

Chapter B17. Two Point Boundary Value Problems

```
! FUNCTION shoot(v) is named "funcv" for use with "newt"
FUNCTION funcv(v)
USE nrtype
USE nr, ONLY : odeint,rkqs
USE sphoot_caller, ONLY : nvar,x1,x2; USE ode_path, ONLY : xp,yp
IMPLICIT NONE
REAL(SP), DIMENSION(:,), INTENT(IN) :: v
REAL(SP), DIMENSION(size(v)) :: funcv
REAL(SP), PARAMETER :: EPS=1.0e-6_sp
      Routine for use with newt to solve a two point boundary value problem for  $N$  coupled
      ODEs by shooting from  $x_1$  to  $x_2$ . Initial values for the ODEs at  $x_1$  are generated from
      the  $n_2$  input coefficients  $v$ , using the user-supplied routine load. The routine integrates
      the ODEs to  $x_2$  using the Runge-Kutta method with tolerance EPS, initial stepsize  $h_1$ ,
      and minimum stepsize  $h_{\min}$ . At  $x_2$  it calls the user-supplied subroutine score to evaluate
      the  $n_2$  functions funcv that ought to be zero to satisfy the boundary conditions at  $x_2$ .
      The functions funcv are returned on output. newt uses a globally convergent Newton's
      method to adjust the values of  $v$  until the functions funcv are zero. The user-supplied
      subroutine derivs(x,y,dydx) supplies derivative information to the ODE integrator (see
      Chapter 16). The module sphoot_caller receives its values from the main program so
      that funcv can have the syntax required by newt. Set nvar =  $N$  in the main program.
REAL(SP) :: h1,hmin
REAL(SP), DIMENSION(nvar) :: y
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:,), INTENT(IN) :: y
    REAL(SP), DIMENSION(:,), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
  SUBROUTINE load(x1,v,y)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x1
    REAL(SP), DIMENSION(:,), INTENT(IN) :: v
    REAL(SP), DIMENSION(:,), INTENT(OUT) :: y
  END SUBROUTINE load
  SUBROUTINE score(x2,y,f)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x2
    REAL(SP), DIMENSION(:,), INTENT(IN) :: y
    REAL(SP), DIMENSION(:,), INTENT(OUT) :: f
  END SUBROUTINE score
END INTERFACE
h1=(x2-x1)/100.0_sp
```

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```

hmin=0.0
call load(x1,v,y)
if (associated(xp)) deallocate(xp,yp)      Prevent memory leak if save_steps set
call odeint(y,x1,x2,EPS,h1,hmin,derivs,rkqs)   to .true.
call score(x2,y,funcv)
END FUNCTION funcv

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!  FUNCTION shootf(v) is named "funcv" for use with "newt"
FUNCTION funcv(v)
USE nrtype
USE nr, ONLY : odeint,rkqs
USE sphfpt_caller, ONLY : x1,x2,xf,nn2; USE ode_path, ONLY : xp,yp
IMPLICIT NONE
REAL(SP), DIMENSION(:, INTENT(IN) :: v
REAL(SP), DIMENSION(size(v)) :: funcv
REAL(SP), PARAMETER :: EPS=1.0e-6_sp
      Routine for use with newt to solve a two point boundary value problem for  $N$  coupled
      ODEs by shooting from  $x_1$  and  $x_2$  to a fitting point  $xf$ . Initial values for the ODEs at
       $x_1$  ( $x_2$ ) are generated from the  $n_2$  ( $n_1$ ) coefficients  $V_1$  ( $V_2$ ), using the user-supplied
      routine load1 (load2). The coefficients  $V_1$  and  $V_2$  should be stored in a single ar-
      ray  $v$  of length  $N$  in the main program, and referenced by pointers as  $v1=>v(1:n_2)$ ,
 $v2=>v(n_2+1:N)$ . Here  $N = n_1 + n_2$ . The routine integrates the ODEs to  $xf$  using
      the Runge-Kutta method with tolerance EPS, initial stepsize  $h_1$ , and minimum stepsize
       $hmin$ . At  $xf$  it calls the user-supplied subroutine score to evaluate the  $N$  functions  $f_1$ 
      and  $f_2$  that ought to match at  $xf$ . The differences funcv are returned on output. newt
      uses a globally convergent Newton's method to adjust the values of  $v$  until the functions
      funcv are zero. The user-supplied subroutine derivs( $x,y,dydx$ ) supplies derivative in-
      formation to the ODE integrator (see Chapter 16). The module sphfpt_caller receives
      its values from the main program so that funcv can have the syntax required by newt.
      Set nn2 =  $n_2$  in the main program.
REAL(SP) :: h1,hmin
REAL(SP), DIMENSION(size(v)) :: f1,f2,y
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:, INTENT(IN) :: y
    REAL(SP), DIMENSION(:, INTENT(OUT) :: dydx
  END SUBROUTINE derivs

  SUBROUTINE load1(x1,v1,y)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x1
    REAL(SP), DIMENSION(:, INTENT(IN) :: v1
    REAL(SP), DIMENSION(:, INTENT(OUT) :: y
  END SUBROUTINE load1

  SUBROUTINE load2(x2,v2,y)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x2
    REAL(SP), DIMENSION(:, INTENT(IN) :: v2
    REAL(SP), DIMENSION(:, INTENT(OUT) :: y
  END SUBROUTINE load2

  SUBROUTINE score(x2,y,f)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x2
    REAL(SP), DIMENSION(:, INTENT(IN) :: y

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REAL(SP), DIMENSION(:, ), INTENT(OUT) :: f
END SUBROUTINE score
END INTERFACE
h1=(x2-x1)/100.0_sp
hmin=0.0
call load1(x1,v,y)                                     Path from x1 to xf with best trial values  $V_1$ .
if (associated(xp)) deallocate(xp,yp)                 Prevent memory leak if save_steps set
call odeint(y,x1,xf,EPS,h1,hmin,derivs,rkqs)        to .true.
call score(xf,y,f1)
call load2(x2,v(nn2+1:),y)                           Path from x2 to xf with best trial values  $V_2$ .
call odeint(y,x2,xf,EPS,h1,hmin,derivs,rkqs)
call score(xf,y,f2)
funcv(:)=f1(:)-f2(:)
END FUNCTION funcv

      *      *      *

SUBROUTINE solvde(itmax,conv,slowc,scalv,indexv,nb,y)
USE nrtype; USE nrutil, ONLY : assert_eq,imaxloc,nrerror
USE nr, ONLY : difeq
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: itmax,nb
REAL(SP), INTENT(IN) :: conv,slowc
REAL(SP), DIMENSION(:, ), INTENT(IN) :: scalv
INTEGER(I4B), DIMENSION(:, ), INTENT(IN) :: indexv
REAL(SP), DIMENSION(:, :, ), INTENT(INOUT) :: y
Driver routine for solution of two point boundary value problems with  $N$  equations by
relaxation.  $itmax$  is the maximum number of iterations.  $conv$  is the convergence criterion
(see text).  $slowc$  controls the fraction of corrections actually used after each iteration.
 $scalv$ , a vector of length  $N$ , contains typical sizes for each dependent variable, used to
weight errors.  $indexv$ , also of length  $N$ , lists the column ordering of variables used to
construct the matrix  $s$  of derivatives. (The  $nb$  boundary conditions at the first mesh point
must contain some dependence on the first  $nb$  variables listed in  $indexv$ .) There are a total
of  $M$  mesh points.  $y$  is the  $N \times M$  array that contains the initial guess for all the dependent
variables at each mesh point. On each iteration, it is updated by the calculated correction.
INTEGER(I4B) :: ic1,ic2,ic3,ic4,it,j,j1,j2,j3,j4,j5,j6,j7,j8,&
j9,jc1,jcf,jv,k,k1,k2,km,kp,m,ne,nvars
INTEGER(I4B), DIMENSION(size(scalv)) :: kmax
REAL(SP) :: err,fac
REAL(SP), DIMENSION(size(scalv)) :: ermax
REAL(SP), DIMENSION(size(scalv),2*size(scalv)+1) :: s
REAL(SP), DIMENSION(size(scalv),size(scalv)-nb+1,size(y,2)+1) :: c
ne=assert_eq(size(scalv),size(indexv),size(y,1),'solvde: ne')
m=size(y,2)
k1=1                                                 Set up row and column markers.
k2=m
nvars=ne*m
j1=1
j2=nb
j3=nb+1
j4=ne
j5=j4+j1
j6=j4+j2
j7=j4+j3
j8=j4+j4
j9=j8+j1
ic1=1
ic2=ne-nb
ic3=ic2+1
ic4=ne
jc1=1
jcf=ic3
do it=1,itmax
  k=k1
  Primary iteration loop.
  Boundary conditions at first point.

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```

call difeq(k,k1,k2,j9,ic3,ic4,indexv,s,y)
call pinvs(ic3,ic4,j5,j9,jc1,k1,c,s)
do k=k1+1,k2
  call difeq(k,k1,k2,j9,ic1,ic4,indexv,s,y)          Finite difference equations at all point
  kp=k-1                                               pairs.
  call difeq(k,k1,k2,j9,ic1,ic4,indexv,s,y)
  call red(ic1,ic4,j1,j2,j3,j4,j9,ic3,jc1,jcf,kp,c,s)
  call pinvs(ic1,ic4,j3,j9,jc1,k,c,s)
end do
k=k2+1
call difeq(k,k1,k2,j9,ic1,ic2,indexv,s,y)          Final boundary conditions.
call red(ic1,ic2,j5,j6,j7,j8,j9,ic3,jc1,jcf,k2,c,s)
call pinvs(ic1,ic2,j7,j9,jcf,k2+1,c,s)
call bksub(ne,nb,jcf,k1,k2,c)
do j=1,ne
  call bksub(ne,nb,jcf,k1,k2,c)                      Backsubstitution.
  do i=1,ne
    c(i)=c(i,j)
  end do
  call scalv(c(:),ne)                                 Convergence check, accumulate average
  km=imaxloc(abs(c(:))+1)                            error.
  km=km+1
end do
ermax(:)=ermax(:)/scalv(:)                         Weighting for each dependent variable.
err=sum(sum(abs(c(indexv(:,1:k1:k2))),dim=2)/scalv(:))/nvars
fac=slowc/max(slowc,err)
ermax(:)=ermax(:)/scalv(:)                         Reduce correction applied when error is large.
y(:,k1:k2)=y(:,k1:k2)-fac*c(indexv(:,1,k1:k2))      Apply corrections.
write(*,'(1x,i4,2f12.6)') it,err,fac
Summary of corrections for this step. Point with largest error for each variable can be
monitored by writing out kmax and ermax.
if (err < conv) RETURN
end do
call nrerror('itmax exceeded in solvde')           Convergence failed.
CONTAINS

SUBROUTINE bksub(ne,nb,jf,k1,k2,c)
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: ne,nb,jf,k1,k2
REAL(SP), DIMENSION(:, :, :), INTENT(INOUT) :: c
  Backsubstitution, used internally by solvde.
INTEGER(I4B) :: im,k,nbf
nbf=ne-nb
im=1
k=k2,k1,-1
do
  Use recurrence relations to eliminate remaining dependences.
  if (k == k1) im=nbf+1                           Special handling of first point.
  c(im:ne,jf,k)=c(im:ne,jf,k)-matmul(c(im:ne,1:nbf,k),c(1:nbf,jf,k+1))
end do
c(1:nb,1,k1:k2)=c(1+nbf:nb+nbf,jf,k1:k2)       Reorder corrections to be in column 1.
c(1+nbf:nb+nbf,1,k1:k2)=c(1:nbf,jf,k1+1:k2+1)
END SUBROUTINE bksub

SUBROUTINE pinvs(ie1,ie2,je1,jsf,jc1,k,c,s)
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: ie1,ie2,je1,jsf,jc1,k
REAL(SP), DIMENSION(:, :, :), INTENT(OUT) :: c
REAL(SP), DIMENSION(:, :, :), INTENT(INOUT) :: s
  Diagonalize the square subsection of the s matrix, and store the recursion coefficients in
  c; used internally by solvde.
INTEGER(I4B) :: i,icoff,id,ipiv,jcoff,je2,jp,jpiv,js1
INTEGER(I4B), DIMENSION(ie2) :: indxr
REAL(SP) :: big,piv,pivinv
REAL(SP), DIMENSION(ie2) :: pscl
je2=je1+ie2-je1
js1=je2+1
pscl(ie1:ie2)=maxval(abs(s(ie1:ie2,je1:je2)),dim=2)
Implicit pivoting, as in §2.1.

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if (any(pscl(ie1:ie2) == 0.0)) &
    call nrerror('singular matrix, row all 0 in pinvs')
pscl(ie1:ie2)=1.0_sp/pscl(ie1:ie2)
indxr(ie1:ie2)=0
do id=ie1,ie2
    piv=0.0
    do i=ie1,ie2
        if (indxr(i) == 0) then
            jp=imaxloc(abs(s(i,je1:je2)))+je1-1
            big=abs(s(i,jp))
            if (big*pscl(i) > piv) then
                ipiv=i
                jpiv=jp
                piv=big*pscl(i)
            end if
        end if
    end do
    if (s(ipiv,jpiv) == 0.0) call nrerror('singular matrix in pinvs')
    indxr(ipiv)=jpiv                                In place reduction. Save column order-
    pivinv=1.0_sp/s(ipiv,jpiv)                      ing.
    s(ipiv,je1:jsf)=s(ipiv,je1:jsf)*pivinv      Normalize pivot row.
    s(ipiv,jpiv)=1.0
    do i=ie1,ie2
        if (indxr(i) /= jpiv .and. s(i,jpiv) /= 0.0) then
            s(i,je1:jsf)=s(i,je1:jsf)-s(i,jpiv)*s(ipiv,je1:jsf)
            s(i,jpiv)=0.0
        end if
    end do
    end do
    jcoff=jc1-js1                                     Sort and store unreduced coefficients.
    icooff=ie1-je1
    c(indxr(ie1:ie2)+icooff,js1+jcoff:jsf+jcoff,k)=s(ie1:ie2,js1:jsf)
END SUBROUTINE pinvs

SUBROUTINE red(iz1,iz2,jz1,jz2,jm1,jm2,jmf,ic1,jc1,jcf,kc,c,s)
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: iz1,iz2,jz1,jz2,jm1,jm2,jmf,ic1,jc1,jcf,kc
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: s
REAL(SP), DIMENSION(:,:,:,:), INTENT(IN) :: c
Reduce columns jz1-jz2 of the s matrix, using previous results as stored in the c matrix.
Only columns jm1-jm2,jmf are affected by the prior results. red is used internally by
solvde.
INTEGER(I4B) :: ic,l,loff
loff=jc1-jm1
ic=ic1
do j=jz1,jz2
    do l=jm1,jm2
        s(iz1:iz2,l)=s(iz1:iz2,l)-s(iz1:iz2,j)*c(ic,l+loff,kc)
    end do
    s(iz1:iz2,jmf)=s(iz1:iz2,jmf)-s(iz1:iz2,j)*c(ic,jcf,kc)  Plus final element.
    ic=ic+1
end do
END SUBROUTINE red
END SUBROUTINE solvde

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f90 km=imaxloc... See discussion of imaxloc on p. 1017.

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MODULE sfroid_data                                Communicates with difeq.
USE nrtype
INTEGER(I4B), PARAMETER :: M=41
INTEGER(I4B) :: mm,n
REAL(SP) :: anorm,c2,h
REAL(SP), DIMENSION(M) :: x
END MODULE sfroid_data

PROGRAM sfroid
USE nrtype; USE nrutil, ONLY : arth
USE nr, ONLY : plgndr,solvde
USE sfroid_data
IMPLICIT NONE
INTEGER(I4B), PARAMETER :: NE=3,NB=1
Sample program using solvde. Computes eigenvalues of spheroidal harmonics  $S_{mn}(x; c)$ 
for  $m \geq 0$  and  $n \geq m$ . In the program,  $m$  is mm,  $c^2$  is c2, and  $\gamma$  of equation (17.4.20)
is anorm.
INTEGER(I4B) :: itmax
INTEGER(I4B), DIMENSION(NE) :: indexv
REAL(SP) :: conv,slowc
REAL(SP), DIMENSION(M) :: deriv,fac1,fac2
REAL(SP), DIMENSION(NE) :: scalv
REAL(SP), DIMENSION(NE,M) :: y
itmax=100
conv=5.0e-6_sp
slowc=1.0
h=1.0_sp/(M-1)
c2=0.0
write(*,*) 'ENTER M,N'
read(*,*) mm,n
indexv(1:3)=merge( (/ 1, 2, 3 /), (/ 2, 1, 3 /), (mod(n+mm,2) == 1) )
No interchanges necessary if n+mm is odd; otherwise interchange  $y_1$  and  $y_2$ .
anorm=1.0                                         Compute  $\gamma$ .
if (mm /= 0) then
  anorm=(-0.5_sp)**mm*product(&
    arth(n+1,1,mm)*arth(real(n,sp),-1.0_sp,mm)/arth(1,1,mm))
end if
x(1:M-1)=arth(0,1,M-1)*h
fac1(1:M-1)=1.0_sp-x(1:M-1)**2                  Compute initial guess.
fac2(1:M-1)=fac1(1:M-1)**(-mm/2.0_sp)
y(1,1:M-1)=plgndr(n,mm,x(1:M-1))*fac2(1:M-1)    $P_n^m$  from §6.8.
deriv(1:M-1)=-(n-mm+1)*plgndr(n+1,mm,x(1:M-1))-(n+1)*&
  x(1:M-1)*plgndr(n,mm,x(1:M-1))/fac1(1:M-1)
Derivative of  $P_n^m$  from a recurrence relation.
y(2,1:M-1)=mm*x(1:M-1)*y(1,1:M-1)/fac1(1:M-1)+deriv(1:M-1)*fac2(1:M-1)
y(3,1:M-1)=n*(n+1)-mm*(mm+1)
x(M)=1.0                                         Initial guess at  $x = 1$  done separately.
y(1,M)=anorm
y(3,M)=n*(n+1)-mm*(mm+1)
y(2,M)=(y(3,M)-c2)*y(1,M)/(2.0_sp*(mm+1.0_sp))
scalv(1:3)=(/ abs(anorm), max(abs(anorm),y(2,M)), max(1.0_sp,y(3,M)) /)
do
  write (*,*) 'ENTER C**2 OR 999 TO END'
  read (*,*) c2
  if (c2 == 999.0) exit
  call solvde(itmax,conv,slowc,scalv,indexv,NB,y)
  write (*,*) ' M = ',mm,' N = ',n,&
    ' C**2 = ',c2,' LAMBDA = ',y(3,1)+mm*(mm+1)
end do                                              Go back for another value of  $c^2$ .
END PROGRAM sfroid

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f90

MODULE sfroid_data This module functions just like a common block to communicate variables with difeq. The advantage of a module is that it allows complete specification of the variables.

anorm=(-0.5_sp)**mm*product(... This statement computes equation (17.4.20) by direct multiplication.

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```
SUBROUTINE difeq(k,k1,k2,jsf,is1,isf,indexv,s,y)
USE nrtype
USE sfroid_data
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: is1,isf,jsf,k,k1,k2
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indexv
REAL(SP), DIMENSION(:, :, ), INTENT(OUT) :: s
REAL(SP), DIMENSION(:, :, ), INTENT(IN) :: y
    Returns matrix s(i,j) for solvde.
REAL(SP) :: temp,temp2
INTEGER(I4B), DIMENSION(3) :: indexv3
indexv3(1:3)=3+indexv(1:3)
if (k == k1) then          Boundary condition at first point.
    if (mod(n+mm,2) == 1) then
        s(3,indexv3(1:3))= (/ 1.0_sp, 0.0_sp, 0.0_sp /)      Equation (17.4.32).
        s(3,jsf)=y(1,1)                                         Equation (17.4.31).
    else
        s(3,indexv3(1:3))= (/ 0.0_sp, 1.0_sp, 0.0_sp /)      Equation (17.4.32).
        s(3,jsf)=y(2,1)                                         Equation (17.4.31).
    end if
else if (k > k2) then      Boundary conditions at last point.
    s(1,indexv3(1:3))= (/ -(y(3,M)-c2)/(2.0_sp*(mm+1.0_sp)),&
        1.0_sp, -y(1,M)/(2.0_sp*(mm+1.0_sp)) /)           Equation (17.4.35).
    s(1,jsf)=y(2,M)-(y(3,M)-c2)*y(1,M)/(2.0_sp*(mm+1.0_sp))   Equation (17.4.33).
    s(2,indexv3(1:3))=(/ 1.0_sp, 0.0_sp, 0.0_sp /)           Equation (17.4.36).
    s(2,jsf)=y(1,M)-anorm                                    Equation (17.4.34).
else                      Interior point.
    s(1,indexv(1:3))=(/ -1.0_sp, -0.5_sp*h, 0.0_sp /)       Equation (17.4.28).
    s(1,indexv3(1:3))=(/ 1.0_sp, -0.5_sp*h, 0.0_sp /)
    temp=h/(1.0_sp-(x(k)+x(k-1))*2*0.25_sp)
    temp2=0.5_sp*(y(3,k)+y(3,k-1))-c2*0.25_sp*(x(k)+x(k-1))*2
    s(2,indexv(1:3))=(/ temp*temp2*0.5_sp,&
        -1.0_sp-0.5_sp*temp*(mm+1.0_sp)*(x(k)+x(k-1)),&
        0.25_sp*temp*(y(1,k)+y(1,k-1)) /)                  Equation (17.4.29).
    s(2,indexv3(1:3))=s(2,indexv(1:3))
    s(2,indexv3(2))=s(2,indexv3(2))+2.0_sp
    s(3,indexv(1:3))=(/ 0.0_sp, 0.0_sp, -1.0_sp /)         Equation (17.4.30).
    s(3,indexv3(1:3))=(/ 0.0_sp, 0.0_sp, 1.0_sp /)
    s(1,jsf)=y(1,k)-y(1,k-1)-0.5_sp*h*(y(2,k)+y(2,k-1))   Equation (17.4.23).
    s(2,jsf)=y(2,k)-y(2,k-1)-temp*((x(k)+x(k-1))*&
        0.5_sp*(mm+1.0_sp)*(y(2,k)+y(2,k-1))-temp2*&
        0.5_sp*(y(1,k)+y(1,k-1)))                           Equation (17.4.24).
    s(3,jsf)=y(3,k)-y(3,k-1)                                Equation (17.4.27).
end if
END SUBROUTINE difeq
```

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```

MODULE sphoot_data                                Communicates with load, score, and derivs.
USE nrtype
INTEGER(I4B) :: m,n
REAL(SP) :: c2,dx,gamma
END MODULE sphoot_data

MODULE sphoot_caller                            Communicates with shoot.
USE nrtype
INTEGER(I4B) :: nvar
REAL(SP) :: x1,x2
END MODULE sphoot_caller

PROGRAM sphoot
  Sample program using shoot. Computes eigenvalues of spheroidal harmonics  $S_{mn}(x; c)$  for
   $m \geq 0$  and  $n \geq m$ . Be sure that routine funcv for newt is provided by shoot (§17.1).
  USE nrtype; USE nrutil, ONLY : arth
  USE nr, ONLY : newt
  USE sphoot_data
  USE sphoot_caller
  IMPLICIT NONE
  INTEGER(I4B), PARAMETER :: NV=3,N2=1
  REAL(SP), DIMENSION(N2) :: v
  LOGICAL(LGT) :: check
  nvar=NV                                         Number of equations.
  dx=1.0e-4_sp                                     Avoid evaluating derivatives exactly at  $x = -1$ .
  do
    write(*,*) 'input m,n,c-squared (999 to end)'
    read(*,*) m,n,c2
    if (c2 == 999.0) exit
    if ((n < m) .or. (m < 0)) cycle
    gamma=(-0.5_sp)**m*product(&               Compute  $\gamma$  of equation (17.4.20).
      arth(n+1,1,m)*(arth(real(n,sp),-1.0_sp,m)/arth(1,1,m)))
    v(1)=n*(n+1)-m*(m+1)+c2/2.0_sp             Initial guess for eigenvalue.
    x1=-1.0_sp+dx                                Set range of integration.
    x2=0.0
    call newt(v,check)                           Find v that zeros function f in score.
    if (check) then
      write(*,*) 'shoot failed; bad initial guess'
      exit
    else
      write(*,'(1x,t6,a)') 'mu(m,n)'
      write(*,'(1x,f12.6)') v(1)
    end if
  end do
END PROGRAM sphoot

SUBROUTINE load(x1,v,y)
USE nrtype
USE sphoot_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x1
REAL(SP), DIMENSION(:), INTENT(IN) :: v
REAL(SP), DIMENSION(:), INTENT(OUT) :: y
  Supplies starting values for integration at  $x = -1 + dx$ .
  REAL(SP) :: y1
  y(3)=v(1)
  y1=merge(gamma,-gamma, mod(n-m,2) == 0 )
  y(2)=-(y(3)-c2)*y1/(2*(m+1))
  y(1)=y1+y(2)*dx
END SUBROUTINE load

```

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```
SUBROUTINE score(x2,y,f)
USE nrtype
USE sphoot_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x2
REAL(SP), DIMENSION(:), INTENT(IN) :: y
REAL(SP), DIMENSION(:), INTENT(OUT) :: f
Tests whether boundary condition at x = 0 is satisfied.
f(1)=merge(y(2),y(1), mod(n-m,2) == 0 )
END SUBROUTINE score
```

f90 MODULE sphoot_data...MODULE sphoot_caller These modules function just like common blocks to communicate variables from sphoot to the various subsidiary routines. The advantage of a module is that it allows complete specification of the variables.

```
SUBROUTINE derivs(x,y,dydx)
USE nrtype
USE sphoot_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: y
REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
Evaluates derivatives for odeint.
dydx(1)=y(2)
dydx(2)=(2.0_sp*x*(m+1.0_sp)*y(2)-(y(3)-c2*x*x)*y(1))/(1.0_sp-x*x)
dydx(3)=0.0
END SUBROUTINE derivs
```

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```
MODULE sphfpt_data
USE nrtype
INTEGER(I4B) :: m,n
REAL(SP) :: c2,dx,gamma
END MODULE sphfpt_data
```

Communicates with load1, load2, score,
and derivs.

```
MODULE sphfpt_caller
USE nrtype
INTEGER(I4B) :: nn2
REAL(SP) :: x1,x2,xf
END MODULE sphfpt_caller
```

Communicates with shootf.

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```

PROGRAM sphfpt
  Sample program using shootf. Computes eigenvalues of spheroidal harmonics  $S_{mn}(x; c)$ 
  for  $m \geq 0$  and  $n \geq m$ . Be sure that routine funcv for newt is provided by shootf (§17.2).
  The routine derivs is the same as for sphoot.
USE nrtype; USE nrutil, ONLY : arth
USE nr, ONLY : newt
USE sphfpt_data
USE sphfpt_caller
IMPLICIT NONE
INTEGER(14B), PARAMETER :: N1=2,N2=1,NTOT=N1+N2
REAL(SP), PARAMETER :: DXX=1.0e-4_sp
REAL(SP), DIMENSION(:), POINTER :: v1,v2
REAL(SP), DIMENSION(NTOT), TARGET :: v
LOGICAL(LGT) :: check
v1=>v(1:N2)
v2=>v(N2+1:NTOT)
nn2=N2
dx=DXX
do
  write(*,*) 'input m,n,c-squared (999 to end)'
  read(*,*) m,n,c2
  if (c2 == 999.0) exit
  if ((n < m) .or. (m < 0)) cycle
  gamma=(-0.5_sp)**m*product(&
    arth(n+1,1,m)*(arth(real(n,sp),-1.0_sp,m)/arth(1,1,m)))
  v1(1)=n*(n+1)-m*(m+1)+c2/2.0_sp
  v2(2)=v1(1)
  v2(1)=gamma*(1.0_sp-(v2(2)-c2)*dx/(2*(m+1)))
  x1=-1.0_sp+dx
  x2=1.0_sp-dx
  xf=0.0
  call newt(v,check)
  if (check) then
    write(*,*) 'shootf failed; bad initial guess'
    exit
  else
    write(*,'(1x,t6,a)') 'mu(m,n)'
    write(*,'(1x,f12.6)') v1(1)
  end if
end do
END PROGRAM sphfpt

```

```

SUBROUTINE load1(x1,v1,y)
USE nrtype
USE sphfpt_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x1
REAL(SP), DIMENSION(:), INTENT(IN) :: v1
REAL(SP), DIMENSION(:), INTENT(OUT) :: y
Supplies starting values for integration at  $x = -1 + dx$ .
REAL(SP) :: y1
y(3)=v1(1)
y1=merge(gamma,-gamma,mod(n-m,2) == 0)
y(2)=- (y(3)-c2)*y1/(2*(m+1))
y(1)=y1+y(2)*dx
END SUBROUTINE load1

```

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```
SUBROUTINE load2(x2,v2,y)
USE nrtype
USE sphfpt_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x2
REAL(SP), DIMENSION(:), INTENT(IN) :: v2
REAL(SP), DIMENSION(:), INTENT(OUT) :: y
      Supplies starting values for integration at  $x = 1 - dx$ .
y(3)=v2(2)
y(1)=v2(1)
y(2)=(y(3)-c2)*y(1)/(2*(m+1))
END SUBROUTINE load2
```

```
SUBROUTINE score(xf,y,f)
USE nrtype
USE sphfpt_data
IMPLICIT NONE
REAL(SP), INTENT(IN) :: xf
REAL(SP), DIMENSION(:), INTENT(IN) :: y
REAL(SP), DIMENSION(:), INTENT(OUT) :: f
      Tests whether solutions match at fitting point  $x = 0$ .
f(1:3)=y(1:3)
END SUBROUTINE score
```



MODULE sphfpt_data...MODULE sphfpt_caller These modules function just like common blocks to communicate variables from sphfpt to the various subsidiary routines. The advantage of a module is that it allows complete specification of the variables.

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