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c=====
c      bisect: Uses bisection to find approximate root
c      of f(x) on interval [xmin .. xmax].  Return value is
c      root located to (relative) tolerance 'xtol'.  Return code
c      'rc' is set to 0 on success, non-zero on failure
c      and routine succeeds (by definition) as long as initial
c      interval *does* bracket at least one root.  Routine
c      performs tracing of algorithm (on stderr) if input
c      argument 'trace' is .true.
c=====

real*8 function bisect(f,xmin,xmax,xtol,trace,rc)

implicit none

real*8      drelabs

real*8      f
external      f

real*8      xmin,           xmax,           xtol
logical      trace
integer      rc

c-----
c      Other variables needed for search.
c-----

integer      mxiter
parameter ( mxiter = 50 )

real*8      xlo,           dx,           sfxmid,
&              sgn
integer      iter

```

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c-----
c      Check that input interval is specified correctly
c      and that it manifestly brackets at least one root:
c      (i.e. the fcn changes sign).
c-----

      if( xmax .le. xmin .or.
      &      f(xmin) * f(xmax) .gt. 0.0d0 ) then
          write(0,*) 'bisect: Input interval is not '//
          &                  'bracketing'
          rc = 1

c-----
c      Returned value is meaningless in this case,
c      but have to return *some* value.
c-----

      bisect = xmin
      return
      end if

c-----
c      Compute 'sgn' such that sgn * f(xmin) < 0, and
c      initialize bracketing interval
c-----

      sgn = 1.0d0
      if( f(xmin) .le. 0.0d0 ) then
          sgn = 1.0d0
      else
          sgn = -1.0d0
      end if
      xlo = xmin
      dx   = xmax - xmin

```

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c-----
c      Bisection loop: continue until root found to
c      specified tolerance or until maximum number of
c      iterations taken
c-----
do iter = 1 , mxiter
    bisect = xlo + 0.5d0 * dx
    if( trace ) then
        write(0,*) xlo, xlo + dx, f(bisect)
    end if
    if( sgn * f(bisect) .lt. 0.0d0 ) then
        xlo = bisect
    end if
    if( drelabs(dx,bisect,1.0d-10) .le. xtol ) go to 900
    dx = 0.5d0 * dx
end do

900    continue
rc = 0
if( trace ) write(0,*)
return

end

```

```
c=====
c      drelabs: Function useful for 'relativizing' quantity
c      being monitored for detection of convergence.
c=====

      real*8 function drelabs(dx,x,xfloor)
      implicit      none

      real*8          dx,        x,        xfloor

      if( abs(x) .lt. abs(xfloor) ) then
          drelabs = abs(dx)
      else
          drelabs = abs(dx/x)
      end if

      return
end
```

```
c=====
c      tbisect: Illustrates root finding using bisection
c      routine 'bisect'.
c
c      Initial bracketing interval must be specified via the
c      command-line, along with optional convergence criteria
c      and output option.
c
c      This program also illustrates the general Fortran
c      techniques (briefly discussed previously) for:
c
c      (1) Writing and using routines which take other routines
c          as arguments.
c      (2) Using a COMMON block to communicate information to
c          a routine in cases where the information cannot be
c          passed via the argument list.
c      (3) Using an "INCLUDE" file (in this case 'comf.inc')
c          to ensure that the same common block structure is defined
c          in all program units.
c
c      Currently set up for computing square roots i.e.
c      solves
c
c          f(x; a) = x**2 - a = 0
c
c      for 'a' specified on command-line
c
c      Outputs a, approximate root (x*) and f(x*; a) on stdout.
c=====
```

program tbisect  
implicit none

```

c-----
c      Declaration of the bisection routine.
c-----
c      real*8          bisect
c-----
c      Name of the specific function whose root we seek.
c      Note use of 'external' to let compiler know 'fsqr'
c      is the name of a function, not a variable.
c-----
c      real*8          fsqr
c      external        fsqr

      integer          i4arg,           iargc
      real*8           r8arg

c-----  

c      For use in detecting bad real*8 command-line value.
c-----
c      real*8          r8_never
c      parameter       ( r8_never = -1.0d-60 )

c-----  

c      Use a common block to pass number whose square root
c      is sought to external function 'fsqr'.
c-----
c      include         'comf.inc'

c-----  

c      Initial bracket, convergence tolerance and output
c      option from command-line; default value for conv.
c      tolerance.

c-----  

c      real*8          xmin,           xmax,           xtol
c      logical          trace

      real*8          default_xtol
c      parameter       ( default_xtol = 1.0d-8 )

```

```

c-----
c      Root and return code from bisection routine.
c-----
c-----  

real*8          root  

integer         rc  

c-----  

c      Argument parsing.  

c-----  

if( iargc() .lt. 3 ) go to 900  

a      = r8arg(1,r8_never)  

xmin  = r8arg(2,r8_never)  

xmax  = r8arg(3,r8_never)  

if( a .eq. r8_never .or. xmin .eq. r8_never .or.  

&   xmax .eq. r8_never ) go to 900  

  

xtol  = r8arg(4,default_xtol)  

trace = iargc() .gt. 4  

c-----  

c      Invoke root finder then write a, sqrt(a), and residual  

c      to standard output.  

c-----  

root = bisect(fsqr,xmin,xmax,xtol,trace,rc)  

if( rc .eq. 0 ) then  

    write(*,*) a, root, fsqr(root)  

else  

    write(0,*) 'tbisect: Bisection failed.'  

end if  

c-----  

c      Normal exit.  

c-----  

stop

```

```

c-----
c      Usage exit.
c-----
900  continue
        write(0,*) 'usage: tbisect <a> <xmin> <xmax> //'
&                      '[<xtol> <trace>] '
        stop

        end

c=====
c      Function whose root is sought. Again, note use of
c      COMMON block to pass additional information (in this
c      case 'a') to the routine.
c=====

        real*8 function fsqr(x)
        implicit      none

        real*8          x

        include      'comf.inc'

        fsqr = x**2 - a

        return
end

```

```
c-----  
c      Common block for communicating value of 'a' from main  
c      to 'fsqr'.  
c-----  
real*8           a  
common   / comf / a
```

```

#####
# Building 'tbisect' and sample output on sgi1
#
# 'tbisect' is set up to compute sqrt(a) via bisection.
#####

sgi1% pwd ; ls
/usr/people/phys410/nonlin/ex1

Makefile      bisect.f      comf.inc      tbisect.f
sgi1% make
f77 -g -64 -c tbisect.f
f77 -g -64 -c bisect.f
f77 -g -64 -L/usr/local/lib tbisect.o bisect.o -lp410f -o tbisect

sgi1% tbisect
usage: tbisect <a> <xmin> <xmax> [<xtol> <trace>]

#####
# Compute +sqrt(2) to default tolerance (1.0d-8)
#
# Note: Exact value to 16 digits is 1.414 2135 6237 3095
#####
sgi1% tbisect 2.0 1.0 2.0
2.0000000000000000          1.414213564246893          5.2999009625409599E-09

#####
# Recompute with higher tolerance (1.0d-12)
#####
sgi1% tbisect 2.0 1.0 2.0 1.0e-12
2.0000000000000000          1.414213562372879          -6.1084470814876113E-13

```



2.000000000000000

1.414213564246893

5.2999009625409599E-09

```

c=====
c      newtsqrt:  Uses Newton's method to find (positive)
c      square root of number supplied on command line, i.e.
c      solves
c
c      f(x) = x^2 - a = 0
c
c      for given 'a'.  Optional second argument specifies
c      convergence criteria (relative dx).
c
c      Tracing output (written to standard error)
c      includes iteration number, estimated root (xn),
c      change in estimate (dxn), log10(dxn), residual and
c      log10(residual).
c=====

program           newtsqrt

implicit          none

integer            iargc
real*8             r8arg,           drelabs

real*8             r8_never
parameter          ( r8_never = -1.0d-60 )

c-----
c      Default convergence tolerance.
c-----

real*8             default_xtol
parameter          ( default_xtol = 1.0d-8 )

c-----
c      Maximum allowed number of Newton iterations.
c-----

integer            mxiter
parameter          ( mxiter = 50 )

```

```

c-----
c      Command-line arguments (see above).
c-----
c      real*8          a,           xtol
c-----
c      Locals used in Newton iteration.
c-----
c      integer          iter
c      real*8          xn,          resn,          dxn
c-----
c      Argument parsing.
c-----
if( iargc() .lt. 1 ) go to 900
a      = r8arg(1,r8_never)
if( a .eq. r8_never .or. a .lt. 0.0d0 ) go to 900
xtol  = r8arg(2,1.0d-8)
if( xtol .le. 0.0d0 ) xtol = 1.0d-8

c-----
c      Un-inspired initial guess: x^(0) = a / 2.
c-----
xn = 0.5d0 * a

```

```

c-----
c      Newton loop.
c-----
      write(0,*) 'Iter          xn          '//  

      &           'dxn      log10(dxn)    rn      log10(rn),  

      write(0,*)
      do iter = 1 , mxiter
         resn = xn**2 - a
         dxn  = resn / (2.0d0 * xn)
         xn   = xn - dxn
         write(0,1000) iter, xn, dxn, log10(abs(dxn)),
      &             resn, log10(abs(resn))
1000    format(i2,1p,e26.16,e12.3,0p,f10.2,1p,e12.3,0p,f10.2)
c-----
c      Jump out of Newton loop if soln has converged.
c-----
      if( drelabs(dxn,xn,1.0d-10) .le. xtol ) go to 100
      end do
c-----
c      No-convergence exit.
c-----
      write(0,*) 'No convergence after ', mxiter,
      &           ' iterations'
      stop
c-----
c      Normal exit, write input and estimated square root
c      to standard output.
c-----
100  continue
      write(0,*)
      write(*,*) a, xn
      stop

```

```

c-----
c      Usage exit.
c-----
900  continue
      write(0,*) 'usage: newtsqrt <a> [<x tol>]'
stop

end

c=====
c      drelabs: Function useful for 'relativizing' quantity
c      being monitored for detection of convergence.
c=====

      real*8 function drelabs(dx,x,xfloor)

      implicit      none

      real*8          dx,        x,        xfloor

      if( abs(x) .lt. abs(xfloop) ) then
          drelabs = abs(dx)
      else
          drelabs = abs(dx/x)
      end if

      return

end

```

```

#####
# Building 'newtsqrt' and sample output on sgi1
#####
sgi1% pwd; ls
/usr/people/phys410/nonlin/ex2
Makefile      newtsqrt.f

sgi1% make
f77 -g -64 -c newtsqrt.f
f77 -g -64 -L/usr/local/lib newtsqrt.o -lp410f -o newtsqrt

sgi1% newtsqrt
usage: newtsqrt <a> [<xtol>]

#####
# Compute +sqrt(10) to default tolerance (1.0d-8)
#
# Note: Exact value to 16 digits is 3.162 2776 6016 8379
#####
sgi1% newtsqrt 10.0
Iter          xn                  dxn    log10(dxn)      rn      log10(rn)
1   3.500000000000000E+00  1.500E+00    0.18  1.500E+01    1.18
2   3.1785714285714284E+00 3.214E-01   -0.49  2.250E+00    0.35
3   3.1623194221508828E+00 1.625E-02   -1.79  1.033E-01   -0.99
4   3.1622776604441363E+00 4.176E-05   -4.38  2.641E-04   -3.58
5   3.1622776601683795E+00 2.758E-10   -9.56  1.744E-09   -8.76

10.00000000000000          3.162277660168380

```

```
#####
# Recompute with higher tolerance---an extra Newton step
# is taken, but the solution was already accurate to
# roughly machine epsilon, so there is very little change
# in the output.
#####
sgi1% newtsqrt 10.0 1.0e-15
Iter          xn            dxn      log10(dxn)      rn      log10(rn)
1   3.500000000000000E+00  1.500E+00    0.18  1.500E+01   1.18
2   3.1785714285714284E+00 3.214E-01   -0.49  2.250E+00   0.35
3   3.1623194221508828E+00 1.625E-02   -1.79  1.033E-01  -0.99
4   3.1622776604441363E+00 4.176E-05   -4.38  2.641E-04  -3.58
5   3.1622776601683795E+00 2.758E-10   -9.56  1.744E-09  -8.76
6   3.1622776601683791E+00 2.809E-16  -15.55  1.776E-15 -14.75

10.00000000000000          3.162277660168379

#####
# Compute +sqrt(1/2) to default tolerance (1.0d-8)
#
# Note: Exact value to 16 digits is 0.7071 0678 1186 5475
#####
sgi1% newtsqrt 0.5
Iter          xn            dxn      log10(dxn)      rn      log10(rn)
1   1.125000000000000E+00  -8.750E-01   -0.06  -4.375E-01  -0.36
2   7.847222222222221E-01  3.403E-01   -0.47  7.656E-01  -0.12
3   7.1094518190757128E-01 7.378E-02   -1.13  1.158E-01  -0.94
4   7.0711714297003669E-01 3.828E-03   -2.42  5.443E-03  -2.26
5   7.0710678126246607E-01 1.036E-05   -4.98  1.465E-05  -4.83
6   7.0710678118654757E-01 7.592E-11  -10.12  1.074E-10 -9.97

0.5000000000000000          0.7071067811865476
```

```

c=====
c      newt2:  Uses multi-dimensional Newton's method
c      to compute a root of simple non-linear system
c      discussed in class
c
c          sin(xy) - 1/2 = 0
c          y^2 - 6x - 2  = 0
c
c      Command line input is initial guess (two numbers)
c      for root, and optional convergence criteria.
c      Estimated root written to standard output.
c      Tracing output similar to that from 'newtsqrt'.
c=====

      program      newt2

      implicit      none

      integer        iargc
      real*8         r8arg,           drelabs,       dvl2norm

      real*8         r8_never
      parameter      ( r8_never = -1.0d-60 )

c-----
c      Size of system.
c-----

      integer        neq
      parameter      ( neq = 2 )

c-----
c      Command-line arguments:  Initial guess will be
c      input directly into 'x' array.
c-----

      real*8         tol

```

```

c-----
c      Variables used in Newton iteration and solution of
c      linear systems via LAPACK routine 'dgesv'.
c-----

      real*8          J(neq,neq) ,    res(neq) ,
      &                  x(neq)
      integer         ipiv(neq)
      integer         ieq,           info

      integer         mxiter,        nrhs
      parameter       ( mxiter = 50,  nrhs = 1 )

      integer         iter
      real*8          nrm2res,      nrm2dx,      nrm2x
c-----

c      Default convergence tolerance.
c-----

      real*8          default_tol
      parameter       ( default_tol = 1.0d-8 )
c-----

c      Argument parsing.
c-----

      if( iargc() .lt. neq ) go to 900
      do ieq = 1 , neq
          x(ieq) = r8arg(ieq,r8_never)
          if( x(ieq) .eq. r8_never ) go to 900
      end do
      tol  = r8arg(neq+1,default_tol)
      if( tol .le. 0.0d0 ) tol = default_tol

```

```

c-----
c      Newton loop.
c-----
      write(0,*)
      &           'Iter          x          y' //'
      write(0,*)
      do iter = 1 , mxiter
c-----
c      Evaluate residual vector.
c-----
      res(1) = sin(x(1)*x(2)) - 0.5d0
      res(2) = x(2)**2 - 6.0d0 * x(1) - 2.0d0
      nrm2res = dvl2norm(res,2)
c-----
c      Set up Jacobian.
c-----
      J(1,1) = x(2) * cos(x(1) * x(2))
      J(1,2) = x(1) * cos(x(1) * x(2))
      J(2,1) = -6.0d0
      J(2,2) = 2.0d0 * x(2)
c-----
c      Solve linear system (J dx = res) for update
c      dx.  Update returned in 'res' vector.
c-----
      call dgesv( neq, nrhs, J, neq, ipiv, res, neq, info )
      if( info .eq. 0 ) then
c-----
c      Update solution.
c-----
      nrm2x  = dvl2norm(x,neq)
      nrm2dx = dvl2norm(res,neq)
      do ieq = 1 , neq
         x(ieq) = x(ieq) - res(ieq)
      end do

```

```

c-----
c      Tracing output: note use of max to prevent
c      taking log10 of 0.
c-----
c      write(0,1000) iter, x(1), x(2),
&          log10(max(nrm2dx,1.0d-60)),
&          log10(max(nrm2res,1.0d-60))
1000      format(i2,1p,2e24.16,0p,2f8.2)
c-----
c      Check for convergence.
c-----
c      if( drelabs(nrm2dx,nrm2x,1.0d-6) .le. tol ) go to 100
else
    write(0,*) 'newt2: dgesv failed.'
    stop
end if
end do
c-----
c      No-convergence exit.
c-----
c      write(0,*) 'No convergence after ', mxiter,
&          ' iterations'
stop

c-----
c      Normal exit, write input and estimated square root
c      to standard output.
c-----
100  continue
write(0,*)
write(*,*) x
stop

```

```

c-----
c      Usage exit.
c-----
900  continue
        write(0,*) 'usage: newt2 <x0> <y0> [<tol>]'
stop

end

c=====
c      dvl2norm: Returns l2-norm of double precision vector.
c=====
real*8 function dvl2norm(v,n)

implicit none

integer n
real*8 v(n)
integer i

dvl2norm = 0.0d0
do i = 1 , n
    dvl2norm = dvl2norm + v(i) * v(i)
end do
if( n .gt. 0 ) then
    dvl2norm = sqrt(dvl2norm / n)
end if

return

end

```

```
c=====
c      drelabs: Function useful for 'relativizing' quantity
c      being monitored for detection of convergence.
c=====

      real*8 function drelabs(dx,x,xfloor)

      implicit      none

      real*8          dx,      x,      xfloor

      if( abs(x) .lt. abs(xfloor) ) then
          drelabs = abs(dx)
      else
          drelabs = abs(dx/x)
      end if

      return

end
```

```

#####
# Building 'newt2' and sample output on sgi1.
#
# Note how different roots are found depending on the initial
# guess and how, in each case, convergence of both dx and
# the residual is quadratic as the solution is approached.
#####
sgi1% pwd ; ls
/usr/people/phys410/nonlin/ex3
Makefile newt2.f

sgi1% make
f77 -g -64 -c newt2.f
f77 -g -64 -L/usr/local/lib newt2.o -lp410f -llapack -lblas -o newt2

sgi1% newt2
usage: newt2 <x0> <y0> [<tol>]

#####
# Start with initial guess (1.0,1.0) and use default tolerance
#####
sgi1% newt2 1.0 1.0
Iter          x                  y          log10(dx) log10(res)
1  -3.2999966453609808E-02  1.4010001006391706E+00  -0.11    0.70
2   3.7660093320946680E-01  2.2207017966697333E+00  -0.19   -0.40
3   2.6508349149835875E-01  1.9187667230923000E+00  -0.64   -0.30
4   2.7416951525985472E-01  1.9092166705387068E+00  -2.03   -1.19
5   2.7423631305849172E-01  1.9092977465351673E+00  -4.13   -3.95
6   2.7423631371214585E-01  1.9092977458408302E+00  -9.17   -8.33

0.2742363137121459      1.909297745840830

```

```

#####
# Start with initial guess (10.0,10.0)
#####
sgi1% newt2 10.0 10.0
Iter          x                  y      log10(dx) log10(res)
1  1.1551311217431483E+01  8.5653933652294452E+00  0.17    1.43
2  5.2821340061728987E+00  6.2494950887340917E+00  0.67    0.26
3  7.9156169056753551E+00  7.0845635560056479E+00  0.29    0.58
4  8.0553488926886114E+00  7.0945184795470357E+00 -1.00   -0.08
5  8.0478800969936373E+00  7.0913532277542579E+00 -2.24   -1.34
6  8.0480621354266173E+00  7.0914295327798440E+00 -3.86   -2.93
7  8.0480622340064549E+00  7.0914295740731097E+00 -7.12   -6.20

8.048062234006455      7.091429574073110

#####
# Start with initial guess (100.0,100.0)
#####
sgi1% newt2 100.0 100.0
Iter         x                  y      log10(dx) log10(res)
1  1.4561314470371522E+02  5.4378394341111459E+01  1.66    3.82
2  1.9021837653952511E+02  3.7701738714769540E+01  1.53    3.17
3  2.0349983567820649E+02  3.5070267397907145E+01  0.98    2.29
4  2.0392234856561154E+02  3.5007684984188487E+01 -0.52    0.70
5  2.0390326095147395E+02  3.5005993323580455E+01 -1.87   -0.53
6  2.0391023928640132E+02  3.5006591323292412E+01 -2.31   -0.59
7  2.0391061250942661E+02  3.5006623302706338E+01 -3.58   -1.92
8  2.0391061457091234E+02  3.5006623479357074E+01 -5.83   -4.18
9  2.0391061457097669E+02  3.5006623479362588E+01 -10.34  -8.68

203.9106145709767     35.00662347936259

```

```

#####
# Start with initial guess (0.0,0.0), generates singular
# Jacobian
#####
sgi1% newt2 0.0 0.0
Iter           x                   y           log10(dx) log10(res)

newt2: dgesv failed.

#####
# Start with initial guess (1.0,1.0) but use more stringent
# tolerance
#####
sgi1% newt2 1.0 1.0 1.0e-15
Iter           x                   y           log10(dx) log10(res)

1 -3.2999966453609808E-02  1.4010001006391706E+00  -0.11    0.70
2  3.7660093320946680E-01  2.2207017966697333E+00  -0.19   -0.40
3  2.6508349149835875E-01  1.9187667230923000E+00  -0.64   -0.30
4  2.7416951525985472E-01  1.9092166705387068E+00  -2.03   -1.19
5  2.7423631305849172E-01  1.9092977465351673E+00  -4.13   -3.95
6  2.7423631371214585E-01  1.9092977458408302E+00  -9.17  -8.33
7  2.7423631371214585E-01  1.9092977458408302E+00 -16.44 -16.41

0.2742363137121459      1.909297745840830

```

```

#####
# Checking 'newt2' using numerical root finding capablities
# of Maple.
#####
sgi1% maple
    |\^/|      Maple V Release 5 (University of Texas at Austin)
 .-\|\  |/_|. Copyright (c) 1981-1997 by Waterloo Maple Inc. All rights
 \ MAPLE / reserved. Maple and Maple V are registered trademarks of
 <---- ----> Waterloo Maple Inc.
    |          Type ? for help.
> Digits := 20;
                                Digits := 20

> f1 := sin(x*y) - 1/2;
                                f1 := sin(x y) - 1/2

> f2 := y^2 - 6*x - 2;
                                2
                                f2 := y  - 6 x - 2

#####
# Locates root found by 'newt2 1.0 1.0'
#####
> ans := fsolve( {f1,f2}, {x,y}, {x=0.25..0.30, y=1.8..2.0});
                                ans := {y = 1.9092977458408301606, x = .27423631371214588082}

```

```

#####
# Compute residuals of root
#####
> r1 := evalf(subs(ans,f1)); r2 := evalf(subs(ans,f2));
                                         -19
r1 := -.1 10

                                         -18
r2 := -.1 10

#####
# Locates root found by 'newt2 10.0 10.0'
#####
> ans := fsolve( {f1,f2}, {x,y}, {x=7..9, y=6..8});
ans := {x = 8.0480622340064835835, y = 7.0914295740731220704}

> r1 := evalf(subs(ans,f1)); r2 := evalf(subs(ans,f2));
                                         -18
r1 := -.35 10

r2 := 0

```

```

#####
# Locates root found by 'newt2 100.0 100.0'
#####
> ans := fsolve( {f1,f2}, {x,y}, {x=203.9..203.95, y=35.0..35.01});
ans := {x = 203.91061457097670060, y = 35.006623479362590528}

> r1 := evalf(subs(ans,f1)); r2 := evalf(subs(ans,f2));
                                         -16
r1 := -.5214 10

r2 := 0

#####
# Another nearby, but distinct, root
#####
> ans := fsolve( {f1,f2}, {x,y}, {x=203..204, y=35.0..35.1});
ans := {x = 203.95052002180667001, y = 35.010043132376172782}

> r1 := evalf(subs(ans,f1)); r2 := evalf(subs(ans,f2));
                                         -16
r1 := .4548 10

r2 := 0

> quit;

```