```
 1     !TweakEngine.F95  Version 1.0
 2    !2018.10.08.0945cdt JMS- Applied numerical partial differentiation.
 3
 4    !  Jeffrey M. Setterholm, 8095 230th St. E., Lakeville, Minnesota 55044, USA
 5    !   I have authored the four Fortran *.f95 source code files listed below.
 6    !                        I hereby place these four files:
 7    !       Tweak-Begin.f95, Tweak-Engine.F95, Tweak-User.F95, & Tweak-Vis.f95
 8    !                and the algorithms which are demonstrated therein,
 9    !                      in the public domain (a.k.a.: "free").
10    !Disclaimer:
11    !       ************************************************************
12    !       **********   Individual cognition is always flawed,  **********
13    !       **********         including yours and mine.         **********
14    !       **********                  - So: -                  **********
15    !       **********      Use this code at your own risk.      **********
16    !       ************************************************************
17
18    !Table of Contents:
19    !Program Tweak
20    !Subroutine EvalFit(RSSL,iP)
21    !Subroutine PrintIter(iP)
22    !Subroutine RSSPartials(jpUL)
23    !Subroutine DatapointPartials
24    !Subroutine Invert(N,A,ValMin,iRank,DetN,iUsed,iP)
25    !Subroutine PrintA(N,A,Noise,iRank,DetN,iRu,jCu,iP)
26    !Subroutine SelectStepMult(iP)
27    !Function om(Value1,Value0,iP)
28    !Subroutine FloatWrite(R16In,a40out)
29    !Subroutine FDate23(DaTime)
30    !Subroutine Beamer(n,nTot)
31    !-------------------------------------------------------------------------------7-9
32
33    Program Tweak
34    !2018.10.09.0820cdt JMS- Empowers numerical partial differentiation to fit
35    !                         the parameters of your model(s) to your datae
36    !                                  with extreme accuracy.
37    !                       "Tweaks" refers to the small deltas of parameter
38    !                              values used to compute the numerical partials.
39    !                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
40    !---                                                                globals
41    !Defined in Tweak-Begin.f95; all named here, as an overview:
42     use Tweakrec,only: jPhase,jMode  ,cVersion,cDateTime & !Tweak's FYI
43                       ,jBOn,jUnClamp,jStepMult,jPrev     & !Solution strategy
44                       ,jpU10,jpU,jpD           ,cFloat40 & !Printout-Alphanumeric
45                       ,jpU3d,TLrec,TL,TLprev,TL2,TLsave  & !Printout-3D
46                       ,jTLmorph,TLiter,omjSave           & !         "
47                       ,jItertot,jIter,jDone              & !Iteration control
48                       ,RSS,RSSbase,Weight,Delta,offon    & !Tweaking & errors
49                       ,AbsDet,NoiseFloor,iRank,kPChanged & !Inverter outputs
50                       ,jMintot,jMin,StepMult,omj         & !Minimization passes !Minim
51                       ,B,BtB,BtZ                         & !Allocated matrices
52                       ,What,Why,How,Who,When,Where1      & !Project context
53                       ,jUserPhase,jUserConfig,cjUserFile & !Use in YouTweak()
54                       ,TweakNml                            !Runtime reconfig.
55     Use KPrec,   only: Kptot,Kp,Kp2,  Pr   ,Pu,PstepMag    !Parameters -to fit to-
56     Use LZrec,   only: Lztot,Lz,      Zr   ,Zu,Zu2,Z0      !Outputs    - of your -
57     use MDrec,   only: Mdtot,Md,MdMax,Datae                !Dataset
58     use NXrec,   only: Nxtot,Nx,      Xr                   !Independent variables
59    !                                  ^^:These are allocated records.
60    !                    ^^:At the outset you size these four values.
61     !---
62     implicit none                                                  !arguments
63      !---                                                          !internals
64      integer*4:: i,j
65      integer*4:: nY
66      integer*4:: jpUL       !Printer argument of Invert() and SelectStepMult()
67      character:: A1*1
68     !real*16  :: RSSL
69      logical  ::LExists       !File existence flag
70
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```
 71      !-----                                                          !end defs
 72     !call fdate(cDateTime)
 73      call FDate23(cDateTime)
 74   !  -------------------------
 75      jPhase = "0: Allocates records based on Kptot,Lztot,Mdtot,& Nxtot"c
 76
 77      call YouTweak(0) !You must size Kptot,Lztot,Mdtot, & Nxtot!
 78
 79   !  Modifying key variables at runtime using NameList:
 80      inquire(file="Tweak-user.nml",exist=LExists)
 81      if(LExists)then
 82        write(6,"('Tweak-user.nml variable changes included...')")
 83        open(unit=jpU10,file  ='Tweak-user.nml',action='read' &
 84            ,access='sequential'  ,status='old' ,err=11)
 85           read(jpU10,nml=TweakNml,err=11)
 86        close(jpU10); goto 12
 87    11  pause "Error reading Tweak-user.nml. Press enter to continue."
 88        close(jpU10)
 89       endif!LExists
 90    12 continue
 91
 92      call TweakAllocateAll !Allocates all but the inverter's internal arrays.
 93
 94      if(jpU < 6) jpD=0       !No output file: no printouts.
 95                  jpUL = jpU
 96      if(jpD < 6) jpUL = 0
 97
 98      if(Weight > 0._16) Zr.Wt    = Weight
 99                         Pr.offon = offon
100
101   !  Using previous values of the parameters:
102      if(jPrev == 0) then
103    20  write(6,"(1x,'Use the last run`s Pr.Pbase values? (0 or 1)'\)");
104        read(5,*,err=20) jPrev
105      endif !jPrev = 0
106      if(jPrev.eq.1) then  !Import the previous values from "Tweak-params.txt":
107        inquire(file="Tweak-params.txt",exist=LExists)
108        if(LExists)then
109          open(unit=jpU10,file  ='Tweak-params.txt',action='read' &
110            ,access='sequential'  ,status='old' ,err=21)
111          read(jpU10,*,err=21) Kptot,Lztot
112          do Kp=1,Kptot; read(jpU10,*) Pr(Kp).P ;enddo!Kp
113        close(jpU10); goto 22
114    21    pause "Error reading Tweak-params.txt. Press enter to continue."
115          close(jpU10)
116         else
117          pause "jPrev==1, but Tweak-params.txt not found. 'Enter` to continue."
118        endif!Lexists
119      endif !jPrev==0
120    22 continue
121
122   !  Open the output file:
123      if((jpU >10).and.(jpD > 0)) &
124        open(unit=jpU,file='Tweak-out.txt',action='write')
125      if(jpD>0) then;   if(jpU>6) write(  6,"(a60/)") cVersion
126                                  write(jpU,"(a60)") cVersion
127                                  write(jpU,"(/'Project Context:')")
128        j=len_trim(What)  ;if(J>0)write(jpU,"(60a1)") (What(i:i)  ,i=1,j)
129        j=len_trim(Why)   ;if(J>0)write(jpU,"(60a1)") (Why(i:i)   ,i=1,j)
130        j=len_trim(How)   ;if(J>0)write(jpU,"(60a1)") (How(i:i)   ,i=1,j)
131        j=len_trim(Who)   ;if(J>0)write(jpU,"(60a1)") (Who(i:i)   ,i=1,j)
132        j=len_trim(When)  ;if(J>0)write(jpU,"(60a1)") (When(i:i),  i=1,j)
133        j=len_trim(Where1);if(J>0)write(jpU,"(60a1)") (Where1(i:i),i=1,j)
134      endif!(jpD>0)
135   !  -------------------------
136      jPhase = "1: You quantify your system model in the allocated arrays"c
137
138      call YouTweak(1)
139   !  Key Tweakrec values:
140      if(jpD >= 1) then
```

```
141       write(jpU,"(/'Tweak`s initial values, after calling YouTweak(1):')")
142       write(jpU,"( ' jBOn     =',i6,6x,' = [     1: ]' )") jBOn
143       write(jpU,"( ' jUnClamp =',i6,6x,' = [     1: ]' )") jUnClamp
144       write(jpU,"( ' jStepMult=',i6,6x,' = [     1,2]' )") jStepMult
145       write(jpU,"( ' jPrev    =',i6,6x,' = [-1,0,1  ]' )") jPrev
146
147       write(jpU,"(/' jpU      =',i6,6x,' = [   0,6,11]')") jpU
148       write(jpU,"( ' jpD      =',i6,6x,' = [   0-8   ]')") jpD    !Details
149       write(jpU,"( ' jpU10    =',i6,6x,' = [       10]')") jpU10
150       write(jpU,"( ' jpU3D    =',i6,6x,' = [   0  ,13]')") jpU3D
151
152       write(jpU,"(/' jItertot =',i6,6x,' = [   0:    ]')") jItertot
153
154       write(jpU,"(/' Weight   =',e12.3,' = [ nom: 1.] ')") Weight
155       write(jpU,"( ' Delta    =',e12.3,' = [small>0.] ')") Delta
156       write(jpU,"( ' offon    =',e12.3,' = [  0., 1.] ')") offon
157
158       write(jpU,"(/' jMintot  =',i6,6x,' = [   1:    ]')") jMintot
159
160       write(jpU,"(/' Kptot    =',i6,6x,' = [   1:    ]')") Kptot
161       write(jpU,"( ' Lztot    =',i6,6x,' = [   1:    ]')") Lztot
162       write(jpU,"( ' Mdtot    =',i6,6x,' = [   1:    ]')") Mdtot
163       write(jpU,"( ' Nxtot    =',i6,6x,' = [   1:    ]')") Nxtot
164     endif !jpD>=1
165
166   !   -------------------------
167     jPhase = "2: Top-of-each iteration: establish baseline residual errors"c
168
169     do jIter = 0,jItertot !Iterate the solution:
170       if((jpU > 5).and.(jpD >=4)) write(jpU,"(/'Iteration:',i3)") jIter
171
172       Zr.RMS   = 0._16
173       Zr.Zmax  = 0._16
174       Zr.Mdmax = 0
175          Md    = 0
176       call YouTweak(2)  !(Re-)Initialize your dataset
177      !Pr.Pbase - holds the baseline parameter values for each iteration.
178       Pr.P = Pr.Pbase
179
180       if(Delta  > 0._16) Pr(1:Kptot).Delta=Delta  !Numerical tweak deltas
181       if((jpD >= 5).and.(Delta > 0._16)) write(jpU,"('Delta=',e12.6)") Delta
182       if(Weight > 0._16) Zr(1:Lztot).Wt =Weight !Output weights
183
184   !   Establish the base values at the start of each iteration:
185       call EvalFit(RSS, 0)
186       if((jIter == 0).and.(jpD >=4)) call PrintIter(jpU)
187       RSSbase=RSS; Zr.Zbase=Zr.Z; Zr.RMSbase=Zr.RMS     ;if(jIter == 0) goto 700
188
189   !   jIter>0:
190
191   !   Compute the numerical partial derivatives two ways:
192   !   -------------------------
193
194       call RSSPartials(jpUL) !Computes Pr(*).Pstep(1,1)'s
195   !   -------------------------
196
197       call DatapointPartials !Computes Pr(*).Pstep(2,1)'s
198   !     Inside the call:
199         jPhase = "3: Populate BtB(Kptot,Kptot) and BtZ(Kptot)"c
200         jPhase = "4: Normalize and invert BtB(Kptot,Kptot)"c
201         jPhase = "5: Inverters stepsize = BtBinv(denormalized)*BtZ"c
202   !   -------------------------
203
204   !   By each of the paths above - Pr(1:Kptot).Pstep's have been computed.
205   !   The .Pstep's are the Tweak-Engine's guess(es) about the vector direction
206   !   in which to change your parameter values so that your mathematical model
207   !   better-fits your dataset. When using jBon=1 on a linear system model
208   !   the length of the vector is just about right on.
209
210   !   My experience has been that non-linear models are locally linear around
```

```
211  !    their solution point; hence they routinely converge very rapidly
212  !    in the last few iterations of a highly-accurate fit. In calibrating
213  !    sensors, model fits with less than .01% error are the norm, rather than
214  !    the exception.
215
216  !    The computations in SelectStepMult() search for a value of StepMult that
217  !    significantly reduces the fit error for non-linear problems.
218
219  !    For non-linear models the opening .Pistep vector may be huge.
220  !    Restricting the magnitude of parameter changes may prevent having
221  !    your model blow up before nears the stable region where it fits your data:
222
223       do Kp2=1,2
224         if(jpD >= 5) then
225           if(Kp2 == 1) write(jpU,"(/'Pr.Pstep(1,1) RSS values:'\)")
226           if(Kp2 == 2) write(jpU,"(/'Pr.Pstep(2,1) Inv values:'\)")
227         endif!jpD>=5
228         Pr.Pstep(Kp2,2) = Pr.Pstep(Kp2,1)
229         if(jIter < jUnClamp) then
230                           PstepMag = 0._16
231           do Kp=1,Kptot; PstepMag = PstepMag +Pr(Kp).Pstep(Kp2,1)**2; enddo!Kp
232           if(PstepMag  > 1._16) then !Shorten Pr.P.Step to magnitude = 1.
233             Pr.Pstep(Kp2,2)=Pr.Pstep(Kp2,1)/sqrt(PstepMag )
234             if(jpD >= 5) write(jpU,"(' Clamped:'\)")
235           endif!(PstepMag  > 1._16)
236         endif!(jIter<=__)
237         if(jpD >= 5) then
238           write(jpu,*)
239           do Kp = 1,Kptot
240             call FloatWrite( Pr(Kp).Pstep(Kp2,2),cFloat40)
241             write(jpU,"(a40,2x,16a1)") cFloat40,(Pr(Kp).Pname(i:i) &
242                                       ,i=1,len_trim(Pr(Kp).Pname)      )
243           enddo!Kp
244         endif!jpD>5
245       enddo!Kp2
246
247  !    Set flag jBOn=_ to:
248       if(jIter <  jBOn) Pr.Pstep(4,1) =  Pr.Pstep(1,2) !Use RSS Partials
249       if(jIter >= jBOn) Pr.Pstep(4,1) =  Pr.Pstep(2,2) !Use Inverter's Partials
250
251  !    --------------------------
252       jPhase = "6: Find an error-reducing actual stepsize"c
253
254  !    Select/Compute StepMult:
255       select case(jStepMult)
256        case(1) !Use inverter's result; excellent for linear models.
257                                 StepMult = 1._16
258         Pr.Pnew = Pr.Pbase + StepMult * Pr.PStep(4,2)
259
260        case(2) !Use SelectStepMult(), esp. when using jBPath=2
261         call SelectStepMult(jpUL)       !(0): no detail
262
263        case default; pause"jStepMult /= [1,2]; press enter to halt."; stop
264
265       end select!(jStepMult)
266                                                       kPChanged = 0
267       do Kp=1,kptot;
268         if(Pr(Kp).Pnew /= Pr(Kp).Pbase) kPChanged = kPChanged + 1
269       enddo!Kp
270       if((kPChanged == 0).and.(jIter > 5)) jDone=1
271
272       Pr.P = Pr.Pnew; call EvalFit(RSS, 0)
273       if(jpD >= 4) call PrintIter(jpU) !Print the results.
274       if(jIter < 101) omjSave(jIter) = omj
275       Pr.Pbase = Pr.Pnew !Use the new baseline parameters.
276  !    --------------------------
277       jPhase = "7: Iterative pass done. Your intervention opportunity:"c
278  !                                      E.g.: to adjust Delta & Pr().onOff's
279   700 call YouTweak(5)
280                        ;if(jDone == 0) cycle
```

```
      NY=2
      if(jpD >= 2) then
        call PrintIter(6)
 710    WRITE(6,"(1X,'Want to quit (N/n or Y/y)?'\)")
        A1=char(0)
        read(5,*) A1
        select case(ichar(A1))
         case(78,110);  NY=1   !Nn
         case(89,121);  NY=2   !Yy
         case default; goto 710
        end select !ichar(A1)
      endif !(jpD>=2)
                                                                  if(NY.EQ.2) exit
    enddo!jIter
!     -------------------------
    jPhase = "8: Tweak is done interating. Export the results & close"c
    Pr.P=Pr.Pbase
    if(jpD == 3) call PrintIter(jpU)
    if(jpD >= 3) write(jpU,"(/'EvalFit final printout:')")
    call EvalFit(RSS,jpU)
    call YouTweak(6) !"Tweak-is-done": your completion-printout opportunity.

    if(jpD > 0) write(jpU,"('Tweak: saving results & deallocating arrays...')")

    if(jpU>10) close(jpU)

!   Save final values, e.g. to use as 'previous' parameters:
    call FDate23(cDateTime)
   !call fdate(cDateTime)
    open(unit=jpU10,file='Tweak-params.txt',action='write',access='sequential')
                 write(jpU10,*) Kptot,Lztot
      do Kp=1,Kptot; write(jpU10,"(e41.32,i5,'  '\)") Pr(Kp).Pbase,Kp
        j=len_trim( Pr(Kp).Pname)
        if(J>0)write(jpU10,"(16a1)") (Pr(Kp).Pname(i:i),i=1,j)
      enddo!Kp
      write(jpU10,"(3x,'^These are the last-iteration`s values'\)")
      write(jpU10,"(    ' at full precision.'/)")

      do Kp=1,Kptot;  call FloatWrite(Pr(Kp).Pbase,cFloat40)
                 write(jpU10,"(1x,i4,' ',a40)") Kp,cFloat40
      enddo!Kp
      write(jpU10,"(/13x,'.123456789012345678901234567890123456789012345')")
      write(jpU10,"( 23x,'1         2         3'\)")
      write(jpU10,"(  6x,'-Floats decimal place counter')")

      Pr.P=Pr.Pbase; call EvalFit(RSS,jpU10)

      write(jpU10,"(/'Project Context:',40x,a23)") cDateTime
      j=len_trim(What)  ;if(J>0)write(jpU10,"(60a1)") (What(i:i)  ,i=1,j)
      j=len_trim(Why)   ;if(J>0)write(jpU10,"(60a1)") (Why(i:i)   ,i=1,j)
      j=len_trim(How)   ;if(J>0)write(jpU10,"(60a1)") (How(i:i)   ,i=1,j)
      j=len_trim(Who)   ;if(J>0)write(jpU10,"(60a1)") (Who(i:i)   ,i=1,j)
      j=len_trim(When)  ;if(J>0)write(jpU10,"(60a1)") (When(i:i),  i=1,j)
      j=len_trim(Where1);if(J>0)write(jpU10,"(60a1)") (Where1(i:i),i=1,j)
      write(jpU10,"(/a60)") cVersion
    close(jpU10)

    deallocate(Pr,Zr,Datae,Xr)
    deallocate(B,BtB,BtZ)
    if(jpU > 10) write(6,"('`Tweak-out.txt` has your run summary.' )")
                 write(6,"('`Tweak-params.txt` has the parametric values.' )")
    pause 'Press `Enter` to exit.'
End Program Tweak
!-------------------------------------------------------------------------------7-9
Subroutine EvalFit(RSSL,iP)
!2018.09.02.1220cdt JMS- Evaluates the residual error(s) of the dataset.
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                  globals
 use Tweakrec,only: jItertot,jIter                    & !Iteration control
                   ,jpU,jpD                ,cFloat40   !Printout
```

```
  Use KPrec,    only:                Pr                    !Parameters -to fit to-
  Use LZrec,    only: Lztot,Lz,      Zr                    !Outputs    - of your -
  use MDrec,    only: Mdtot,Md,MdMax,Datae                 !Dataset
  use NXrec,    only: Nxtot,Nx,      Xr                    !Independent variables
  !---
  implicit none                                            !arguments
   real*16  ::RSSL
   integer*4::iP
   !---                                                     !internals
   real*16  ::temp
   integer*4::i
    !-----                                                  !end defs
    if(iP > 5) write(iP,"(/'EvalErr:')")
    RSSL=0._16
    Md = 0
    call YouTweak(2)

    Zr.Zmax  = 0._16
    Zr.Mdmax = 0
    Zr.RMS   = 0._16
       RSSL  = 0._16
    if(iP > 5) &
      write(iP,"('Data# Out#',9x,'Error  : results comparison',11x,'dataID')")

    do Md = 1,Mdtot
      call YouTweak(3)
      call YouTweak(4)
      do Lz=1,Lztot
                                  temp = Zr(Lz).Z
        Zr(Lz).RMS  = Zr(Lz).RMS+temp*temp
       !if(jIter.le.jItertot) cycle
        if(Md == 1) then
               Zr(Lz).Zmax      = temp; Zr(Lz).Mdmax=1; endif!Md=1
        if(abs(Zr(Lz).Zmax) < abs(temp)) then
               Zr(Lz).Zmax      = temp; Zr(Lz).Mdmax=Md;endif
      enddo!Lz
    enddo!Md

    do Lz=1,Lztot
       Zr(Lz).RMS =sqrt(Zr(Lz).RMS/Mdtot)
       RSSL=RSSL + Zr(Lz).RMS*Zr(Lz).RMS
    enddo!Lz
    RSSL=sqrt(RSSL)

  ! Md = 0
  ! call YouTweak(2)
                                                  !if(jIter < jItertot) return
                                                   if(iP    <    6    ) return
    write(iP,"('EvalFit Summary:')")
                                call FloatWrite(RSSL,cFloat40)
    write(iP,"(  'Mdtot=',i7,a40,' SRSS')") Mdtot,cFloat40
    do Lz=1,Lztot;                                  Mdmax =Zr(Lz).Mdmax
                                  call FloatWrite(Zr(Lz).RMS ,cFloat40)
      write(iP,  "('  Lz= ',i7,a40,' RMS')")     Lz,           cFloat40
      if(MdMax > 0) then
                                  call FloatWrite(Zr(Lz).Zmax,cFloat40)
        write(iP,"(' @Md= ',i7,a40,' Max(abs)')")    Mdmax,      cFloat40
           Nx=0
          write(iP,"(i13,f10.0,31x,16a1)")Nx,Datae(Nx    ,Mdmax) &
                                  ,(Xr(Nx).Xname(i:i),i=1,len_trim(Xr(Nx).Xname))
        do Nx=1,Nxtot
               call FloatWrite(Datae(Nx      ,Mdmax),cFloat40)
          write(iP,"(i13,a40,1x,16a1)")   Nx,          cFloat40  &
                                  ,(Xr(Nx).Xname(i:i),i=1,len_trim(Xr(Nx).Xname))
        enddo!Nx
               call FloatWrite(Datae(NxTot+LZ,Mdmax),cFloat40)
        write(  iP,"(13x,a40,1x,16a1)")               cFloat40  &
                                  ,(Zr(Lz).Zname(i:i),i=1,len_trim(Zr(Lz).Zname))
      endif !(McMax>0)
    enddo!Lz
```

```
  421     write(iP,"(49x,'^^^^: exponents, if any.')")
  422     write(iP,  "(i13,'  Iterations')") jIter;                                  return
  423   End Subroutine EvalFit
  424   !-------------------------------------------------------------------------------7-9
  425
  426   Subroutine PrintIter(iP)
  427   !2018.09.26.1150cdt JMS- Using FloatWrite
  428   !                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
  429    !---                                                                      globals
  430    use Tweakrec,only:                              cDateTime & !Tweak's FYI
  431                     ,jBOn,jUnClamp,jStepMult               & !Solution strategy
  432                     ,jpU,jpD                      ,cFloat40 & !Printout
  433                     ,      jItertot,jIter,jDone       & !Iteration
  434                     ,RSS                              & !Tweaking & errors
  435                     ,jMintot,jMin,StepMult,omj          !Minimization passes
  436    Use KPrec,    only: Kptot,Kp,Kp2,  Pr               !Parameters -to fit to-
  437    Use LZrec,    only: Lztot,Lz,      Zr               !Outputs    - of your -
  438    use MDrec,    only: Mdtot,Md                        !Dataset
  439    !---
  440    implicit none                                                        !arguments
  441     integer*4::iP
  442     !---                                                                 !internals
  443     real*16  ::change,delta
  444     integer*4::KpL
  445     character::C1*1
  446      !-----                                                               end defs
  447     if(jpD < 3) return
  448     call FDate23(cDateTime)
  449     if(jMin > jMintot) write(iP,"('Lower value of error not found.')")
  450     if(jIter == 0) write(iP,"(/35x,'om = an order-of-magnitude change scale.')")
  451     if(jIter == 0) write(iP,"(/'Stopwatch - 24-hour local time (msec val'\)")
  452     if(jIter == 0) write(iP,"( 'ues stick):     Year Mo D  Hr Mn Sec~ms')")
  453     write(iP,"(/   'Pass',i3,' of',i4,\)") jIter,jItertot
  454     if(jBOn  > jIter) write(iP,"('  RSS partials',\)")
  455     if(jBOn <= jIter) write(iP,"('  BtB & BtZ    ',\)")
  456     if(jUnClamp >  jIter) write(iP,"(' -clamped  ',\)")
  457     if(jUnClamp <= jIter) write(iP,"('           ',\)")
  458     write(iP,"('om = ',a9,3x,a23)") omj,cDateTime
  459                          call FloatWrite(RSS,cFloat40)
  460     write(iP,"('RSS = ',a40,e14.6,' /',i2)") cFloat40,RSS,jMin
  461     write(iP,"('Lz#   ',13x,'Residual Error',16x,'Change',8x,'weight')")
  462     do Lz=1,Lztot
  463       call FloatWrite(Zr(Lz).RMS,cFloat40)
  464       change=Zr(Lz).RMS-Zr(Lz).RMSbase
  465                          C1="*"
  466       if(abs(change) > 0) C1=" "
  467         write(iP,"(1x,i4,a1,a40,\)") Lz,C1,cFloat40
  468       if(abs(change) > .000001_16) then
  469         write(iP,"(1x,f17.8 ,2x,f13.9)") dble(change),dble(Zr(Lz).Wt)
  470        else;
  471         write(iP,"(1x,e17.10,2x,f13.9)") dble(change),dble(Zr(Lz).Wt)
  472       endif !(change not tiny)
  473     enddo!Lz
  474     write(iP,"('----- ----.12345678901234567890123456789012345')")
  475     write(iP,"(     '     *:unchanged    1         2         3'\)")
  476     write(iP,"(  9x,'-Floats decimal place counter'/)")
  477
  478     write(iP,"('Kp#   ',17x,'Value',21x,'Change',9x,'delta')")
  479     do Kp=1,Kptot
  480       call FloatWrite(Pr(Kp).P,cFloat40)
  481       change = Pr(Kp).P-Pr(Kp).Pbase
  482       KpL    = Kp
  483       delta  = Pr(Kp).Delta
  484
  485       if(abs(change) > 0) then
  486             write(iP,"(1x,i4,' ',a40,\)") KpL,cFloat40
  487        else; write(iP,"(1x,i4,'*',a40,\)") KpL,cFloat40
  488       endif!(|Change|>0)
  489       if(abs(change) > .000001_16) then
  490         write(iP,"(1x,f17.8 \)") dble(change)
```

```
491         else;
492          write(iP,"(1x,e17.10\)") dble(change)
493        endif !(change not tiny)
494        if(abs(delta) >= 1.e-9_16) then
495          write(iP,"(2x,f13.9)") dble(delta)
496         else;
497          write(iP,"(2x,e13.7)") dble(delta)
498        endif !(change not tiny)
499      enddo!Kp
500      write(iP,"('----- ----.12345678901234567890123456789012345')")
501      write(iP,"(      '     *:unchanged    1          2         3'\)")
502      write(iP,"(  9x,'-Floats decimal place counter'/)")
503      write(iP,*)
504      Md=0
505      if((iP == 6).and.(jDone == 0)) pause "... by PrintIter"
506                                                                    return
507  End Subroutine PrintIter
508  !-------------------------------------------------------------------------7-9
509
510  Subroutine RSSPartials(jpUL)
511  !2018.09.26.1150cdt JMS- Uses the partial derivatives of the entire dataset
512  !                       to compute a single gradient vector.
513  !                    - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
514   !---                                                           globals
515   use Tweakrec,only:     jpD                 ,cFloat40  &!Printout
516                     ,RSS,RSSbase                          !Tweaking & errors
517  !                  ,B,BtB,BtZ                            !Allocated matrices
518   Use KPrec,    only: Kptot,Kp,Kp2,  Pr    ,Pu,PstepMag    !Parameters -to fit to-
519  !Use LZrec,    only: Lztot,Lz,      Zr                   !Outputs    - of your -
520  !use MDrec,    only: Mdtot,Md,MdMax,Datae                !Dataset
521   !---
522   implicit none                                                !arguments
523    integer*4::jpUL
524    !---                                                       !internals
525    real*16  ::RSSL
526    integer*4::i
527     !-----                                                    !end defs
528  !  Reset the point from which numerical partial differentiation will occur:
529       Pr.P     = Pr.Pbase              ;call EvalFit(RSS,jPUL)
530  !  Compute the numerical partial derivatives of each parameter vs. RSS:
531     PstepMag  = 0._16
532     do Kp = 1,Kptot !Tweak each of the parameters in turn:
533       Pr(Kp).P = Pr(Kp).P+Pr(Kp).Delta ;call EvalFit(RSSL,jPUL) !Delta parameter
534                                        !     Evaluates the entire dataset
535  !    Insert the numerical partial derivative into Pr(Kp).Pstep(1,1):
536       Pr(Kp).Pstep(1,1) = (RSS-RSSL)/Pr(Kp).Delta
537       PstepMag          = PstepMag  + Pr(Kp).Pstep(1,1) * Pr(Kp).Pstep(1,1)
538       Pr(Kp).P          = Pr(Kp).Pbase          !un-Delta parameter
539     enddo!Kp
540       Pr.P              = Pr.Pbase               ;call EvalFit(RSS,jpUL)
541     if(abs(PstepMag )  > 1.e-30_16) then
542       PstepMag          = RSS/sqrt(PstepMag )
543       Pr.Pstep(1,1)     = PstepMag  * Pr.Pstep(1,1)
544     endif!(PstepMag  not tiny)
545
546
547     if(jpUL >= 5) then
548                  call FloatWrite( PstepMag   ,cFloat40)
549       write(jpUL,"('RSSPartials:  PstepMag =',a40)") cFloat40
550       do Kp = 1,KpTot
551         call FloatWrite( Pr(Kp).Pstep(1,1),cFloat40)
552         write(jpUL,"(a40,2x,16a1)") cFloat40,(Pr(Kp).Pname(i:i) &
553                                    ,i=1,len_trim(Pr(Kp).Pname)      )
554       enddo!Kp
555     endif!(jpUL>=5)
556                                                                    return
557  End Subroutine RSSPartials
558  !-------------------------------------------------------------------------7-9
559
560  Subroutine DatapointPartials
```

```
!2018.09.09.0735cdt JMS- Using the partial derivatives of individual datapoints
!                        to compute B(:,:) & hence BtB() and BtZ
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                globals
 use Tweakrec,only: jPhase                              & !Tweak's FYI
                   ,jpU,jpD                  ,cFloat40 & !Printout
                   ,AbsDet,NoiseFloor,iRank           & !Inverter outputs
                   ,B,BtB,BtZ                           !Allocated matrices
 Use KPrec,   only: Kptot,Kp,Kp2,  Pr                   !Parameters -to fit to-
 Use LZrec,   only: Lztot,Lz,      Zr                   !Outputs    - of your -
 use MDrec,   only: Mdtot,Md,MdMax,Datae                !Dataset
 !---
 implicit none                                                      !arguments
  !---                                                             !internals
  integer*4:: i
  integer*4:: jpUL         !Printer argument of Invert() and SelectStepMult()

   !-----                                                          !end defs
            jpUL = jpU
   if(jpD<6) jpUL=0

!  Zero the matrix accumulators:
   BtZ         = 0._16
   BtB         = 0._16
!  Populate the key matrixes using the full dataset:
          Md = 0
   call YouTweak(2)  !(Re-)Initialize your dataset
   do Md = 1,Mdtot !For each dataset:
              if(MdTot > 1000) &
     call beamer(Md,Mdtot) !DOS-screen progress bar - mitigates angst
                                                 ! while huge datasets process.
     call YouTweak(3) !Pull in the next datapoint
     call YouTweak(4) !Compute outputs for the current datapoint
     Zr.Zbase = Zr.Z  !Compute each outputs un-tweaked value

!    Compute the numerical partial derivatives of each parameter:
     do Kp = 1,Kptot !Tweak each of the parameters in turn:
       Pr(Kp).P = Pr(Kp).P+Pr(Kp).Delta !   Delta parameter
       call YouTweak(4)                !Evaluate the outputs

!      Insert the numerical partial derivative into B():
       B(1:Lztot,Kp)=((Zr.Zbase-Zr.Z)/Pr(Kp).Delta)*Pr(Kp).offon
       Pr(Kp).P = Pr(Kp).Pbase         !un-Delta parameter
     enddo!Kp

     if(jpD >= 5) then  !Print B()
       write(jpU,"('Md# = ',i16/'Lz# =')")Md
       do Lz=1,Lztot;   write(jpU,  &
                "(i5,4x,g12.6,' Zr( Lz        ).Zbase'/'  '\)") Lz,Zr(Lz).Zbase
         do Kp=1,Kptot; write(jpU,"(g12.6\)") B(Lz,Kp)             ;enddo!Kp
                        write(jpU,"(' B(  Lz,1:Kptot)'/'  '\)")
         do Kp=1,Kptot; write(jpU,"(g12.6\)") B(Lz,Kp)*Zr(Lz).Zbase ;enddo!kp
                        write(jpU,"(' BtZ(   1:Kptot)')")
       enddo!Lz
     endif!((jpU>5)&(jpD>6))

!    Accumulate B() into -BtZ() and BtB:
     do Lz=1,Lztot
       do Kp=1,Kptot      !Vector add:
         BtZ(Kp)=BtZ(Kp)+B(Lz,Kp)*Zr(Lz).Zbase
         do Kp2 = 1,Kptot !Outer product of B() with itself (~covariance):
           BtB(Kp2,Kp) = BtB(Kp2,Kp) +    B(Lz,Kp2)  *  B(Lz,Kp)
         enddo!Kp2
       enddo!Kp2
     enddo!Lz
   enddo!Md
!  BtB(), BtZ(), and BnZ() have been computed.

!  ------------------------

```

```
631     jPhase = "4: Normalize and invert BtB(Kptot,Kptot)"c
632
633     if(jpD >= 6) then  !Print BtB() & BtZ()
634       write(jpU,"(/'Kp#   BtB(Kptot,Kptot) | BtZ(Kptot)=  (normalized)')")
635       do Kp=1,Kptot;    write(jpU,"(i4,'  ',\)") Kp
636         do Kp2=1,Kptot; write(jpU,"(     g18.9\)") BtB(Kp,Kp2); enddo!Kp2
637                         write(jpU,"(' |',g18.9 )") BtZ(Kp)
638       enddo;            write(jpU,"('')")
639     endif!((jpU>5)&(jpD>=6))
640
641   !  Pr.BtBnorm will be used to normalize BtB() with 1.'s on the diagonal:
642     do Kp=1,Kptot; Pr(Kp).BtBnorm = abs(BtB(Kp,Kp))
643                 if(Pr(Kp).BtBnorm > 1.e-20_16) then !This threshold is a wag,
644   !                                                          ...explore it.
645                    Pr(Kp).BtBnorm = sqrt(Pr(Kp).BtBnorm)
646                  else
647                    Pr(Kp).BtBnorm = 1._16
648                 endif!Pr(Kp).BtBnorm not tiny
649       if((jpU > 5).and.(jpD >= 6)) &
650         write(jpU,"('Pr(',i4,').BtBnorm=',e13.6)") Kp,Pr(Kp).BtBnorm
651     enddo !Kp
652
653   !  Pr.BtBnorm = 1._16 !<- Disables BtBnorm normalization.
654
655   !  Normalize BtB()
656     do Kp=1,Kptot
657       do Kp2=1,Kptot
658         BtB(Kp,Kp2) = BtB(Kp,Kp2)/(Pr(Kp).BtBnorm*Pr(Kp2).BtBnorm)
659       enddo!Kp2
660     enddo!Kp
661
662     if(jpD >= 5) then  !Print BtB() & BtZ()
663       write(jpU,"(/'Kp#   BtB(Kptot,Kptot) | BtZ(Kptot)=')")
664       do Kp=1,Kptot;    write(jpU,"(i4,'  ',\)") Kp
665         do Kp2=1,Kptot; write(jpU,"(     g18.9\)") BtB(Kp,Kp2); enddo!Kp2
666                         write(jpU,"(' |',g18.9 )") BtZ(Kp)
667       enddo;            write(jpU,"('')")
668     endif!((jpU>5)&(jpD>=6))
669
670     !---
671     call invert( Kptot        &  !Input : dimensions of BtB(Kptot,Kptot)
672                , BtB          &  !In/Out: matrix to be inverted
673                , NoiseFloor   &  !Output: noise floor of the inversion
674                , iRank        &  !        Rank of BtBinverse <= Kptot
675                , AbsDet       &  !        abs(Determinant) of BtB
676                , Pr.Inverted  &  !        =0. linearly   dependent param.
677                               &  !        =1. linearly independent param.
678                , jpUL          ) !input : >5: Print unit number
679                                  !        =0: No printout
680
681   !  -------------------------
682     jPhase = "5: Inverters stepsize = BtBinv(denormalized)*BtZ"c
683
684     do Kp=1,Kptot
685       do Kp2=1,Kptot
686         BtB(Kp,Kp2) =  BtB(Kp,Kp2)/( Pr(Kp).BtBnorm*Pr(Kp2).BtBnorm )
687       enddo!Kp2
688     enddo!Kp
689
690     if(jpD >= 5) then  !Print BtBinv() & BtZ()
691       write(jpU,"(/'Kp#   BtBinv(Kptot,Kptot) | BtZ(Kptot)=')")
692       do Kp=1,Kptot;    write(jpU,"(i4,'  ',\)") Kp
693         do Kp2=1,Kptot; write(jpU,"(     g18.9\)") BtB(Kp,Kp2); enddo!Kp2
694                         write(jpU,"(' |',g18.9 )") BtZ(Kp)
695       enddo;            write(jpU,"('')")
696     endif!((jpU>5)&(jpD>=6))
697
698     Pr.Pstep(2,1) = 0._16
699     do Kp=1,Kptot      !Compute the step vector:
700       do Kp2=1,Kptot
```

```
701         Pr(Kp).Pstep(2,1) = Pr(Kp).Pstep(2,1) + BtB(Kp,Kp2) * BtZ(Kp2)
702       enddo!Kp2
703     enddo!Kp
704
705     Pr.P = Pr.Pbase
706     if(jpD >= 5) then
707       write(jpU,"(/'Inverter`s full Pr(Kp).Pstep(2,1):')")
708       do Kp = 1,KpTot
709         call FloatWrite( Pr(Kp).Pstep(2,1),cFloat40)
710         write(jpU,"(a40,2x,16a1)") cFloat40,(Pr(Kp).Pname(i:i), &
711                                    i=1,len_trim(Pr(Kp).Pname)        )
712       enddo!Kp
713     endif!jpD>=5
714                                                                          return
715   End Subroutine DatapointPartials
716   !-------------------------------------------------------------------------7-9
717
718   Subroutine Invert(N,A,ValMin,iRank,DetN,iUsed,iP)
719   !2010.01.06.1205cst JMS- Traveler2/Athlon64/WinXPPro-32/APF9.0-32
720   !2006.05.25.0715cdt JMS- An instantiation of the "Setterholm Matrix Inverter"
721   !---                                                          No globals
722    implicit none                                                !arguments
723     integer*4:: N
724     real*16  :: A(N,N)
725     real*16  :: ValMin
726     integer*4:: iRank
727     real*16  :: DetN    !Abs(determinant product) for each iteration
728     integer*4:: iUsed(N)
729     integer*4:: iP
730     !---                                                          !internals
731     integer*4,allocatable::iRu(:)
732     integer*4,allocatable::jCu(:)
733     real*16  ,allocatable::Temp(:)
734     integer*4::i,iu,iu2,j,ju,ju2,L
735     real*16  ::Amult,ValMax
736     integer*8::iBinSum
737     integer*4::iAlloc
738      !-----                                                       !end defs
739      if(iP.gt.5) write(iP,"('Overwriting Matrix Inversion:')")
740      DetN=0._16 ;iUsed(1:N)=0 ;iRank=0
741      !---
742      allocate(iRu(N),stat=iAlloc)
743      if(iAlloc.ne.0) stop 'Invert: iRu(N) allocation error. Halt.'
744      iRu=0
745      allocate(jCu(N),stat=iAlloc)
746      if(iAlloc.ne.0) stop 'Invert: jCu(N) allocation error. Halt.'
747      jCu=0
748      allocate(Temp(N),stat=iAlloc)
749      if(iAlloc.ne.0) stop 'Invert: Temp(N) allocation error. Halt.'
750      Temp=0._16
751      !---
752        Temp=0._16; iRu   =0 ;jCu   =0 ;ValMin=0._16
753      do i=1,N    ;iRu(i)=i ;jCu(i)=i                ;end do
754              if(iP.gt.5) call PrintA(N,A,ValMin,iRank,DetN,iRu,jCu,iP) !*********
755   !  Inversion Loop:
756      do L=1,N ;iU=0     ;jU=0     ;ValMax =0._16
757        do i=1,N  ;if(iRu(i).lt.0) cycle
758          do j=1,N ;if(jCu(j).lt.0) cycle
759            if(ValMax.ge.abs(A(i,j))) cycle
760              ValMax=abs(A(i,j)) ;iu=i ;ju=j
761          enddo!j
762        enddo!i
763        if(L.eq.1) ValMin=ValMax*1.d-20  !Establishes the "noise floor".
764        if(iU.eq.0) Exit
765        if(ValMax.lt.ValMin) Exit
766        iRank=iRank+1
767        DetN=ValMax
768        ValMax=A(iu,ju) ;iu2=jCu(ju) ;ju2=iRu(iu)
769       !if(iP.gt.5) write(iP,"(3i3,f15.6)")  L,iu,ju,ValMax
770        if(iP.gt.5) write(iP,"(1x,2i4,f15.9,'   :iu ju pivot, & value')") &
```

```
                                                  iu,ju,        ValMax
      Temp(1:N)=A(1:N,ju)                                 ;i=iRu(iu)
                A(1:N,ju)=A(1:N,ju2)                      ;  iRu(iu)=iRu(iu2)
                          A(1:N,ju2)=Temp(1:N)            ;          iRu(iu2)=-abs(i)
      Temp(1:N)=A(iu,1:N)                                 ;j=jCu(ju)
                A(iu,1:N)=A(iu2,1:N)                      ;  jCu(ju)=jCu(ju2)
                          A(iu2,1:N)=Temp(1:N)/ValMax     ;          jCu(ju2)=-abs(j)
      do i=1,N ;if(i.eq.iu2) cycle ;Amult=A(i,ju2)
        do j=1,N ;A(i,j)=A(i,j)-A(iu2,j)*Amult ;enddo!j
        A(i,ju2)=-Amult/ValMax
      enddo; A(iu2,ju2)=1._16/ValMax
           if(iP.gt.5) call PrintA(N,A,ValMin,iRank,DetN,iRu,jCu,iP) !*********
    enddo!L  Inversion loop- done.

    iBinSum=0
    do i=1,n
      if((iRu(i).lt.0).and.(i.lt.63)) iBinsum=iBinSum+2**(i-1)
       if(iRu(i).lt.0) iUsed(i)=1
!     Zero linearly-dependent rows and columns, if any:
       if(iRu(i).gt.0) A(i,1:N)=0._16
       if(jCu(i).gt.0) A(1:N,i)=0._16
    enddo!i
    if((iP >5).and.(iu == 0)) then
      write(iP,"('Linear dependency dealt with. Partial inverse results:')")
      write(iP,"(b63.2,' -Kp unused flag')") iBinSum !For the first 62 Kp's
                        call PrintA(N,A,ValMin,iRank,DetN,iRu,jCu,iP) !*********
    endif!iP>5 & iu==0
    if(iP.gt.5) write(iP,"('Overwriting Inverter- done.')")
    deallocate(iRu)
    deallocate(jCu)
    deallocate(Temp)
    return
End Subroutine Invert
!-------------------------------------------------------------------------------7-9

Subroutine PrintA(N,A,Noise,iRank,DetN,iRu,jCu,iP)
!2018.09.04.1340cdt JMS- Prints Invert's progress.
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                  No globals
 implicit none                                                        !arguments
  integer*4:: N
  real*16  :: A(N,N)
  real*16  :: Noise
  integer*4:: iRank
  real*16  :: DetN
  integer*4:: iRu(N)
  integer*4:: jCu(N)
  integer*4:: iP
  !---                                                                 !internals
  integer*4::i,j
   !-----                                                              !end defs
                                                                  if(iP < 6) return
   write(iP,"('Inverter: @ Rank =',i5,8x,'abs(Det)=',f39.30/2x\)") iRank,DetN
   do j=1,N;   write(iP,"(i18,\)") jCu(j) ; enddo; write(iP,"('')")
   do i=1,N;   write(iP,"(i5,' ' ,\)") iRu(i)
     do j=1,N; write(iP,"(f18.9\)") A(i,j); enddo; write(iP,"('')")
   enddo!i
   write(iP,"('')");                                                       return
End Subroutine PrintA
!-------------------------------------------------------------------------------7-9

Subroutine SelectStepMult(iP)
!2018.10.03.1630cdt JMS- Rescales Pr.Pstep(4,1) to reduce Zr.Zbase error.
!                     & reports Pr.Pstep(4,2) = Pr.Pstep(4,1) * X(32)
!            Pr.Pnew = Pr.Pbase + Pr.Pstep(4,2)
!                     - X(32) is the multiplier with the smallest RSS Z error
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                   globals
 use Tweakrec,only:                          cDateTime & !Tweak's FYI
                            ,jpD             ,cFloat40 & !Printout-Alphanumeric
```

```
                                      ,jDone                & !Iteration control
                     ,RSS,RSSbase                           & !Tweaking & errors
                     ,jMintot,jMin,StepMult,omj               !Minimization passes
   Use KPrec,    only: Kptot,Kp,Kp2,   Pr      ,PstepMag     !Parameters -to fit to-
   Use LZrec,    only: Lztot,Lz,       Zr                    !Outputs    - of your -
   use MDrec,    only: Mdtot,Md                              !Dataset
   !---
   implicit none                                                          !arguments
    integer*4::iP
    !--                                                                    internals
    real*16,parameter:: Del =1.e-3_16 !Hard coded.
    real*16  :: X( 32)
    real*16  :: Z( 31)
    real*16  :: C(1:3,0:2)
    real*16  :: Delta
    real*16  :: Discrim
    integer*4:: i, iQ, k, nX, nX0, nXT
 ! real*16  :: Da
    real*16  :: B0,B1,S0,S1,S2,X0,X1,Z0,Z1
    character:: om*9
     !-----                                                              !end defs
     X( 1) =  -.1_16
     X( 2) =   .0_16
     X( 3) =          +Del
     X( 4) =          +Del*2._16
     X( 5) =   .1_16
     X( 6) =   .2_16
     X( 7) =   .3_16
     X( 8) =   .4_16
     X( 9) =   .5_16
     X(10) =   .6_16
     X(11) =   .7_16
     X(12) =   .8_16
     X(13) =   .9_16
     X(14) =  1.0_16
     X(15) =  1.0_16  +Del
     X(16) =  1.0_16  +Del*2._16
     X(17) =  1.1_16
     nX0    = 17 ! X( 1:17) are  canned  multipliers of Pr.Pstep(4,1)
     nXT    = 31 ! X(18:31) are computed multipliers of Pr.Pstep(4,1)
 !             ! x( 32  ) is the multiplier used.

     do jMin = 1,jMintot
       Delta = 2._16**(jMin-1)
       if(iP.gt.0) write(iP,"('SelectStepMult minimization pass',i3,':')") jMin
       jDone = 0
       X(nX0+1:nXT+1) = 0._16
       Z              = 0._16
       C              = 0._16

       do i =1,nX0
         Pr.P = Pr.Pbase+X(i)*Pr.Pstep(4,1)/Delta; call EvalFit(Z(i), 0)
       enddo!i

 !     The following two inverse quadratic matrix solvers are exact:
 !     Quadratic at StepMult = 0._16, Del=.001_16,  AbsDet = 2.e-9 exactly.
       C(1,0) = + 500000._16*Z( 2) -1000000._16*Z( 3) +500000._16*Z( 4) !A0
       C(2,0) = -   1500._16*Z( 2) +   2000._16*Z( 3) -   500._16*Z( 4) !B0
       C(3,0) = +            Z( 2)                                      !C0
 !     Quadratic at StepMult = 1._16, Del=.001_16,  AbsDet = 2.e-9 exactly.
       C(1,1) = + 500000._16*Z(14) -1000000._16*Z(15) +500000._16*Z(16) !A1
       C(2,1) = -1001500._16*Z(14) +2002000._16*Z(15)-1000500._16*Z(16) !B1
       C(3,1) = + 501501._16*Z(14) -1002000._16*Z(15) +500500._16*Z(16) !C1
 !     Pass  1 of  40           om =  -26e.713          2018.10.03 14:25:27:750
 !     RSS =    0.000001584256005357190219467317 2E-20 X(30) V intersect
 !                        ^
 !     In a linear testcase, less roundoff error did not result from using:
 !     C(1,0) = (              Z( 2) -2.000_16*Z( 3)          +Z( 4) ) * 5.e5_16
 !     C(2,0) = ( -3.000000_16*Z( 2) +4.000_16*Z( 3)          -Z( 4) ) * 5.e2_16
 !     C(3,0) =                Z( 2)
```

```
!     C(1,1) = (   .500000_16*Z(14) -1.000_16*Z(15)  +.5000_16*Z(16) ) * 1.e6_16
!     C(2,1) = ( -1.001500_16*Z(14) +2.002_16*Z(15) -1.0005_16*Z(16) ) * 1.e6_16
!     C(3,1) = (  +.501501_16*Z(14) -1.002_16*Z(15)  +.5005_16*Z(16) ) * 1.e6_16
!     Pass  1 of  40             om =  -26e.713          2018.10.03 15:57:36:781
!     RSS =    0.000001584412508105244183944676OE-20 X(30) V intersect
!                      ^

!     Quadratic difference
      C(1:3,2) = C(1:3,1) - C(1:3,0)

      if(iP > 5) then
        write(iP,"(5x,'A',23x,'B',23x,'C')")
        do iQ=0,2
          write(iP,"(3e24.15\)") C(1:3,iQ)
          if(iQ == 0) write(iP,"(' @0.')")
          if(iQ == 1) write(iP,"(' @1.')")
          if(iQ == 2) write(iP,"(' dif')")
        enddo!iQ
      endif!iP>5

      do iQ=0,2; nX = nX0 + 4 * iQ
        if(abs(C(1,iQ)) > 1.e-28) then !Quadratic
          Discrim = C(2,iQ)*C(2,iQ) - 4._16*C(1,iQ)*C(3,iQ) != B*B - 4.*A*C
          if(Discrim >= 0._16) then
            X(nX+1)= (-C(2,iQ) -sqrt(Discrim)) / (2._16*C(1,iQ))
            X(nX+3)= (-C(2,iQ) +sqrt(Discrim)) / (2._16*C(1,iQ))
          endif!Discrim>=0.
          if(C(1,iQ) /= 0._16) &
            X(nX+2) =       -C(2,iQ)                / (2._16*C(1,iQ))
         elseif(abs(C(2,iQ)) > 1.e-18) then
            X(nX+4) =       -C(3,iQ)                / (2._16*C(2,iQ))
        endif!C(1,iQ)  not zero
      enddo!iQ

!     V Intersect: (Uses the slopes computed by the quadratic solvers.)
      X0 = X( 2); S0 =                C(2,0); Z0 = Z( 2); B0 = Z0-X0*S0
      X1 = X(14); S1 = 2._16*C(1,1) + C(2,1); Z1 = Z(14); B1 = Z1-X1*S1
                  S2 =                        Z1 - Z0
!     Error = 0. Intersect:
      if((S1-S0) /= 0._16) X(30) = (B0-B1)/(S1-S0)
      if(  S2    /= 0._16) X(31) =   -Z0  /  S2

      if(iP > 5)  &
        write(iP,"(' #',5x,'Xnom',3x,'X(#)used',11x,'om',8x,'Z(#)error')")

      do i = 1,nXT
        if(iP > 5) write(iP,"(i2,1x,f8.3\)") i,dble(X(i))
        if(X(i) < -2.0_16) X(i) = -2.0_16
        if(X(i) > +2.0_16) X(i) = +2.0_16
        if(iP > 5) write(iP,"(f19.15\)") dble(X(i))
        if((i > nX0) .and.(abs(X(i)) > 0._16)) then
          Pr.P = Pr.Pbase+X(i)*Pr.Pstep(4,1)*Delta; call EvalFit(Z(i), 0)
        endif !i>nX
        if(iP > 5) then
            write(iP,"(a9\)") om(Z(i),RSSbase,0)

            call FloatWrite(Z(i),cFloat40)
            write(iP,"(a40)")    cFloat40

          select case(i)
           case(17); write(iP,*) "M=0. Poly"
           case(21); write(iP,*) "M=1. Poly"
            case(25); write(iP,*) "Diff.Poly"
           case(29); write(iP,*) "V Intersect"
           case(30); write(iP,*) "0.Intersect"
           case(31); write(iP,*) "Using:"
          end select !(i)
        endif !iP>5
      enddo!i
                                                  K=2
```

```
      do i = 1,nXT; if(i == 2) cycle
        if( (X(i) /= 0._16) .and. (Z(i) < Z(K)) ) K=i
      enddo!i
      X(32)    = X(k)
      StepMult = X(k)
      if(K == 2) jDone=1
      Pr.P           = Pr.Pbase + StepMult * Pr.Pstep(4,1)
      Pr.Pstep(4,2) =           + StepMult * Pr.Pstep(4,1)

      if(iP > 5) then
                       call FloatWrite(Z(K),cFloat40)
        write(iP,"(i2,9x,f19.15,a9,a40)")  &
                       K,X(K),om(Z(k),RSSbase,0),cFloat40
      endif!(iP>5)

      call EvalFit(RSS, 0)
      omj     = om(Z(k),RSSbase,0)
      Pr.Pnew = Pr.P

      if(K == 3) jDone=1;                                        if(k.gt.1) return
    enddo!jMin
    if(iP > 5) write(iP,"(1x/1x,'lower value of error not found.')");     return
End Subroutine SelectStepMult
!-------------------------------------------------------------------------------7-9
!Example X() values & om values solving Non-Linear Equation: Z=P1*X**P2
!                                  Set jpD=6 to printout this level of detail.
!            ... in this case V-intersect prevailed.

!SelectStepMult minimization pass  1:
!     A                        B                          C
!  -0.414516409594126E-01  -0.140501747823906E+01   0.140504987721336E+01 @0.
!   0.251661992428589E+01  -0.400476300816663E+01   0.195385476930220E+01 @1.
!   0.255807156524530E+01  -0.259974552992757E+01   0.548804892088839E+00 dif
! #     Xnom   X(#)used           om        Z(#)error
! 1    -0.100 -0.100000000000000  +1e.110  1.5451410593139114173282020766252800O
! 2     0.000  0.000000000000000  +1e.1    1.4050498772133646065121277301300300O
! 3     0.001  0.001000000000000  -0e.999  1.4036448182834845885967105958510300O
! 4     0.002  0.002000000000000  -0e.998  1.4022396764503226518561097885710800O
! 5     0.100  0.100000000000000  -0e.900  1.2641461157081127273503992445912110O
! 6     0.200  0.200000000000000  -0e.799  1.1225788324186468638803782773072600O
! 7     0.300  0.300000000000000  -0e.698  0.9808450081609988255292976425840030O
! 8     0.400  0.400000000000000  -0e.598  0.8400720772840563839458885524557304O
! 9     0.500  0.500000000000000  -0e.500  0.7026285251787715898603658678030620O
!10     0.600  0.600000000000000  -0e.408  0.5735176209024664671446512138419972O
!11     0.700  0.700000000000000  -0e.330  0.4635024730286748764969311925521300O
!12     0.800  0.800000000000000  -0e.280  0.3940172736813381685290744558771421O
!13     0.900  0.900000000000000  -0e.280  0.3929328189916826723018731587198220O
!14     1.000  1.000000000000000  -0e.331  0.4657116854214696117286979443371740O
!15     1.001  1.001000000000000  -0e.332  0.4667426788817990550917540585193934O
!16     1.002  1.002000000000000  -0e.333  0.4677787055819770702386269127277800O
!17     1.100  1.100000000000000  -0e.420  0.5896640651707571184195240775714490O
! M=0. Poly
!18     0.972  0.972141384261836  -0e.313  0.4391266939182541564119166581793550O
!19   -16.948 -2.000000000000000  +1e.322  4.5259939488746612435225705705220920O
!20   -34.867 -2.000000000000000  +1e.322  4.5259939488746612435225705705220920O
!21     0.000  0.000000000000000  - e.000  0.0000000000000000000000000000000E+00
! M=1. Poly
!22     0.000  0.000000000000000  - e.000  0.0000000000000000000000000000000E+00
!23     0.796  0.795663057722752  -0e.282  0.3957869673186825493221965980317773O
!24     0.000  0.000000000000000  - e.000  0.0000000000000000000000000000000E+00
!25     0.000  0.000000000000000  - e.000  0.0000000000000000000000000000000E+00
! Diff.Poly
!26     0.299  0.299163738467439  -0e.699  0.9820284821706654251010188928374064O
!27     0.508  0.508145582251970  -0e.492  0.6917039006079792815011268119149143O
!28     0.717  0.717127426036501  -0e.319  0.4479385526210309218718649088359733O
!29     0.000  0.000000000000000  - e.000  0.0000000000000000000000000000000E+00
! V Intersect
!30     0.809  0.808637610994461  -0e.278  0.3908902091673827930728067940846300O
! 0.Intersect
!31     1.496  1.495787022704859  -0e.913  1.2823551405605819574004272065162240O
```

```
 1051 ! Using:
 1052 !30           0.808637610994461  -0e.278  0.39089020916738279307280679408463000
 1053
 1054 !Pass  5 of  40            om =   -0e.278               2018.10.03 13:59:49:906
 1055 !RSS =    0.39089020916738279307280679408463000  0.390890E+00 / 1
 1056 !Lz#                Residual Error                Change        weight
 1057 !    1    0.39089020916738279307280679408463000      -1.01415967    1.000000000
 1058 !----- ----.12345678901234567890123456789012345
 1059 !     *:unchanged    1         2         3        -Floats decimal place counter
 1060
 1061 !Kp#                     Value                     Change         delta
 1062 !    1    3.0644781163677558959170486544163910O      0.13343492    0.000001000
 1063 !    2    2.2046961983250071880359627235936120O     -0.02030151    0.000001000
 1064 !----- ----.12345678901234567890123456789012345
 1065 !     *:unchanged    1         2         3        -Floats decimal place counter
 1066
 1067 !Non-Linear Equation: Z=P1*X**P2 :
 1068 !om results, by iteration, were:                          Elapsed time: ~.07sec
 1069 !Pass  0 of  40           om = undefined               2018.10.03 13:59:49:890
 1070 !Pass  1 of  40           om =   -0e.995  RSS X(19)    2018.10.03 13:59:49:890
 1071 !Pass  2 of  40           om =   -0e.555  RSS X(18)    2018.10.03 13:59:49:906
 1072 !Pass  3 of  40           om =   -0e.115  RSS X(18)    2018.10.03 13:59:49:906
 1073 !Pass  4 of  40           om =   -1e.719      X(18)    2018.10.03 13:59:49:906
 1074 !Pass  5 of  40           om =   -0e.278      X(30)    2018.10.03 13:59:49:906
 1075 !Pass  6 of  40           om =   -1e.385      X(18)    2018.10.03 13:59:49:921
 1076 !Pass  7 of  40           om =   -2e.129      X(18)    2018.10.03 13:59:49:921
 1077 !Pass  8 of  40           om =   -5e.556      X(18)    2018.10.03 13:59:49:921
 1078 !Pass  9 of  40           om =   -7e.707      X(18)    2018.10.03 13:59:49:937
 1079 !Pass 10 of  40           om =  -11e.388      X(31)    2018.10.03 13:59:49:937
 1080 !                            =  -11e.370  for X(14): BtBinv*BtZ was a contender
 1081 !Pass 11 of  40           om =   -0e.394      X(13)    2018.10.03 13:59:49:937
 1082 !Pass 12 of  40           om =   -0e.768      X(17)    2018.10.03 13:59:49:953
 1083 !Pass 13 of  40           om =   -0e.891      X(30)    2018.10.03 13:59:49:953
 1084 !Pass 14 of  40           om =   -0e.370      X( 2)    2018.10.03 13:59:49:953
 1085 !Pass 15 of  40           om =   +1e.1                 2018.10.03 13:59:49:953
 1086 !RSS =    0.00000000029516472331573768861320E-20 0.295165E-29 / 1
 1087 !Lz#                Residual Error                Change        weight
 1088 !    1*   0.00000000029516472331573768861320E-20 0.0000000000E+00    1.000000000
 1089 !----- ----.12345678901234567890123456789012345
 1090 !     *:unchanged    1         2         3        -Floats decimal place counter
 1091
 1092 !Kp#                     Value                     Change         delta
 1093 !    1*   3.1000000000000000000000000000002000 0.0000000000E+00  0.1000000E-27
 1094 !    2*   2.2000000009999999999999999999995300 0.0000000000E+00  0.1000000E-27
 1095 !----- ----.12345678901234567890123456789012345
 1096 !     *:unchanged    1         2         3        -Floats decimal place counter
 1097
 1098 !Solving Linear Equation: log10(Z) = log10(P1)+log10(P2)*X :
 1099 !om results, by iteration, were:                           Elapsed time: ~.015sec
 1100 !Pass  0 of  40           om = undefined               2018.10.03 14:25:27:734
 1101 !Pass  1 of  40           om =  -26e.713 /1.4e26  X(30) 2018.10.03 14:25:27:750
 1102 !Pass  2 of  40           om =   -5e.170 /590000. X(14) 2018.10.03 14:25:27:750
 1103 !Pass  3 of  40           om =   -0e.957 /1.04    X(12) 2018.10.03 14:25:27:750
 1104 !Pass  4 of  40           om =   -0e.997          X(12) 2018.10.03 14:25:27:765
 1105 !Pass  5 of  40           om =   +1e.1                  2018.10.03 14:25:27:765
 1106 !                                                    ^: best X multiplier
 1107 !Numerical roundoff errors degrade locating analytical minima at the extreme
 1108 !  lower end. In this example, multiplier X(12) = .8 prevailed.
 1109
 1110 !In pass 1 the V Intersect edged out the Inverter solution by a factor of 2,
 1111 !  but X(14) = 1.0 produced om = -25e.144, and V Intersect was operating solely
 1112 !  along the Inverter's Pr(1:2).Pstep(2,1) direction.
 1113 !  The direction was about +77.4 degrees (CW)  for a distance of ~ 2.254e0.
 1114 !RSS =    0.00000158425600535719021946731720E-20  X(30)
 1115
 1116 !To get the pass 2 om = -5e.170,
 1117 !  the direction was about -49.4 (CCW) degrees for a distance of ~ .85e-25.
 1118 !RSS =    0.00000000002686378879975318568600E-20  X(14)
 1119
 1120 !X(12)'s two poke-&-hopes in iterations 3 & 4 yielded a minor improvement:
```

```
!RSS =    0.00000000000257078103911025839 98E-20  X(12)
!The granularity of the least significant bits is evident.

!The Fortran environment being use here is 32-bit, so real*16's are 128 bits.
!Using a 64 bit environment with 256-bit quad precision reals will improve the
!potential accuracy of these  results by an additional om ~= -32e.100

!Real measurements are usually noisy, with noise floors far above om = -18e.100

!-------------------------------------------------------------------------------7-9

Function om(Value1,Value0,iP)
!2018.10.03.1245cdt JMS- My "Order of Magnitude" scale.
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
!The objective: to quickly grasp large numeric order-of-magnitude changes.

!om   = Function omScale(Value1,Value0,iP)
!Expresses the value1/Value0 ratio of positive numbers in exponential form, &
! places the signed exponent on the left side of the result.
!Exponents > 0 represent ratios >= 1.
!Exponents <=0 represent ratios <  1.
!1. > mantissa >= .1, except when Value1 = 0.
!                          (Actual arguments are "_16" quad-precision values.)
!Examples:    Value1    Value0  = Value1/Value0  = om character expression
! omScale(    6.5   ,   4.32 ,_) = .150462963e+1  = "  +1e.150"
! omScale(    6.5   ,  43.2  ,_) = .150462963e+0  = "  -0e.150"
! omScale(    6.5e5 ,  43.2e1,_) = .150462963e+4  = "  +4e.150"
! omScale(   43.2e1 ,   6.5e5,_) = .664615e-3     = "  -3e.665"
! omScale(   43.2   ,   6.5  ,_) = .664615e+1     = "  +1e.665"
! omScale(    6.5e12,  43.2e1,_) = .150462963e+11 = " +11e.150"
!                                                  "__sme.nnn" <-9 characters
!                                                  "_smme.nnn"   "
!Special cases:                                    "__s_e.***"   "
! omScale(    6.5   ,   6.5  ,_) = .100000e+1     = "  +1e.1  "  equal
! omScale(   -6.5   ,   4.32 ,_) = .100000e+1     = "    e.err"  outside range
! omScale(    0.0   ,   0.0  ,_) = .000000e+0     = "    e.nul"  both zero
! omScale(    0.0   ,   4.32 ,_) = .000000e+0     = "  - e.000"  Value1=0.
! omScale(    6.5   ,   0.0  ,_) = .000000e+0     = "  + e.inf"  Value0=0.
 !---                                                          No globals
 implicit none                                                 !arguments
  real*16  :: Value1  !Value- ending/current                         >0.
  real*16  :: Value0  !     - beginning/reference/previous           >0.
  character:: om*9    !     - Value1/Value0 measured in omScale units.
  integer*4:: iP
  !---                                                         !internals
  real*16  :: Ratio
  integer*4:: eFactor
  real*16  :: Mantissa
   !-----                                                      !end defs
   if((Value1 > 0._16).and.(Value0 > 0._16)) then
     Ratio    = Value1/value0
     eFactor  = floor(log10(Ratio)+1.e-30) + 1
     Mantissa = Ratio/(10._16**eFactor)
     if(Mantissa > .999_16) Mantissa = .999_16
     if(eFactor > 9) then
       write(om,"(' +' ,i2,'e',SS,f4.3)") efactor,Mantissa
      elseif(eFactor > 0) then
       write(om,"('  +' ,i1,'e',SS,f4.3)") efactor,Mantissa
      elseif(eFactor > -10) then
       write(om,"('  -' ,i1,'e',SS,f4.3)") abs(efactor),Mantissa
      else
       write(om,"(' -' ,i2,'e',SS,f4.3)") abs(efactor),Mantissa
     endif!eFactor>9
     if(abs((Value1-Value0)/Value0) <1.e-28_16 )  om= "  +1e.1  ";goto 10
   endif! Value1>0. & Value0>0.
   if((Value1 <0._16).or. (Value1 =="NAN")) then; om= "    e.err";goto 10;endif
   if((Value0 <0._16).or. (Value0 =="NAN")) then; om= "    e.err";goto 10;endif
   if((Value1==0._16).and.(Value0 ==0._16)) then; om= "    e.nul";goto 10;endif
   if(Value1 ==0._16)                       then; om= "  - e.000";goto 10;endif
   if(Value0 ==0._16)                       then; om= "  + e.inf";goto 10;endif
```

```
!  Conversion error:
                                                    om= "  + e.unk"
10 continue                                           ;         if(iP < 6) return
   write(iP,"(/a9,' = omScale(',e20.12,',',e20.12,',', i2,')')") &
              om                ,Value1,   Value0 ,   iP
   write(iP,"(20x,e20.12,i5,e20.12/)") Ratio,eFactor,Mantissa
                                                                          return
End Function om
!-------------------------------------------------------------------------------7-9

Subroutine FloatWrite(R16In,a40out)
!2013.10.23.1300cdt JMS- converts r16's to a 41-character-float string.
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                  No globals
 implicit none                                                        !arguments
  real*16  ::R16In
  character::a40out*40
  !---                                                                !internals
  real*16  ::Real16InL
   !---
   Real16InL=R16In
   if(      abs(R16In).gt. 1.e30_16) then; write(a40out,"(e40.32   )") R16In
     elseif(abs(R16In).gt. 1.e20_16) then; write(a40out,"(f40.12   )") R16In
     elseif(abs(R16In).gt. 1.e10_16) then; write(a40out,"(f40.21   )") R16In
     elseif(abs(R16In).gt.999.e0_16) then; write(a40out,"(f40.29   )") R16In
     elseif(abs(R16In).gt.1.e-10_16) then
                          write(a40out,"(f40.32       )")               R16In
     elseif(abs(R16In).gt.1.e-20_16) then
                          write(a40out,"(f36.31,'E-10')") Real16InL*10._16**10
     elseif(abs(R16In).gt.1.e-30_16) then
                          write(a40out,"(f36.31,'E-20')") Real16InL*10._16**20
     elseif(abs(R16In).gt.1.e-40_16) then
                          write(a40out,"(f36.31,'E-30')") Real16InL*10._16**30
     else                                ; write(a40out,"(e40.31   )") R16In
   endif!
   return
End Subroutine FloatWrite
!-------------------------------------------------------------------------------7-9

Subroutine FDate23(DaTime)                                !Year Mo D  Hr Mn Sec~ms
 !A snapshot of the computers current date & time:      2018.09.20 06:12:20:390
 !-----
 implicit none                                                        !arguments
  character::DaTime*23
 !integer*4::i,iDMY(3),iHMS(3)
  integer*4::MyValues(8)
 !----------
  !call iDate(iDMY)
  !call iTime(iHMS)
   call DATE_AND_TIME(Values=MyValues)
  !write(DaTime,"(i4,'.',i2.2,'.',i2.2,'.',i2.2,i2.2'.',i2.2,' L')")  &
  !             (iDMY(i),i=3,1,-1)       ,(iHMS(i),i=1,3),0
  !write(DaTime,"(i4,'.',i2.2,'.',i2.2,'.',i2.2,i2.2,':',i2.2,':',i3.3)")  &
   write(DaTime,"(i4,'.',i2.2,'.',i2.2,' ',i2.2,':',i2.2,':',i2.2,':',i3.3)")&
                 MyValues(1:3)           ,MyValues(5:8)                ;return
End Subroutine Fdate23
!-------------------------------------------------------------------------------7 9

Subroutine Beamer(n,nTot)
!2018.08.27.1155cdt JMS- DOS screen iteration-progress bar (2% increments)
!                          -&- cumulative time predictor (seconds) .
!                     - Traveler2/Athlon64/WinXPPro-32/APF9.0-32
 !---                                                                  No globals
 implicit none                                                        !arguments
  integer*4::n
  integer*4::nTot
  !---                                                                !internals
  integer*4::Init=0
  real*4   ::dT,tarray(2),dTime
  integer*4::nm
```

```
 1261    !-----                                                                !end defs
 1262    if(    n       ==    1) then; write(6,"('Beamer '\)"); dT=dtime(tarray)
 1263                                   nm=nTot/50; if(nm==0) nm =1      ;return;endif
 1264    if(    n       == nTot) then; write(6,"(' done.' )")                  ;endif
 1265    if(mod(n,nm)   /=    1)                                          return
 1266    if(    n/nm    ==    1) then;                                dT=dtime(tarray)
 1267                                   write(6,"(f9.2,'sec.'\)") dT*50.d0      ;endif
 1268    if(mod(n,nm*5) ==    1) then; write(6,"('*'\)")                      ;return;endif
 1269                                   write(6,"(':'\)")                      ;return
 1270 End Subroutine Beamer
 1271 !-------------------------------------------------------------------------------7-9
 1272
```