).le. 1.1 .and. &
477     min(csrcp_raw,csrcc_raw,csrbn_raw).ge. -0.1) then
478         err_flag = 0
479         go to 321
480     end if
481
482     if (tcu < 0.15 .and. min(csrcp_raw,csrcc_raw,csrbn_raw)< -0.100) then

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483     err_flag = 1           ! Low Grade flag, likely round-off errors or high As value
484     if (csrbn_raw < -0.100) then
485         if (idebug .eq. 1) &
486             write(62,'(a,3f7.3)') ' cpbnc raw ->',csrccp_raw,csrbn_raw,csrcc_raw
487         go to 400
488     end if
489     else if (csrbn_raw < -0.100) then
490         err_flag = 2           ! Elevated FSCu relative to CNCu, potentially oxidized
491         if (idebug .eq. 1) &
492             write(62,'(a,3f7.3)') ' cpbnc raw ->',csrccp_raw,csrbn_raw,csrcc_raw
493         go to 400
494     else if (csrccp_raw < -0.100) then
495         err_flag = 3           ! Elevated CNCu relative to FSCu
496     else
497         err_flag = 4           ! Undefined error
498     end if
499 !
500 ! Adjust mineral csr for csrccp < 0 and csrbn < 0
501 321 continue
502     if (csrccp_raw .lt. 0.000) then
503         csrccp1 = 0.0000
504     else if (csrbn_raw .lt. 0.000) then
505         csrccp1 = csrccp_raw/(csrccp_raw + csrcc_raw)
506     else
507         csrccp1 = csrccp_raw
508     end if
509
510     if (csrbn_raw .lt. 0.000) then
511         csrcc1 = csrcc_raw/(csrccp_raw + csrcc_raw)
512         csrbn1 = 0.0000
513     else
514         csrcc1 = csrcc_raw
515         csrbn1 = csrbn_raw
516     end if
517 !
518 ! Second-stage adjustment, for csrccp1 > 1 and csrcc1 < 0
519     if (csrccp1 .gt. 1.000) then
520         csrccp = csrccp1/(csrccp1 + csrbn1)
521     else
522         csrccp = csrccp1
523     end if
524
525     if (csrcc1 .lt. 0.000) then
526         csrcc = 0.0000
527     else
528         csrcc = csrcc1/(csrccp1 + csrcc1 + csrbn1)
529     end if
530
531     csrbn = 1 - csrccp - csrcc
532     csrccv = 0.0000
533     csrgo = 0.0000
534     csrbr = 0.0000
535     csrxc = 0.0000

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```

536
537     if (idebug .eq. 1) &
538     write(62, '(a,3f7.3,a,3f7.3)') ' cpbncc raw ->', csrnp_raw, csrbn_raw, csrcc_raw, &
539     ' cpbncc final -> ', csrnp, csrbn, csrcc
540     go to 600
541 !
542 ! Calculation of chalcopyrite-bornite-covellite association, executed for
543 ! samples with ind_bn = 1 and negative chalcocite from previous section
544 330 continue
545     csrnp_raw = ((cvrcn*bnrfs)-(cvrfs*bnrcn)+(bnrcn-cvrcn)*fscu_rat &
546     + (cvrfs-bnrfs)*cncu_rat)/d_cpcvbn
547     csrnp_raw = ((bnrcn*cprfs)-(bnrfs*cprcn)+(bnrfs-cprfs)*cncu_rat &
548     + (cprcn-bnrcn)*fscu_rat)/d_cpcvbn
549     csrbn_raw = 1-csrnp_raw-csrnp_raw
550     csrcc_raw = 0.0
551
552 ! Set error flag for calculated csr value that exceed tolerances of 10%
553     if (max(csrnp_raw,csrnp_raw,csrbn_raw).le. 1.1 .and. &
554     min(csrnp_raw,csrnp_raw,csrbn_raw).ge. -0.1) then
555         err_flag = 0
556         go to 331
557     end if
558
559     if (tcu < 0.15 .and. min(csrnp_raw,csrnp_raw,csrbn_raw)< -0.1) then
560         err_flag = 1 ! Low Grade flag, likely round-off errors or high As value
561     else if (csrbn_raw > 1.1) then
562         err_flag = 2 ! Elevated FSCu relative to CNCu, in cp-cc-bn association
563     else if (csrnp_raw < -0.1) then
564         err_flag = 3 ! Elevated CNCu relative to FSCu
565     else
566         err_flag = 4 ! Undefined error
567     end if
568 !
569 ! Adjust mineral csr for csrnp < 0 and csrbn < 0
570 331 continue
571     if (csrnp_raw .lt. 0.0) then
572         csrnp1 = 0.0
573     else if (csrnp_raw .lt. 0.0) then
574         csrnp1 = csrnp_raw/(csrnp_raw + csrbn_raw)
575     else
576         csrnp1 = csrnp_raw
577     end if
578
579     if (csrnp_raw .lt. 0.0) then
580         csrbn1 = csrbn_raw/(csrnp_raw + csrbn_raw)
581         csrnp1 = 0.0
582     else
583         csrnp1 = csrnp_raw
584         csrbn1 = csrbn_raw
585     end if
586 !
587 ! Second-stage adjustment, for csrnp1 > 1 and csrbn1 < 0
588     if (csrnp1 .gt. 1.0) then
589         csrnp = csrnp1/(csrnp1 + csrnp1)

```

```

590     else
591         csrctp = csrctp1
592     end if
593
594     if (csrbn1 .lt. 0.0) then
595         csrbn = 0.0
596     else
597         csrbn = csrbn1/(csrctp1 + csrctv1 + csrbn1)
598     end if
599
600     csrctv = 1.0000 - csrctp - csrbn
601     csrctc = 0.0000
602     csrgo = 0.0000
603     csrbr = 0.0000
604     csrxc = 0.0000
605
606     if(idebug .eq. 1) &
607     write(62,'(a,3f7.3,a,3f7.3)') ' cpbncv raw ->',csrctp_raw,csrbn_raw,csrctv_raw, &
608     ' cpbncv final -> ', csrctp, csrbn, csrctv
609     go to 600
610 ! -----
611 ! End of Sulfide mineral associations
612
613 ! Start Oxide/Mixed mineral associations
614 ! -----
615 400 continue
616 ! Initialize modified assay and calculate PtXt ratios
617     scu_rat = scu/tcu
618     fscu_rat = fscu/tcu
619     cncu_rat = cncu/tcu
620     tcumod = tcu
621 ! Initialize bornite and enargite components
622     csrbn = 0.0000
623     en_wtpct = 0.000
624     cspen = 0.000
625
626 ! Check for sulfide sulfur, Oxide to goe-cc-br-xc
627     if (s2 .le. 0.15 .and. s2 .ge. 0) go to 410
628
629 ! Check for cpy as insol mineral, go to cp-cc-br-xc
630     if (cncu > scu) go to 420
631
632 ! Calculation of normative minerals, goe-cc-br-xc mineral association
633 410 continue
634 ! Initialize normative mineral matrices
635 ! Mineral 1 = Cugoethite, Mineral 2 = Chalcocite, Mineral 3 = Brochantite
636 ! Mineral 4 = Chrysocolla
637     m_min1 = m_goccbrrxc
638     m_min2 = m_goccbrrxc
639     m_min3 = m_goccbrrxc
640     m_min4 = m_goccbrrxc
641 ! Insert PtXt ratios into the end-member mineral matrices and find determinant
642     m_min1(2,1) = cncu_rat

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643     m_min1(3,1) = rscu_rat
644     m_min1(4,1) = scu_rat
645     d_min1 = m44det (m_min1)
646
647     m_min2(2,2) = cncu_rat
648     m_min2(3,2) = fscu_rat
649     m_min2(4,2) = scu_rat
650     d_min2 = m44det (m_min2)
651
652     m_min3(2,3) = cncu_rat
653     m_min3(3,3) = fscu_rat
654     m_min3(4,3) = scu_rat
655     d_min3 = m44det (m_min3)
656
657     m_min4(2,4) = cncu_rat
658     m_min4(3,4) = fscu_rat
659     m_min4(4,4) = scu_rat
660     d_min4 = m44det (m_min4)
661
662 ! Calculation of raw CSR values
663     csrgo_raw = d_min1/d_goccbrrxc
664     csrcc_raw = d_min2/d_goccbrrxc
665     csrbr_raw = d_min3/d_goccbrrxc
666     csrrc_raw = d_min4/d_goccbrrxc
667
668 ! Initialize error flag and check for valid csr calculations
669     err_flag = 0
670     csr_max = max(csrgo_raw,csrcc_raw,csrbr_raw,csrrc_raw)
671     csr_min = min(csrgo_raw,csrcc_raw,csrbr_raw,csrrc_raw)
672     if (csr_max .lt. 1.00001 .and. csr_min .gt. -0.00001) then
673         csrgo1 = csrgo_raw
674         csrcc1 = csrcc_raw
675         csrbr1 = csrbr_raw
676         csrrc1 = csrrc_raw
677         go to 411
678     end if
679
680 ! Check for error in each end-member correct CSR and set error flag if necessary
681     if (csrbr_raw .lt. 0.000) then
682         if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 5
683         csrbr1 = 0.0000
684         csrcc1 = max (0.0000, csrbr_raw + csrcc_raw)
685         csrrc1 = max (0.0000, csrrc_raw)
686         csrgo1 = max (0.0000, csrgo_raw)
687         go to 411
688     end if
689
690     if (csrcc_raw .lt. 0.000 .or. csrrc_raw .lt. 0.000) then
691         if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 6
692         csrgo1 = max (0.0000, csrgo_raw)
693         csrcc1 = max (0.0000, csrcc_raw)
694         csrrc1 = max (0.0000, csrrc_raw)
695         csrbr1 = max (0.0000, csrbr_raw)
696         go to 411

```

```

697     end if
698
699     if (csrgo_raw .lt. 0.000) then
700         if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 7
701         csrgol = 0.0000
702         csrcc1 = max (0.000, csrcc_raw)
703         csrxcl = max (0.000, csrxc_raw)
704         csrbr1 = max (0.000, csrbr_raw)
705         go to 411
706     end if
707
708     if (csrmax .gt. 1.100) err_flag = 8
709     csrgol = csrgo_raw
710     csrcc1 = csrcc_raw
711     csrxcl = csrxc_raw
712     csrbr1 = csrbr_raw
713
714 411 continue
715 ! Normalize adjusted csr value and set missing normative minerals to zero
716     sumcsr1 = csrgol + csrcc1 + csrxcl + csrbr1
717     csrgo = csrgol/sumcsr1
718     csrcc = csrcc1/sumcsr1
719     csrbr = csrbr1/sumcsr1
720     csrxc = csrxcl/sumcsr1
721     csrccp = 0.0000
722     csrccv = 0.0000
723
724     if(idebug .eq. 1) &
725     write(62,'(a,4f7.3,a,4f7.3)') ' goccbrxc raw ->',csrgo_raw,csrcc_raw,csrbr_raw, &
726     csrxc_raw,' goccbrxc final -> ', csrgo, csrcc, csrbr,csrxc
727     go to 600
728
729 ! Calculation of normative minerals, cp-cc-br-xc mineral association
730 420 continue
731 ! Initialize normative mineral matrices
732 ! Mineral 1 = Chalcopyrite, Mineral 2 = Chalcocite, Mineral 3 = Brochantite
733 ! Mineral 4 = Chrysocolla
734     m_min1 = m_cpccbrxc
735     m_min2 = m_cpccbrxc
736     m_min3 = m_cpccbrxc
737     m_min4 = m_cpccbrxc
738
739 ! Insert PtXt ratios into the end-member mineral matrices and find determinant
740     m_min1(2,1) = cncu_rat
741     m_min1(3,1) = fscu_rat
742     m_min1(4,1) = scu_rat
743     d_min1 = m44det (m_min1)
744
745     m_min2(2,2) = cncu_rat
746     m_min2(3,2) = fscu_rat
747     m_min2(4,2) = scu_rat
748     d_min2 = m44det (m_min2)
749
750     m_min3(2,3) = cncu_rat

```

```

750     m_min3(2,3) = cncu_rat
751     m_min3(3,3) = fscu_rat
752     m_min3(4,3) = scu_rat
753     d_min3 = m44det (m_min3)
754
755     m_min4(2,4) = cncu_rat
756     m_min4(3,4) = fscu_rat
757     m_min4(4,4) = scu_rat
758     d_min4 = m44det (m_min4)
759
760 ! Calculation of raw CSR values
761     csrctp_raw = d_min1/d_cpccbrxc
762     csrcc_raw = d_min2/d_cpccbrxc
763     csrbr_raw = d_min3/d_cpccbrxc
764     csrxc_raw = d_min4/d_cpccbrxc
765
766 ! Initialize error flag and check for valid csr calculations
767     err_flag = 0
768     csr_max = max(csrctp_raw, csrcc_raw, csrbr_raw, csrxc_raw)
769     csr_min = min(csrctp_raw, csrcc_raw, csrbr_raw, csrxc_raw)
770     if (csr_max .lt. 1.000 .and. csr_min .gt. 0.000) then
771         csrctp1 = csrctp_raw
772         csrcc1 = csrcc_raw
773         csrbr1 = csrbr_raw
774         csrxc1 = csrxc_raw
775         go to 421
776     end if
777
778 ! Check for error in each end-member correct CSR and set error flag if necessary
779 ! Samples with negative chrysocolla is diagnostic of normative CV, take cpcccvbr branch
780     if (csrxc_raw .lt. -0.010) then
781         if (idebug .eq. 1) &
782             write(62, '(a,4f7.3)') ' cpccbrxc raw ->', csrctp_raw, csrcc_raw, csrbr_raw, csrxc_raw
783         go to 430
784     end if
785
786     if (csrctp_raw .lt. 0.000) then
787         if (csrbr_raw .lt. 0.000) then
788             if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 9
789             csrxc1 = max (0.0000, csrxc_raw + csrctp_raw)
790             csrcc1 = max (0.0000, csrcc_raw + csrbr_raw)
791             csrctp1 = 0.0000
792             csrbr1 = 0.0000
793             go to 421
794         end if
795         csrctp1 = 0.0000
796         csrcc1 = max (0.0000, csrcc_raw)
797         csrbr1 = max (0.0000, csrbr_raw)
798         csrxc1 = max (0.0000, csrxc_raw)
799         go to 421
800     end if
801
802     if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 10
803     csrctp1 = max (0.000, csrctp_raw)

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```

804     csrcc1 = max (0.000, csrcc_raw)
805     csrxcl = max (0.000, csrxcl_raw)
806     csrbr1 = max (0.000, csrbr_raw)
807
808 421 continue
809 ! Normalize adjusted csr value and set missing normative minerals to zer
810     sumcsr1 = csrcl1 + csrcc1 + csrxcl + csrbr1
811     csrcl = csrcl1/sumcsr1
812     csrcc = csrcc1/sumcsr1
813     csrbr = csrbr1/sumcsr1
814     csrxcl = csrxcl1/sumcsr1
815     csrgo = 0.0000
816     csrcl = 0.0000
817
818     if(idebug .eq. 1) &
819     write(62,'(a,4f7.3,a,4f7.3)') ' cpcclbrxc raw ->', csrcl_raw, csrcc_raw, csrbr_raw, &
820     csrxcl_raw, ' cpcclbrxc final -> ', csrcl, csrcc, csrbr, csrxcl
821     go to 600
822
823 ! Calculation of normative minerals, cp-cl-cv-br mineral association
824 430 continue
825 ! Initialize normative mineral matrices
826 ! Mineral 1 = Chalcocite, Mineral 2 = Chalcocite, Mineral 3 = Covellite
827 ! Mineral 4 = Brochantite
828     m_min1 = m_cpcccvbr
829     m_min2 = m_cpcccvbr
830     m_min3 = m_cpcccvbr
831     m_min4 = m_cpcccvbr
832
833 ! Insert PtXt ratios into the end-member mineral matrices and find determinant
834     m_min1(2,1) = cncu_rat
835     m_min1(3,1) = fscu_rat
836     m_min1(4,1) = scu_rat
837     d_min1 = m44det (m_min1)
838
839     m_min2(2,2) = cncu_rat
840     m_min2(3,2) = fscu_rat
841     m_min2(4,2) = scu_rat
842     d_min2 = m44det (m_min2)
843
844     m_min3(2,3) = cncu_rat
845     m_min3(3,3) = fscu_rat
846     m_min3(4,3) = scu_rat
847     d_min3 = m44det (m_min3)
848
849     m_min4(2,4) = cncu_rat
850     m_min4(3,4) = fscu_rat
851     m_min4(4,4) = scu_rat
852     d_min4 = m44det (m_min4)
853
854 ! Calculation of raw CSR values
855     csrcl_raw = d_min1/d_cpcccvbr
856     csrcc_raw = d_min2/d_cpcccvbr
857     csrxcl_raw = d_min3/d_cpcccvbr

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857     csrbr_raw = d_min4/d_cpcccvbr
858     csrbr_raw = d_min4/d_cpcccvbr
859
860 ! Initialize error flag and check for valid csr calculations
861     err_flag = 0
862     csr_max = max(csr_cp_raw,csrcc_raw,csrbr_raw,csrcv_raw)
863     csr_min = min(csr_cp_raw,csrcc_raw,csrbr_raw,csrcv_raw)
864     if (csr_max .lt. 1.000 .and. csr_min .gt. 0.000) then
865         csr_cp1 = csr_cp_raw
866         csrcc1 = csrcc_raw
867         csr_cv1 = csr_cv_raw
868         csr_br1 = csrbr_raw
869         go to 431
870     end if
871
872 ! Check for error in each end-member correct CSR and set error flag if necessary
873
874     if (csr_max .gt. 1.100 .or. csr_min .lt. -0.100) err_flag = 11
875     csr_cp1 = max (0.000, csr_cp_raw)
876     csrcc1 = max (0.000, csrcc_raw)
877     csr_cv1 = max (0.000, csr_cv_raw)
878     csr_br1 = max (0.000, csrbr_raw)
879
880 431 continue
881 ! Normalize adjusted csr value and set missing normative minerals to zer
882     sumcsr1 = csr_cp1 + csrcc1 + csr_cv1 + csr_br1
883     csr_cp = csr_cp1/sumcsr1
884     csrcc = csrcc1/sumcsr1
885     csrbr = csrbr1/sumcsr1
886     csr_cv = csr_cv1/sumcsr1
887 432 continue
888     csrgo = 0.0000
889     csrxc = 0.0000
890
891     if(idebug .eq. 1) &
892     write(62,'(a,4f7.3,a,4f7.3)') ' cpcccvbr raw ->',csr_cp_raw,csrcc_raw,csr_cv_raw, &
893     csrbr_raw,' cpcccvbr final -> ', csr_cp, csrcc, csr_cv,csrbr
894     go to 600
895 ! End of Oxide normative CSR calculations
896 !-----
897 !
898 ! Calculation of CSP, copper mineral abundance, and pyrite
899 600 continue
900 ! Set Low Grade error flag
901     if (err_flag > 0 .and. tcu .lt. 0.15) err_flag = 1
902
903 ! Calculation of Copper Source Percent (CSP))
904     cspcp = tcumod * csr_cp
905     cspcc = tcumod * csrcc
906     cspcv = tcumod * csr_cv
907     csprbn = tcumod * csrbrn
908     csprgo = tcumod * csrgo
909     csprxc = tcumod * csrxc
910     csprbr = tcumod * csrbr

```

```

911 ! Calculation of mineral abundance (wt. %)
912     cp_wtpct = cspcp / cpxcu
913     cc_wtpct = cspcc / ccxcu
914     cv_wtpct = cspcv / cvxcu
915     bn_wtpct = cspbn / bnxcu
916     go_wtpct = cspgo / goxcu
917     xc_wtpct = cspxc / xcxcu
918     br_wtpct = cspbr / brxcu
919
920 ! Calculation of pyrite based on Fe content
921     if (fe .lt. 0) then
922         py_fe = -99.
923         xfe = -99.
924     else
925         cusul_fe = cp_wtpct*cpxfe + cc_wtpct*ccxfe + cv_wtpct*cvxfe &
926                 + bn_wtpct*bnxfe + en_wtpct*enxfe
927         py_fe = max (0.000, (fe - cusul_fe)/0.466)
928     end if
929
930 ! Calculation of pyrite based on S content
931     if (s2 .lt. 0) then
932         py_best = -99.                ! Sample missing both S and Fe assay
933         xfe = -99.
934         go to 610
935     else
936         cusul_s = cp_wtpct*cpxs + cc_wtpct*ccxs + cv_wtpct*cvxs &
937                 + bn_wtpct*bnxs + en_wtpct*enxs
938         py_s = max (0.0, (s2 - cusul_s)/0.534)
939     end if
940
941 ! Select minimum pyrite value as best estimate. Pooled analytical uncertainty is 11%
942
943     if (py_fe .lt. 0.0) then
944         py_best = py_s                ! Check for missing Fe assay only
945         xfe = -99.
946         go to 610
947     end if
948
949     ave_est = (py_fe+py_s)/2.0
950     if (abs(ave_est) .lt. 0.001) then
951         py_best = 0.000                ! Check for divide by zero
952         go to 610
953     end if
954
955     if ((abs(py_fe-py_s)/ave_est) .le. 0.11) then
956         py_best = ave_est
957     else
958         py_best = min(py_fe,py_s)
959     end if
960
961 ! Calculate excess iron (non-sulfide Fe)
962     xfe = fe - cusul_fe - py_best*0.466
963     if (xfe .lt. 0.0) xfe = 0.0
964

```

```

965 610 continue
966
967 ! Calculate volume percent sulfides from user-supplied whole rock density and
968 ! mineral densities published by mindat.org
969 !
970 ! Assignment of mineral densities (g/cc) from www.mindat.com
971     sg_py = 5.01      ! Calculated value pyrite
972     sg_cp = 4.18      ! Calculated value chalcopyrite
973     sg_cc = 5.75      ! Calculated for djurleite, near top of measured cc range
974     sg_cv = 4.60      ! Calculated value covellite
975     sg_bn = 5.09      ! Calculated value bornite
976     sg_en = 4.40      ! Calculated value enargite
977     sg_xc = 2.10      ! Mid-range of measured values, chrysocolla
978     sg_br = 3.97      ! Measured value brochantite
979     sg_go = 4.28      ! Mid-range of measured values, goethite
980
981 !
982 ! Rock density provided by data base, with default value assigned where measured
983 ! value is missing
984 !
985 ! If default density is set to zero, skip calculations
986     if (density .lt. 0.01) then
987         cp_volpct = -99.
988         cc_volpct = -99.
989         cv_volpct = -99.
990         bn_volpct = -99.
991         en_volpct = -99.
992         py_volpct = -99.
993         xc_volpct = -99.
994         br_volpct = -99.
995         go_volpct = -99.
996         go to 620
997     end if
998 !
999 ! Calculation of volume percent
1000     cp_volpct = cp_wtpct * density / sg_cp
1001     cc_volpct = cc_wtpct * density / sg_cc
1002     cv_volpct = cv_wtpct * density / sg_cv
1003     bn_volpct = bn_wtpct * density / sg_bn
1004     en_volpct = en_wtpct * density / sg_en
1005     xc_volpct = xc_wtpct * density / sg_xc
1006     br_volpct = br_wtpct * density / sg_br
1007     go_volpct = go_wtpct * density / sg_go
1008     if (py_best .lt. 0) then
1009         py_volpct = -99.
1010     else
1011         py_volpct = py_best * density / sg_py
1012     end if
1013 !
1014 ! =====
1015 ! Calculations complete
1016 ! Print normative mineralogy to file using cvs formatting functions
1017 ! THIS SECTION TO BE REPLACED BY DIRECT IO TO DATABASE

```

```

1018 !=====
1019 ! Modified Aug 2022, Version 2.3, Added tcu, fe, and s2 to output record
1020 620 continue
1021     rec_out = ' '
1022
1023     call csv_record_append_s  (dhname, rec_out)
1024     call csv_record_append_r4 (f_int, rec_out)
1025     call csv_record_append_r4 (t_int , rec_out)
1026     call csv_record_append_s  (sampid, rec_out)
1027     call csv_record_append_i4 (err_flag, rec_out)
1028     call csv_record_append_i4 (minzon, rec_out)
1029     call csv_record_append_i4 (ind_bn, rec_out)
1030     call csv_record_append_r4 (tcu, rec_out)
1031     call csv_record_append_r4 (fe, rec_out)
1032     call csv_record_append_r4 (s2, rec_out)
1033     call csv_record_append_r4 (csrcp, rec_out)
1034     call csv_record_append_r4 (csrcc, rec_out)
1035     call csv_record_append_r4 (csrcv, rec_out)
1036     call csv_record_append_r4 (csrbn, rec_out)
1037     call csv_record_append_r4 (csrgo, rec_out)
1038     call csv_record_append_r4 (csrbr, rec_out)
1039     call csv_record_append_r4 (csrxc, rec_out)
1040     call csv_record_append_r4 (cspcp, rec_out)
1041     call csv_record_append_r4 (cspcc, rec_out)
1042     call csv_record_append_r4 (cspcv, rec_out)
1043     call csv_record_append_r4 (cspbn, rec_out)
1044     call csv_record_append_r4 (cspgo, rec_out)
1045     call csv_record_append_r4 (cspbr, rec_out)
1046     call csv_record_append_r4 (cspxc, rec_out)
1047     call csv_record_append_r4 (cspen, rec_out)
1048     call csv_record_append_r4 (cp_wtpct, rec_out)
1049     call csv_record_append_r4 (cc_wtpct, rec_out)
1050     call csv_record_append_r4 (cv_wtpct, rec_out)
1051     call csv_record_append_r4 (bn_wtpct, rec_out)
1052     call csv_record_append_r4 (go_wtpct, rec_out)
1053     call csv_record_append_r4 (br_wtpct, rec_out)
1054     call csv_record_append_r4 (xc_wtpct, rec_out)
1055     call csv_record_append_r4 (en_wtpct, rec_out)
1056     call csv_record_append_r4 (py_best, rec_out)
1057     call csv_record_append_r4 (xfe, rec_out)
1058     call csv_record_append_r4 (cp_volpct, rec_out)
1059     call csv_record_append_r4 (cc_volpct, rec_out)
1060     call csv_record_append_r4 (cv_volpct, rec_out)
1061     call csv_record_append_r4 (bn_volpct, rec_out)
1062     call csv_record_append_r4 (go_volpct, rec_out)
1063     call csv_record_append_r4 (br_volpct, rec_out)
1064     call csv_record_append_r4 (xc_volpct, rec_out)
1065     call csv_record_append_r4 (en_volpct, rec_out)
1066     call csv_record_append_r4 (py_volpct, rec_out)
1067
1068     call csv_file_record_write (outputcsv, 61, rec_out )
1069 !=====
1070 ! Record output complete
1071 !=====

```

```

1072
1073 ! Write progress indicator to screen
1074     if (mod(ndata,50).eq. 0) write (*,'(i6,a)') ndata,' records processed'
1075
1076 ! Read next line
1077     go to 200
1078
1079 ! Data file read. End program
1080 900 continue
1081     ndata = ndata - 1
1082     write (*,'(i6,a)') ndata, " records processed. Run completed."
1083     close (51)
1084     close (61)
1085     if (idebug .eq. 1) close (62)
1086     stop
1087 END PROGRAM norminv2
1088 !
1089 !=====
1090 !=====
1091 ! Begin subroutine and function programming.
1092 ! These are subprograms that are called in the MAIN program
1093 !-----
1094 ! Begin subroutines for input and output of CSV formatted files
1095 !-----
1096 ! Subroutines to parse data record from input record
1097 ! Separate subroutines for character, integer, and R4 real data types
1098 ! Minor error checking - when error is encountered, variable is set to 'missing'
1099 ! indicator, record_status is set to value > 0, and control is returned to calling
1100 ! statement.
1101 !-----
1102
1103 subroutine get_char (xdata,icol, csv_record, csv_value, csv_len, record_status)
1104 ! Subroutine to extract character data type from csv record
1105 ! icol is location in record, from 1 to value count as per parameter file input
1106 ! Written by Richard K. Preece
1107 ! August 19, 2019
1108
1109
1110     character (len = 25) xdata, cdata
1111     character csv_char
1112     character csv_char_old
1113     integer ( kind = 4) csv_len
1114     integer ( kind = 4) csv_loc
1115     character ( len = *) csv_record
1116     integer ( kind = 4) record_status
1117     integer ( kind = 4) value_count
1118     integer ( kind = 4) csv_value
1119     integer ( kind = 4) word_length
1120
1121 ! Initiate counters
1122     value_count = 0
1123     record_status = 0
1124     word_length = 0

```

```

1125     csv_char_old = ','
1126
1127 ! Check to determine if variable is missing from the input file
1128     if (icol .eq. 0) then
1129         xdata = '-99'
1130         return
1131     end if
1132
1133     do csv_loc = 1, csv_len
1134         csv_char = csv_record(csv_loc:csv_loc)
1135         !
1136         ! Check for start of new value field
1137         if (csv_char_old == ',') then
1138             value_count = value_count + 1
1139             word_length = 1
1140         else
1141             word_length = word_length + 1
1142         end if
1143         if (csv_char == ',') then
1144             if (value_count == icol) go to 100
1145         end if
1146         csv_char_old = csv_char
1147     end do
1148
1149     if (csv_loc == csv_len) then
1150         ! data column not found, set data to -99 and return with error code
1151         record_status = 1
1152         xdata = ''
1153         return
1154     else
1155         !Unknown reason for early termination, set value to -99 and return with error code
1156         record_status = 9
1157         xdata = ''
1158         go to 101
1159     end if
1160
1161     ! Data column found. Calculate column location, read real value, and return
1162 100 continue
1163     mloc = csv_loc
1164     nloc = mloc - (word_length-1)
1165     read (csv_record(nloc:mloc), *,err=101,iostat=record_status) cdata
1166     xdata = trim(cdata)
1167
1168 101 continue
1169
1170 return
1171 end
1172
1173 subroutine get_integer (xdata,icol,csv_record,csv_value,csv_len,record_status)
1174 ! Subroutine to extract integer data type from csv record
1175 ! icol is location in record, from 1 to value count as per parameter file input
1176 ! Written by Richard K. Preece
1177 ! August 19, 2019
1178

```

```

1179
1180     integer (kind = 4) xdata
1181     character csv_char
1182     character csv_char_old
1183     integer ( kind = 4) csv_len
1184     integer ( kind = 4) csv_loc
1185     character ( len = *) csv_record
1186     integer ( kind = 4) record_status
1187     integer ( kind = 4) value_count
1188     integer ( kind = 4) csv_value
1189     integer ( kind = 4) word_length
1190
1191 ! Initiate counters
1192     value_count = 0
1193     record_status = 0
1194     word_length = 0
1195     csv_char_old = ','
1196
1197 ! Check to determine if variable is missing from the input file
1198     if (icol .eq. 0) then
1199         xdata = -99
1200         return
1201     end if
1202
1203     do csv_loc = 1, csv_len
1204         csv_char = csv_record(csv_loc:csv_loc)
1205         !
1206         ! Check for start of new value field
1207         if (csv_char_old == ',') then
1208             value_count = value_count + 1
1209             word_length = 1
1210         else
1211             word_length = word_length + 1
1212         end if
1213         if (csv_char == ',') then
1214             if (value_count == icol) go to 100
1215         end if
1216         csv_char_old = csv_char
1217     end do
1218
1219     if (csv_loc == csv_len) then
1220         ! data column not found, set data to -99 and return with error code
1221         record_status = 1
1222         xdata = -99
1223         return
1224     else
1225         !Unknown reason for early termination, set value to -99 and return with error code
1226         record_status = 9
1227         xdata = -99
1228         go to 101
1229     end if
1230
1231     ! Data column found. Calculate column location, read real value, and return

```

```

1232 100 continue
1233     mloc = csv_loc
1234     nloc = mloc - (word_length-1)
1235     read (csv_record(nloc:mloc), *,err=101,iostat=record_status) zdata
1236     xdata = int(zdata)
1237
1238 101 continue
1239
1240 return
1241 end
1242
1243 subroutine get_real (xdata,icol,csv_record,csv_value,csv_len,record_status)
1244 ! Subroutine to extract real data type from csv record
1245 ! icol is location in record, from 1 to value count as per parameter file input
1246 ! Written by Richard K. Preece
1247 ! August 16, 2019
1248
1249
1250     real (kind = 4) xdata
1251     character csv_char
1252     character csv_char_old
1253     integer ( kind = 4) csv_len
1254     integer ( kind = 4) csv_loc
1255     character ( len = *) csv_record
1256     integer ( kind = 4) record_status
1257     integer ( kind = 4) value_count
1258     integer ( kind = 4) csv_value
1259     integer ( kind = 4) word_length
1260
1261 ! Initiate counters
1262     value_count = 0
1263     record_status = 0
1264     word_length = 0
1265     csv_char_old = ','
1266
1267 ! Check to determine if variable is missing from the input file
1268     if (icol .eq. 0) then
1269         xdata = -99.0
1270         return
1271     end if
1272
1273     do csv_loc = 1, csv_len
1274         csv_char = csv_record(csv_loc:csv_loc)
1275         !
1276         ! Check for start of new value field
1277         if (csv_char_old == ',') then
1278             value_count = value_count + 1
1279             word_length = 1
1280         else
1281             word_length = word_length + 1
1282         end if
1283         if (csv_char == ',') then
1284             if (value_count == icol) go to 100
1285         end if

```



```

1286         csv_char_old = csv_char
1287     end do
1288
1289     ! Check if item is in last value on line
1290     if (value_count == icol) then
1291         word_length = word_length + 1
1292         go to 100
1293     end if
1294
1295     if (csv_loc == csv_len) then
1296         ! data column not found, set data to -99 and return with error code
1297         record_status = 1
1298         xdata = -99.0
1299         return
1300     else
1301         !Unknown reason for early termination, set value to -99 and return with error code
1302         record_status = 9
1303         xdata = -99.0
1304         go to 101
1305     end if
1306
1307     ! Data column found. Calculate column location, read real value, and return
1308100 continue
1309     mloc = csv_loc
1310     nloc = mloc - (word_length-1)
1311     read (csv_record(nloc:mloc), *,err=101,iostat=record_status) xdata
1312
1313101 continue
1314
1315 return
1316 end
1317 !-----
1318 ! Public domain subroutines to manage CSV-formatted input and output files
1319 !-----
1320 subroutine csv_value_count(csv_record, csv_record_status, value_count, csv_len)
1321
1322     !*****80
1323     !
1324     !! CSV_COUNT counts the number of values in a CSV record.
1325     !
1326     !   Licensing:
1327     !
1328     !     This code is distributed under the GNU LGPL license.
1329     !
1330     !   Modified:
1331     !
1332     !     28 November 2008
1333     !
1334     !   Author:
1335     !
1336     !     John Burkardt
1337     !
1338     !   Parameters:

```

```

1339      !
1340      implicit none
1341
1342      character csv_char
1343      character csv_char_old
1344      integer ( kind = 4) csv_len
1345      integer ( kind = 4) csv_loc
1346      character ( len = *) csv_record
1347      integer ( kind = 4) csv_record_status
1348      character :: TAB = achar(9)
1349      integer ( kind = 4) value_count
1350      integer ( kind = 4) word_length
1351      !
1352      !   No values so far.
1353      !
1354      value_count = 0
1355      !
1356      !   We begin in "unquoted" status.
1357      !
1358      csv_record_status = 0
1359      !
1360      !   How many characters in the record?
1361      !
1362      csv_len = len_trim(csv_record)
1363      !
1364      !   Count number of characters in each word.
1365      !
1366      word_length = 0
1367      !
1368      !   Consider each character.
1369      !
1370      csv_char_old = ','
1371
1372      do csv_loc = 1, csv_len
1373
1374          csv_char = csv_record(csv_loc:csv_loc)
1375          !
1376          !   Each comma divides one value from another.
1377          !
1378          if (csv_char_old == ',') then
1379
1380              value_count = value_count + 1
1381              word_length = 0
1382              !
1383              !   For quotes, try using CSV_RECORD_STATUS to count the number of
1384              !   quoted characters.
1385              !
1386          else if (csv_char == '"') then
1387
1388              if (0 < csv_record_status) then
1389                  csv_record_status = 0
1390              else
1391                  csv_record_status = csv_record_status + 1
1392              end if

```

```

1393         !
1394         !   Ignore blanks
1395         !
1396         else if (csv_char == ' ' .or. csv_char == TAB) then
1397             !
1398             !   Add character to length of word.
1399             !
1400         else
1401
1402             word_length = word_length + 1
1403
1404             if (value_count == 0) then
1405                 value_count = 1
1406             end if
1407
1408         end if
1409
1410         csv_char_old = csv_char
1411
1412     end do
1413
1414     return
1415 end
1416 subroutine csv_file_close_read(csv_file_name, csv_file_unit)
1417
1418     !*****80
1419     !
1420     !! CSV_FILE_CLOSE_READ closes a CSV file for reading.
1421     !
1422     !   Licensing:
1423     !
1424     !       This code is distributed under the GNU LGPL license.
1425     !
1426     !   Modified:
1427     !
1428     !       29 November 2008
1429     !
1430     !   Author:
1431     !
1432     !       John Burkardt
1433     !
1434     !   Parameters:
1435     !
1436     !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1437     !
1438     !       Input, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1439     !
1440     implicit none
1441
1442     character ( len = *) csv_file_name
1443     integer ( kind = 4) csv_file_unit
1444
1445     close ( unit = csv_file_unit)

```

```

1447     return
1448 end
1449 subroutine csv_file_close_write(csv_file_name, csv_file_unit)
1450
1451     !*****80
1452     !
1453     !! CSV_FILE_CLOSE_WRITE closes a CSV file for writing.
1454     !
1455     !   Licensing:
1456     !
1457     !       This code is distributed under the GNU LGPL license.
1458     !
1459     !   Modified:
1460     !
1461     !       22 November 2008
1462     !
1463     !   Author:
1464     !
1465     !       John Burkardt
1466     !
1467     !   Parameters:
1468     !
1469     !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1470     !
1471     !       Input, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1472     !
1473     implicit none
1474
1475     character ( len = *) csv_file_name
1476     integer ( kind = 4) csv_file_unit
1477
1478     close ( unit = csv_file_unit)
1479
1480     return
1481 end
1482 subroutine csv_file_header_write(csv_file_name, csv_file_unit, header)
1483
1484     !*****80
1485     !
1486     !! CSV_FILE_HEADER_WRITE writes a header to a CSV file.
1487     !
1488     !   Licensing:
1489     !
1490     !       This code is distributed under the GNU LGPL license.
1491     !
1492     !   Modified:
1493     !
1494     !       22 November 2008
1495     !
1496     !   Author:
1497     !
1498     !       John Burkardt
1499     !

```

```

1500      !   Parameters:
1501      !
1502      !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1503      !
1504      !       Input, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1505      !
1506      !       Input, character ( len = * ) HEADER, the header.
1507      !
1508      implicit none
1509
1510      character ( len = *) csv_file_name
1511      integer ( kind = 4) csv_file_unit
1512      character ( len = *) header
1513
1514      write ( csv_file_unit, '(a)') trim(header)
1515
1516      return
1517 end
1518 subroutine csv_file_line_count(csv_file_name, line_num)
1519
1520      !*****80
1521      !
1522      !! CSV_FILE_LINE_COUNT counts the number of lines in a CSV file.
1523      !
1524      !   Discussion:
1525      !
1526      !       This routine does not try to distinguish the possible header line,
1527      !       blank lines, or cases where a single CSV record extends over multiple
1528      !       lines. It simply counts the number of lines.
1529      !
1530      !   Licensing:
1531      !
1532      !       This code is distributed under the GNU LGPL license.
1533      !
1534      !   Modified:
1535      !
1536      !       22 November 2008
1537      !
1538      !   Author:
1539      !
1540      !       John Burkardt
1541      !
1542      !   Parameters:
1543      !
1544      !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1545      !
1546      !       Output, integer ( kind = 4 ) LINE_NUM, the number of lines.
1547      !
1548      implicit none
1549
1550      character ( len = *) csv_file_name
1551      integer ( kind = 4) ierror
1552      integer ( kind = 4) input_status
1553      integer ( kind = 4) input_unit

```

```

1553 integer ( kind = 4) input_unit
1554 character ( len = 1023) line
1555 integer ( kind = 4) line_num
1556
1557 line_num = -1
1558
1559 call get_unit(input_unit)
1560
1561 open ( unit = input_unit, file = csv_file_name, status = 'old', &
1562 iostat = input_status)
1563
1564 if (input_status /= 0) then
1565     write ( *, '(a)') ' '
1566     write ( *, '(a)') 'CSV_FILE_LINE_COUNT - Fatal error!'
1567     write ( *, '(a,i8)') ' Could not open "' // trim(csv_file_name) // '". '
1568     stop
1569 end if
1570
1571 line_num = 0
1572
1573 do
1574
1575     read ( input_unit, '(a)', iostat = input_status) line
1576
1577     if (input_status /= 0) then
1578         ierror = line_num
1579         exit
1580     end if
1581
1582     line_num = line_num + 1
1583
1584 end do
1585
1586 close ( unit = input_unit)
1587
1588 return
1589 end
1590 subroutine csv_file_record_write(csv_file_name, csv_file_unit, record)
1591
1592     !*****80
1593     !
1594     !! CSV_FILE_RECORD_WRITE writes a record to a CSV file.
1595     !
1596     !   Licensing:
1597     !
1598     !       This code is distributed under the GNU LGPL license.
1599     !
1600     !   Modified:
1601     !
1602     !       22 November 2008
1603     !
1604     !   Author:
1605     !
1606     !       John Burkardt

```

```

1607      !
1608      !   Parameters:
1609      !
1610      !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1611      !
1612      !       Input, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1613      !
1614      !       Input, character ( len = * ) RECORD, the record.
1615      !
1616      implicit none
1617
1618      character ( len = *) csv_file_name
1619      integer ( kind = 4) csv_file_unit
1620      character ( len = *) record
1621
1622      write ( csv_file_unit, '(a)') trim(record)
1623
1624      return
1625 end
1626 subroutine csv_file_open_read(csv_file_name, csv_file_unit)
1627
1628      !*****80
1629      !
1630      !! CSV_FILE_OPEN_READ opens a CSV file for reading.
1631      !
1632      !   Licensing:
1633      !
1634      !       This code is distributed under the GNU LGPL license.
1635      !
1636      !   Modified:
1637      !
1638      !       29 November 2008
1639      !
1640      !   Author:
1641      !
1642      !       John Burkardt
1643      !
1644      !   Parameters:
1645      !
1646      !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1647      !
1648      !       Output, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1649      !
1650      implicit none
1651
1652      character ( len = *) csv_file_name
1653      integer ( kind = 4) csv_file_status
1654      integer ( kind = 4) csv_file_unit
1655
1656      call get_unit(csv_file_unit)
1657
1658      open ( unit = csv_file_unit, file = csv_file_name, status = 'old', &
1659      iostat = csv_file_status)
1660

```

```

1661     if (csv_file_status /= 0) then
1662         write ( *, '(a)') ' '
1663         write ( *, '(a)') 'CSV_FILE_OPEN_READ - Fatal error!'
1664         write ( *, '(a,i8)') ' Could not open "' // trim(csv_file_name) // '".'
1665         csv_file_unit = -1
1666         stop
1667     end if
1668
1669     return
1670 end
1671 subroutine csv_file_open_write(csv_file_name, csv_file_unit)
1672
1673     !*****80
1674     !
1675     !! CSV_FILE_OPEN_WRITE opens a CSV file for writing.
1676     !
1677     !   Licensing:
1678     !
1679     !       This code is distributed under the GNU LGPL license.
1680     !
1681     !   Modified:
1682     !
1683     !       22 November 2008
1684     !
1685     !   Author:
1686     !
1687     !       John Burkardt
1688     !
1689     !   Parameters:
1690     !
1691     !       Input, character ( len = * ) CSV_FILE_NAME, the name of the file.
1692     !
1693     !       Output, integer ( kind = 4 ) CSV_FILE_UNIT, the unit number
1694     !
1695     implicit none
1696
1697     character ( len = *) csv_file_name
1698     integer ( kind = 4) csv_file_status
1699     integer ( kind = 4) csv_file_unit
1700
1701     call get_unit(csv_file_unit)
1702
1703     open ( unit = csv_file_unit, file = csv_file_name, status = 'replace', &
1704         iostat = csv_file_status)
1705
1706     if (csv_file_status /= 0) then
1707         write ( *, '(a)') ' '
1708         write ( *, '(a)') 'CSV_FILE_OPEN_WRITE - Fatal error!'
1709         write ( *, '(a,i8)') ' Could not open "' // trim(csv_file_name) // '".'
1710         stop
1711     end if
1712
1713     return

```



```

1714 end
1715 subroutine csv_record_append_i4(i4, record)
1716
1717 !*****80
1718 !
1719 !! CSV_RECORD_APPEND_I4 appends an I4 to a CSV record.
1720 !
1721 !   Licensing:
1722 !
1723 !       This code is distributed under the GNU LGPL license.
1724 !
1725 !   Modified:
1726 !
1727 !       24 November 2008
1728 !
1729 !   Author:
1730 !
1731 !       John Burkardt
1732 !
1733 !   Parameters:
1734 !
1735 !       Input, integer ( kind = 4 ) I4, the integer to be appended
1736 !
1737 !       Input/output, character ( len = * ) RECORD, the CSV record.
1738 !
1739 implicit none
1740
1741 character ( len = 5) fmat
1742 integer ( kind = 4) i
1743 integer ( kind = 4) i4
1744 integer ( kind = 4) i4_len
1745 integer ( kind = 4) i4_width
1746 character ( len = *) record
1747 !
1748 !   Locate last used location in RECORD.
1749 !
1750 i = len_trim(record)
1751 !
1752 !   Append comma.
1753 !
1754 if (0 < i) then
1755     i = i + 1
1756     record(i:i) = ','
1757 end if
1758 !
1759 !   Determine "width" of I4.
1760 !
1761 i4_len = i4_width(i4)
1762 !
1763 !   Create format for I4.
1764 !
1765 write ( fmat, '(a,i2,a)' ) '(i', i4_len, ')'
1766 !
1767 !   Write I4 to RECORD.

```

```

1768      !
1769      write ( record(i + 1:i + i4_len), fmat) i4
1770
1771      return
1772 end
1773 subroutine csv_record_append_r4(r4, record)
1774
1775      !*****80
1776      !
1777      !! CSV_RECORD_APPEND_R4 appends an R4 to a CSV record.
1778      !
1779      !   Licensing:
1780      !
1781      !       This code is distributed under the GNU LGPL license.
1782      !
1783      !   Modified:
1784      !
1785      !       29 November 2008
1786      !
1787      !   Author:
1788      !
1789      !       John Burkardt, modified by R.K. Preece 19 Aug 2019
1790      !
1791      !   Parameters:
1792      !
1793      !       Input, real ( kind = 8 ) R4, the value to be appended
1794      !
1795      !       Input/output, character ( len = * ) RECORD, the CSV record.
1796      !
1797      implicit none
1798
1799      character ( len = 5) fmat
1800      character ( len = 7) fmat2
1801      integer ( kind = 4) i
1802      integer ( kind = 4) i4
1803      integer ( kind = 4) i4_len
1804      integer ( kind = 4) i4_width
1805      real ( kind = 4) r4
1806      character ( len = *) record
1807      !
1808      !   Locate last used location in RECORD.
1809      !
1810      i = len_trim(record)
1811      !
1812      !   Append comma.
1813      !
1814      if (0 < i) then
1815          i = i + 1
1816          record(i:i) = ','
1817      end if
1818
1819      if (r4 == 0.0) then
1820          i = i + 1

```

```

1821     record(i:i) = '0'
1822     else if (r4 == real ( int ( r4), kind = 4)) then
1823         i4 = int ( r4)
1824         i4_len = i4_width(i4)
1825         write ( fmat, '(a,i2,a)') '(i', i4_len, ')'
1826         write ( record(i + 1:i + i4_len), fmat) i4
1827     else
1828 ! This branch for writing R4 variable modified by RK Preece, 19 August 2019
1829 ! Changed from gl8.7 format to variable width f*.3 format
1830         i4 = int (r4*1000)
1831         i4_len = i4_width(i4) + 2
1832         if (i4_len .lt. 5) then
1833             if (r4 .lt. 0) then
1834                 i4_len = 6
1835             else
1836                 i4_len = 5
1837             end if
1838         end if
1839         write ( fmat2, '(a,i2,a)') '(f', i4_len, '.3)'
1840         write ( record(i + 1:i + i4_len), fmat2) r4
1841 !         write ( record(i + 1:i + 8), '(f8.3)') r4
1842     end if
1843
1844     return
1845 end
1846 subroutine csv_record_append_r8(r8, record)
1847
1848     !*****80
1849     !
1850     !! CSV_RECORD_APPEND_R8 appends an R8 to a CSV record.
1851     !
1852     !   Licensing:
1853     !
1854     !       This code is distributed under the GNU LGPL license.
1855     !
1856     !   Modified:
1857     !
1858     !       29 November 2008
1859     !
1860     !   Author:
1861     !
1862     !       John Burkardt
1863     !
1864     !   Parameters:
1865     !
1866     !       Input, real ( kind = 8 ) R8, the value to be appended
1867     !
1868     !       Input/output, character ( len = * ) RECORD, the CSV record.
1869     !
1870     implicit none
1871
1872     character ( len = 5) fmat
1873     integer ( kind = 4) i
1874     integer ( kind = 4) i4

```

```

1875     integer ( kind = 4) i4_len
1876     integer ( kind = 4) i4_width
1877     real ( kind = 8) r8
1878     character ( len = *) record
1879     !
1880     !  Locate last used location in RECORD.
1881     !
1882     i = len_trim(record)
1883     !
1884     !  Append comma.
1885     !
1886     if (0 < i) then
1887         i = i + 1
1888         record(i:i) = ','
1889     end if
1890
1891     if (r8 == 0.0D+00) then
1892         i = i + 1
1893         record(i:i) = '0'
1894     else if (r8 == real ( int ( r8), kind = 8)) then
1895         i4 = int ( r8)
1896         i4_len = i4_width(i4)
1897         write ( fmat, '(a,i2,a)') '(i', i4_len, ')'
1898         write ( record(i + 1:i + i4_len), fmat) i4
1899     else
1900         write ( record(i + 1:i + 14), '(g14.6)') r8
1901     end if
1902
1903     return
1904 end
1905 subroutine csv_record_append_s(s, record)
1906
1907     !*****80
1908     !
1909     !! CSV_RECORD_APPEND_S appends a string to a CSV record.
1910     !
1911     !  Licensing:
1912     !
1913     !      This code is distributed under the GNU LGPL license.
1914     !
1915     !  Modified:
1916     !
1917     !      26 November 2008
1918     !
1919     !  Author:
1920     !
1921     !      John Burkardt
1922     !
1923     !  Parameters:
1924     !
1925     !      Input, character ( len = * ) S, the string to be appended
1926     !
1927     !      Input/output, character ( len = * ) RECORD, the CSV record.

```

```

1928      !
1929      implicit none
1930
1931      integer ( kind = 4) i
1932      character ( len = *) record
1933      character ( len = *) s
1934      integer ( kind = 4) s_len
1935      !
1936      !   Locate last used location in RECORD.
1937      !
1938      i = len_trim(record)
1939      !
1940      !   Append a comma.
1941      !
1942      if (0 < i) then
1943          i = i + 1
1944          record(i:i) = ','
1945      end if
1946      !
1947      !   Prepend a quote.
1948      !
1949      !i = i + 1
1950      !record(I:i) = '"'
1951      !
1952      !   Write S to RECORD.
1953      !
1954      s_len = len_trim(s)
1955      record(i + 1:i + s_len) = s(1:s_len)
1956      i = i + s_len
1957      !
1958      !   Postpend a quote
1959      !
1960      !i = i + 1
1961      !record(i:i) = '"'
1962
1963      return
1964 end
1965 subroutine get_unit(iunit)
1966
1967      !*****80
1968      !
1969      !! GET_UNIT returns a free FORTRAN unit number.
1970      !
1971      !   Discussion:
1972      !
1973      !       A "free" FORTRAN unit number is an integer between 1 and 99 which
1974      !       is not currently associated with an I/O device.  A free FORTRAN unit
1975      !       number is needed in order to open a file with the OPEN command.
1976      !
1977      !       If IUNIT = 0, then no free FORTRAN unit could be found, although
1978      !       all 99 units were checked (except for units 5, 6 and 9, which
1979      !       are commonly reserved for console I/O).
1980      !
1981      !       Otherwise, IUNIT is an integer between 1 and 99, representing a

```

```

1982      !   free FORTRAN unit.  Note that GET_UNIT assumes that units 5 and 6
1983      !   are special, and will never return those values.
1984      !
1985      !   Licensing:
1986      !
1987      !   This code is distributed under the GNU LGPL license.
1988      !
1989      !   Modified:
1990      !
1991      !   26 October 2008
1992      !
1993      !   Author:
1994      !
1995      !   John Burkardt
1996      !
1997      !   Parameters:
1998      !
1999      !   Output, integer ( kind = 4 ) IUNIT, the free unit number.
2000      !
2001      implicit none
2002
2003      integer ( kind = 4) i
2004      integer ( kind = 4) ios
2005      integer ( kind = 4) iunit
2006      logical lopen
2007
2008      iunit = 0
2009
2010      do i = 1, 99
2011
2012         if (i /= 5 .and. i /= 6 .and. i /= 9) then
2013
2014            inquire ( unit = i, opened = lopen, iostat = ios)
2015
2016            if (ios == 0) then
2017               if (.not.lopen) then
2018                  iunit = i
2019                  return
2020               end if
2021            end if
2022
2023         end if
2024
2025      end do
2026
2027      return
2028 end
2029 function i4_log_10(i)
2030
2031      !*****80
2032      !
2033      !! I4_LOG_10 returns the integer part of the logarithm base 10 of an I4.
2034      !

```

```

2035 ! Discussion:
2036 !
2037 !   I4_LOG_10 ( I ) + 1 is the number of decimal digits in I.
2038 !
2039 !   An I4 is an integer ( kind = 4 ) value.
2040 !
2041 ! Example:
2042 !
2043 !       I   I4_LOG_10
2044 !   -----
2045 !       0     0
2046 !       1     0
2047 !       2     0
2048 !       9     0
2049 !      10     1
2050 !      11     1
2051 !      99     1
2052 !     100     2
2053 !     101     2
2054 !     999     2
2055 !    1000     3
2056 !    1001     3
2057 !    9999     3
2058 !   10000     4
2059 !
2060 ! Licensing:
2061 !
2062 !   This code is distributed under the GNU LGPL license.
2063 !
2064 ! Modified:
2065 !
2066 !   08 June 2003
2067 !
2068 ! Author:
2069 !
2070 !   John Burkardt
2071 !
2072 ! Parameters:
2073 !
2074 !   Input, integer ( kind = 4 ) I, the number whose logarithm base 10
2075 !   is desired.
2076 !
2077 !   Output, integer ( kind = 4 ) I4_LOG_10, the integer part of the
2078 !   logarithm base 10 of the absolute value of X.
2079 !
2080 implicit none
2081
2082 integer ( kind = 4 ) i
2083 integer ( kind = 4 ) i_abs
2084 integer ( kind = 4 ) i4_log_10
2085 integer ( kind = 4 ) ten_pow
2086
2087 if ( i == 0 ) then
2088

```

```

2089         i4_log_10 = 0
2090
2091     else
2092
2093         i4_log_10 = 0
2094         ten_pow = 10
2095
2096         i_abs = abs(i)
2097
2098         do while (ten_pow <= i_abs)
2099             i4_log_10 = i4_log_10 + 1
2100             ten_pow = ten_pow * 10
2101         end do
2102
2103     end if
2104
2105     return
2106 end
2107 function i4_width(i)
2108
2109     !*****80
2110     !
2111     !! I4_WIDTH returns the "width" of an I4.
2112     !
2113     ! Discussion:
2114     !
2115     ! The width of an integer is the number of characters necessary to print it.
2116     !
2117     ! The width of an integer can be useful when setting the appropriate output
2118     ! format for a vector or array of values.
2119     !
2120     ! An I4 is an integer ( kind = 4 ) value.
2121     !
2122     ! Example:
2123     !
2124     !      I   I4_WIDTH
2125     !  -----
2126     !    -1234    5
2127     !     -123    4
2128     !      -12    3
2129     !       -1    2
2130     !        0    1
2131     !         1    1
2132     !        12    2
2133     !       123    3
2134     !      1234    4
2135     !     12345    5
2136     !
2137     ! Licensing:
2138     !
2139     ! This code is distributed under the GNU LGPL license.
2140     !
2141     ! Modified:

```



```

2142      !
2143      !      04 December 2004
2144      !
2145      !      Author:
2146      !
2147      !      John Burkardt
2148      !
2149      !      Parameters:
2150      !
2151      !      Input, integer ( kind = 4 ) I, the number whose width is desired.
2152      !
2153      !      Output, integer ( kind = 4 ) I4_WIDTH, the number of characters
2154      !      necessary to represent the integer in base 10, including a negative
2155      !      sign if necessary.
2156      !
2157      implicit none
2158
2159      integer ( kind = 4 ) i
2160      integer ( kind = 4 ) i4_log_10
2161      integer ( kind = 4 ) i4_width
2162
2163      if (0 < i) then
2164         i4_width = i4_log_10(i) + 1
2165      else if (i == 0) then
2166         i4_width = 1
2167      else if (i < 0) then
2168         i4_width = i4_log_10(i) + 2
2169      end if
2170
2171      return
2172 end
2173 subroutine timestamp()
2174
2175      !*****80
2176      !
2177      !! TIMESTAMP prints the current YMDHMS date as a time stamp.
2178      !
2179      !      Example:
2180      !
2181      !      31 May 2001   9:45:54.872 AM
2182      !
2183      !      Licensing:
2184      !
2185      !      This code is distributed under the GNU LGPL license.
2186      !
2187      !      Modified:
2188      !
2189      !      18 May 2013
2190      !
2191      !      Author:
2192      !
2193      !      John Burkardt
2194      !
2195      !      Parameters:

```

```

2196      !
2197      !      None
2198      !
2199      implicit none
2200
2201      character ( len = 8) ampm
2202      integer ( kind = 4) d
2203      integer ( kind = 4) h
2204      integer ( kind = 4) m
2205      integer ( kind = 4) mm
2206      character ( len = 9), parameter, dimension(12) :: month = (/ &
2207      'January ', 'February ', 'March ', 'April ', &
2208      'May ', 'June ', 'July ', 'August ', &
2209      'September', 'October ', 'November ', 'December ' /)
2210      integer ( kind = 4) n
2211      integer ( kind = 4) s
2212      integer ( kind = 4) values(8)
2213      integer ( kind = 4) y
2214
2215      call date_and_time(values = values)
2216
2217      y = values(1)
2218      m = values(2)
2219      d = values(3)
2220      h = values(5)
2221      n = values(6)
2222      s = values(7)
2223      mm = values(8)
2224
2225      if (h < 12) then
2226          ampm = 'AM'
2227      else if (h == 12) then
2228          if (n == 0 .and. s == 0) then
2229              ampm = 'Noon'
2230          else
2231              ampm = 'PM'
2232          end if
2233      else
2234          h = h - 12
2235          if (h < 12) then
2236              ampm = 'PM'
2237          else if (h == 12) then
2238              if (n == 0 .and. s == 0) then
2239                  ampm = 'Midnight'
2240              else
2241                  ampm = 'AM'
2242              end if
2243          end if
2244      end if
2245
2246      write ( *, '(i2,1x,a,1x,i4,2x,i2,a1,i2.2,a1,i2.2,a1,i3.3,1x,a)' ) &
2247      d, trim(month(m)), y, h, ': ', n, ': ', s, '.', mm, trim(ampm)
2248
2249      return

```

```

2249 !      return
2250 end
2251 !
2252 !-----
2253 ! Begin functions for finding the determinant of an algebraic matrix
2254 ! These are calls from within an equation of the MAIN program
2255 ! In both functions, the array is passed to function A and the calculated determinant
2256 ! is returned to the calling equation
2257 !-----
2258 FUNCTION M33DET (A) RESULT (DET)
2259 ! *****
2260 ! M33DET - Function to compute the determinant of a 3x3 matrix.
2261 ! Programmer: David G. Simpson
2262 !             NASA Goddard Space Flight Center
2263 !             Greenbelt, Maryland 20771
2264 ! Date:       July 22, 2005
2265 ! Language:   Fortran-90
2266 ! Version:    1.00a
2267 ! *****
2268
2269     IMPLICIT NONE
2270     real (kind = 8), DIMENSION(3,3), INTENT(IN) :: A
2271     real (kind = 8) :: DET
2272
2273
2274     DET = A(1,1)*A(2,2)*A(3,3) &
2275           - A(1,1)*A(2,3)*A(3,2) &
2276           - A(1,2)*A(2,1)*A(3,3) &
2277           + A(1,2)*A(2,3)*A(3,1) &
2278           + A(1,3)*A(2,1)*A(3,2) &
2279           - A(1,3)*A(2,2)*A(3,1)
2280
2281     RETURN
2282
2283 END FUNCTION M33DET
2284 FUNCTION M44DET (A) RESULT (DET)
2285 ! *****
2286 ! Function:      M44DET
2287 ! Programmer:    David G. Simpson
2288 !               NASA Goddard Space Flight Center
2289 !               Greenbelt, Maryland 20771
2290 ! Date:          February 6, 2009
2291 ! Language:      Fortran-90
2292 ! Version:       1.00a
2293 ! Description:   Computes the determinant a 4x4 matrix
2294 ! *****
2295
2296     IMPLICIT NONE
2297     real (kind = 8), DIMENSION(4,4), INTENT(IN) :: A
2298     real (kind = 8) :: DET
2299
2300     DET = A(1,1)*(A(2,2)*(A(3,3)*A(4,4)-A(3,4)*A(4,3)))+A(2,3)*(A(3,4)*A(4,2)-A(3,2)*A(4,4))
2301           -A(3,3)*A(4,2))-A(1,2)*(A(2,1)*(A(3,3)*A(4,4)-A(3,4)*A(4,3)))+A(2,3)*(A(3,4)*A(4,
2302           A(2,4)*(A(3,1)*A(4,3)-A(3,3)*A(4,1)))+A(1,3)*(A(2,1)*(A(3,2)*A(4,4)-A(3,4)*A(4,2)

```

C:/Users/rkpre/Documents/NetBeansProjects/NorMin_v2/NorMin_v2.f90

```
2303      A(3,1)*A(4,4))+A(2,4)*(A(3,1)*A(4,2)-A(3,2)*A(4,1)))-A(1,4)*(A(2,1)*(A(3,2)*A(4,
2304      A(2,2)*(A(3,3)*A(4,1)-A(3,1)*A(4,3))+A(2,3)*(A(3,1)*A(4,2)-A(3,2)*A(4,1)))
2305
2306      RETURN
2307
2308 END FUNCTION M44DET
2309
2310
2311
```