# C1. Listing of Utility Modules (nrtype and nrutil)

## C1.1 Numerical Recipes Types (nrtype)

The file supplied as nrtype.f90 contains a single module named nrtype, which in turn contains definitions for a number of named constants (that is, PARAMETERS), and a couple of elementary derived data types used by the sparse matrix routines in this book. Of the named constants, by far the most important are those that define the KIND types of virtually all the variables used in this book: I4B, I2B, and I1B for integer variables, SP and DP for real variables (and SPC and DPC for the corresponding complex cases), and LGT for the default logical type.

```
Symbolic names for kind types of 4-, 2-, and 1-byte integers:

INTEGER, PARAMETER :: I4B = SELECTED_INT_KIND(9)

INTEGER, PARAMETER :: I2B = SELECTED_INT_KIND(4)

INTEGER, PARAMETER :: I1B = SELECTED_INT_KIND(2)

Symbolic names for kind types of single- and double-precision reals:

INTEGER, PARAMETER :: SP = KIND(1.0)
```

MODULE nrtype

INTEGER, PARAMETER :: DP = KIND(1.0D0)

Symbolic names for kind types of single- and double-precision complex:

INTEGER, PARAMETER :: SPC = KIND((1.0,1.0))

INTEGER, PARAMETER :: DPC = KIND((1.0D0,1.0D0))

Symbolic name for kind type of default logical:

INTEGER, PARAMETER :: LGT = KIND(.true.)
Frequently used mathematical constants (with precision to spare):

REAL(SP), PARAMETER :: PI=3.141592653589793238462643383279502884197\_sp
REAL(SP), PARAMETER :: PIO2=1.57079632679489661923132169163975144209858\_sp
REAL(SP), PARAMETER :: TWOPI=6.283185307179586476925286766559005768394\_sp
REAL(SP), PARAMETER :: SQRT2=1.41421356237309504880168872420969807856967\_sp

REAL(SP), PARAMETER :: EULER=0.5772156649015328606065120900824024310422\_sp
REAL(DP), PARAMETER :: PI\_D=3.141592653589793238462643383279502884197\_dp
REAL(DP), PARAMETER :: PIO2\_D=1.57079632679489661923132169163975144209858\_dp
REAL(DP), PARAMETER :: TWOPI\_D=6.283185307179586476925286766559005768394\_dp

Derived data types for sparse matrices, single and double precision (see use in Chapter B2): TYPE sprs2\_sp

INTEGER(I4B) :: n,len
REAL(SP), DIMENSION(:), POINTER :: val
INTEGER(I4B), DIMENSION(:), POINTER :: irow
INTEGER(I4B), DIMENSION(:), POINTER :: jcol
END TYPE sprs2\_sp
TYPE sprs2\_dp

INTEGER(14B) :: n,len
REAL(DP), DIMENSION(:), POINTER :: val

```
INTEGER(14B), DIMENSION(:), POINTER :: irow
INTEGER(14B), DIMENSION(:), POINTER :: jcol
END TYPE sprs2_dp
END MODULE nrtype
```

### About Converting to Higher Precision

You might hope that changing all the Numerical Recipes routines from single precision to double precision would be as simple as redefining the values of SP and DP in nrtype. Well ... not quite.

Converting algorithms to a higher precision is not a purely mechanical task because of the distinction between "roundoff error" and "truncation error." (Please see Volume 1, §1.2, if you are not familiar with these concepts.) While increasing the precision implied by the kind values SP and DP will indeed reduce a routine's roundoff error, it will not reduce any truncation error that may be intrinsic to the algorithm. Sometimes, a routine contains "accuracy parameters" that can be adjusted to reduce the truncation error to the new, desired level. In other cases, however, the truncation error cannot be so easily reduced; then, a whole new algorithm is needed. Clearly such new algorithms are beyond the scope of a simple mechanical "conversion."

If, despite these cautionary words, you want to proceed with converting some routines to a higher precision, here are some hints:

If your machine has a kind type that is distinct from, and has equal or greater precision than, the kind type that we use for DP, then, in nrtype, you can simply redefine DP to this new highest precision and redefine SP to what was previously DP. For example, DEC machines usually have a "quadruple precision" real type available, which can be used in this way. You should not need to make any further edits of nrtype or nrutil.

If, on the other hand, the kind type that we already use for DP is the highest precision available, then you must leave DP defined as it is, and redefine SP in nrtype to be this same kind type. Now, however, you will also have to edit nrutil, because some overloaded routines that were previously distinguishable (by the different kind types) will now be seen by the compiler as indistinguishable — and it will object strenuously. Simply delete all the "\_dp" function names from the list of overloaded procedures (i.e., from the MODULE PROCEDURE statements). Note that it is not necessary to delete the routines from the MODULE itself. Similarly, in the interface file nr.f90 you must delete the "\_dp" interfaces, except for the sprs... routines. (Since they have TYPE(sprs2\_dp) or TYPE(sprs2\_sp), they are treated as distinct even though they have functionally equivalent kind types.)

Finally, the following table gives some suggestions for changing the accuracy parameters, or constants, in some of the routines. Please note that this table is not necessarily complete, and that higher-precision performance is not guaranteed for all the routines, *even if* you make all the changes indicated. The above edits, and these suggestions, do, however, work in the majority of cases.

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In routine	change	to
beschb	NUSE1=5, NUSE2=5	NUSE1=7, NUSE2=8
bessi	IACC=40	IACC=200
bessik	EPS=1.0e-10 <b>_</b> dp	EPS=epsilon(x)
bessj	IACC=40	IACC=160
bessjy	EPS=1.0e-10 <b>_</b> dp	EPS=epsilon(x)
broydn	TOLF=1.0e-4_sp	TOLF=1.0e-8_sp
	TOLMIN=1.0e-6_sp	TOLMIN=1.0e-12_sp
fdjac	EPS=1.0e-4 <b>_</b> sp	EPS=1.0e-8_sp
frprmn	EPS=1.0e-10 <b>_</b> sp	EPS=1.0e-18_sp
gauher	EPS=3.0e-13_dp	EPS=1.0e-14_dp
gaujac	EPS=3.0e-14_dp	EPS=1.0e-14_dp
gaulag	EPS=3.0e-13_dp	EPS=1.0e-14_dp
gauleg	EPS=3.0e-14_dp	EPS=1.0e-14_dp
hypgeo	EPS=1.0e-6_sp	EPS=1.0e-14_sp
linmin	TOL=1.0e-4_sp	TOL=1.0e-8_sp
newt	TOLF=1.0e-4_sp	TOLF=1.0e-8_sp
	TOLMIN=1.0e-6_sp	TOLMIN=1.0e-12_sp
probks	EPS1=0.001_sp	EPS1=1.0e-6_sp
	EPS2=1.0e-8 <b>_</b> sp	EPS2=1.0e-16_sp
qromb	EPS=1.0e-6_sp	EPS=1.0e-10_sp
qromo	EPS=1.0e-6_sp	EPS=1.0e-10_sp
qroot	TINY=1.0e-6_sp	TINY=1.0e-14_sp
qsimp	EPS=1.0e-6 <b>_</b> sp	EPS=1.0e-10 <u></u> sp
qtrap	EPS=1.0e-6_sp	EPS=1.0e-10 <u>_</u> sp
rc	ERRTOL=0.04_sp	ERRTOL=0.0012_sp
rd	ERRTOL=0.05_sp	ERRTOL=0.0015_sp
rf	ERRTOL=0.08_sp	ERRTOL=0.0025_sp
rj	ERRTOL=0.05_sp	ERRTOL=0.0015_sp
sfroid	conv=5.0e-6_sp	conv=1.0e-14 <u>sp</u>
shoot	EPS=1.0e-6_sp	EPS=1.0e-14 <u>sp</u>
shootf	EPS=1.0e-6 <b>_</b> sp	EPS=1.0e-14 <u>sp</u>
simplx	EPS=1.0e-6 <b>_</b> sp	EPS=1.0e-14 <u>sp</u>
sncndn	CA=0.0003 <u></u> sp	CA=1.0e-8 <u>-</u> sp
sor	EPS=1.0e-5 <b>_d</b> p	EPS=1.0e-13 <u>d</u> p
sphfpt	DXX=1.0e-4_sp	DXX=1.0e-8 <b>_</b> sp
sphoot	dx=1.0e-4 <u></u> sp	dx=1.0e-8 <u>_</u> sp
svdfit	TOL=1.0e-5 <b>_</b> sp	TOL=1.0e-13 <u>s</u> sp
zroots	EPS=1.0e-6 <b>_</b> sp	EPS=1.0e-14 <u>sp</u>

# C1.2 Numerical Recipes Utilities (nrutil)

The file supplied as nrutil.f90 contains a single module named nrutil, which contains specific implementations for all the Numerical Recipes utility functions described in detail in Chapter 23.

The specific implementations given are something of a compromise between demonstrating parallel techniques (when they can be achieved in Fortran 90) and running efficiently on conventional, serial machines. The parameters at the beginning of the module (names beginning with NPAR.) are typically related to array lengths below which the implementations revert to serial operations. On a purely serial machine, these can be set to large values to suppress many parallel constructions.

The length and repetitiveness of the nrutil.f90 file stems in large part from its extensive use of overloading. Indeed, the file would be even longer if we overloaded versions for all the applicable data types that each utility could, in principle, instantiate. The descriptions in Chapter 23 detail both the full set of intended data types and shapes for each routine, and also the types and shapes actually here implemented (which can also be gleaned by examining the file). The intended result of all this overloading is, in essence, to give the utility routines the desirable properties of many of the Fortran 90 intrinsic functions, namely, to be both *generic* (apply to many data types) and *elemental* (apply element-by-element to arbitrary shapes). Fortran 95's provision of user-defined elemental functions will reduce the multiplicity of overloading in some of our routines; unfortunately the necessity to overload for multiple data types will still be present.

Finally, it is worth reemphasizing the following point, already made in Chapter 23: The purpose of the nrutil utilities is to remove from the Numerical Recipes programs just those programming tasks and "idioms" whose efficient implementation is *most* hardware and compiler dependent, so as to allow for specific, efficient implementations on different machines. One should therefore not expect the utmost in efficiency from the general purpose, one-size-fits-all, implementation listed here.

Correspondingly, we would encourage the incorporation of efficient nrutil implementations, and/or comparable capabilities under different names, with as broad as possible a set of overloaded data types, in libraries associated with specific compilers or machines. In support of this goal, we have specifically put this Appendix C1, and the files nrtype.f90 and nrutil.f90, into the public domain.

### MODULE nrutil

TABLE OF CONTENTS OF THE NRUTIL MODULE:

routines that move data:
 array\_copy, swap, reallocate
routines returning a location as an integer value
 ifirstloc, imaxloc, iminloc
routines for argument checking and error handling:
 assert\_eq, nrerror
routines relating to polynomials and recurrences
 arth, geop, cumsum, cumprod, poly, polyterm,
 zroots\_unity
routines for "outer" operations on vectors
 outerand, outersum, outerdiff, outerprod, outerdiv
routines for scatter-with-combine
 scatter\_add, scatter\_max
routines for skew operations on matrices
 diagadd, diagmult, get\_diag, put\_diag,

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```
unit_matrix, lower_triangle, upper_triangle
        miscellaneous routines
USE nrtype
   Parameters for crossover from serial to parallel algorithms (these are used only within this
   nrutil module):
IMPLICIT NONE
INTEGER(I4B), PARAMETER :: NPAR_ARTH=16,NPAR2_ARTH=8
                                                           Each NPAR2 must be \leq the
INTEGER(I4B), PARAMETER :: NPAR_GEOP=4,NPAR2_GEOP=2
                                                               corresponding NPAR.
INTEGER(I4B), PARAMETER :: NPAR_CUMSUM=16
INTEGER(I4B), PARAMETER :: NPAR_CUMPROD=8
INTEGER(I4B), PARAMETER :: NPAR_POLY=8
INTEGER(I4B), PARAMETER :: NPAR_POLYTERM=8
   Next, generic interfaces for routines with overloaded versions. Naming conventions for ap-
   pended codes in the names of overloaded routines are as follows: r=real, d=double pre-
   cision, i=integer, c=complex, z=double-precision complex, h=character, l=logical. Any of
   r,d,i,c,z,h,l may be followed by v=vector or m=matrix (v,m suffixes are used only when
   needed to resolve ambiguities).
   Routines that move data:
INTERFACE array_copy
    MODULE PROCEDURE array_copy_r, array_copy_d, array_copy_i
END INTERFACE
INTERFACE swap
    MODULE PROCEDURE swap_i,swap_r,swap_rv,swap_c, &
        swap_cv,swap_cm,swap_z,swap_zv,swap_zm, &
        masked_swap_rs,masked_swap_rv,masked_swap_rm
END INTERFACE
INTERFACE reallocate
    MODULE PROCEDURE reallocate_rv,reallocate_rm,&
        reallocate_iv,reallocate_im,reallocate_hv
END INTERFACE
   Routines returning a location as an integer value (ifirstloc, iminloc are not currently over-
   loaded and so do not have a generic interface here):
INTERFACE imaxloc
    MODULE PROCEDURE imaxloc_r,imaxloc_i
END INTERFACE
   Routines for argument checking and error handling (nrerror is not currently overloaded):
INTERFACE assert
   MODULE PROCEDURE assert1,assert2,assert3,assert4,assert_v
END INTERFACE
INTERFACE assert eq
    MODULE PROCEDURE assert_eq2,assert_eq3,assert_eq4,assert_eqn
   Routines relating to polynomials and recurrences (cumprod, zroots_unity are not currently
   overloaded):
INTERFACE arth
   MODULE PROCEDURE arth_r, arth_d, arth_i
END INTERFACE
INTERFACE geop
    MODULE PROCEDURE geop_r, geop_d, geop_i, geop_c, geop_dv
END INTERFACE
INTERFACE cumsum
   MODULE PROCEDURE cumsum_r,cumsum_i
END INTERFACE
INTERFACE poly
    MODULE PROCEDURE poly_rr,poly_rrv,poly_dd,poly_ddv,&
       poly_rc,poly_cc,poly_msk_rrv,poly_msk_ddv
END INTERFACE
INTERFACE poly_term
    MODULE PROCEDURE poly_term_rr,poly_term_cc
END INTERFACE
   Routines for "outer" operations on vectors (outerand, outersum, outerdiv are not currently
```

overloaded): INTERFACE outerprod Sample page from NUMERICAL RECIPES IN FORTRAN 90: The Art of PARALLEL Scientific Computing (ISBN 0-521-57439-0) Copyright (C) 1986-1996 by Cambridge University Press. Programs Copyright (C) 1986-1996 by Numerical Recipes Software. Permission is granted for internet users to make one paper copy for their own personal use. Further reproduction, or any copying of machine-readable files (including this one) to any server computer, is strictly prohibited. To order Numerical Recipes books, diskettes, or CDROMs visit website http://www.nr.com or call 1-800-872-7423 (North America only), or send email to trade@cup.cam.ac.uk (outside North America). from NUMERICAL RECIP ) 1986-1996 by Cambridge granted for internet users PES IN FORTRAN 90: The Art of PARA University Press. Programs Copyright to make one paper copy for their own ms Copyright (C) 19

```
MODULE PROCEDURE outerprod_r,outerprod_d
END INTERFACE
INTERFACE outerdiff
   MODULE PROCEDURE outerdiff_r,outerdiff_d,outerdiff_i
END INTERFACE
   Routines for scatter-with-combine, scatter_add, scatter_max:
INTERFACE scatter_add
   MODULE PROCEDURE scatter_add_r,scatter_add_d
END INTERFACE
INTERFACE scatter max
   MODULE PROCEDURE scatter_max_r,scatter_max_d
END INTERFACE
   Routines for skew operations on matrices (unit_matrix, lower_triangle, upper_triangle not
   currently overloaded):
INTERFACE diagadd
    MODULE PROCEDURE diagadd_rv,diagadd_r
END INTERFACE
INTERFACE diagnult
   MODULE PROCEDURE diagmult_rv,diagmult_r
END INTERFACE
INTERFACE get_diag
   MODULE PROCEDURE get_diag_rv, get_diag_dv
END INTERFACE
INTERFACE put_diag
   MODULE PROCEDURE put_diag_rv, put_diag_r
END INTERFACE
   Other routines (vabs is not currently overloaded):
CONTAINS
   Routines that move data:
SUBROUTINE array_copy_r(src,dest,n_copied,n_not_copied)
   Copy array where size of source not known in advance.
REAL(SP), DIMENSION(:), INTENT(IN) :: src
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src),size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_r
SUBROUTINE array_copy_d(src,dest,n_copied,n_not_copied)
REAL(DP), DIMENSION(:), INTENT(IN) :: src
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src), size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_d
SUBROUTINE array_copy_i(src,dest,n_copied,n_not_copied)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: src
INTEGER(14B), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src),size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_i
SUBROUTINE swap_i(a,b)
   Swap the contents of a and b.
INTEGER(I4B), INTENT(INOUT) :: a,b
INTEGER(I4B) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_i
```

```
SUBROUTINE swap_r(a,b)
REAL(SP), INTENT(INOUT) :: a,b
REAL(SP) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_r
SUBROUTINE swap_rv(a,b)
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
REAL(SP), DIMENSION(SIZE(a)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_rv
SUBROUTINE swap_c(a,b)
COMPLEX(SPC), INTENT(INOUT) :: a,b
COMPLEX(SPC) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_c
SUBROUTINE swap_cv(a,b)
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: a,b
COMPLEX(SPC), DIMENSION(SIZE(a)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_cv
SUBROUTINE swap_cm(a,b)
COMPLEX(SPC), DIMENSION(:,:), INTENT(INOUT) :: a,b
COMPLEX(SPC), DIMENSION(size(a,1),size(a,2)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_cm
SUBROUTINE swap_z(a,b)
COMPLEX(DPC), INTENT(INOUT) :: a,b
COMPLEX(DPC) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_z
SUBROUTINE swap_zv(a,b)
COMPLEX(DPC), DIMENSION(:), INTENT(INOUT) :: a,b
COMPLEX(DPC), DIMENSION(SIZE(a)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_zv
SUBROUTINE swap_zm(a,b)
COMPLEX(DPC), DIMENSION(:,:), INTENT(INOUT) :: a,b
COMPLEX(DPC), DIMENSION(size(a,1),size(a,2)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_zm
SUBROUTINE masked_swap_rs(a,b,mask)
REAL(SP), INTENT(INOUT) :: a,b
LOGICAL(LGT), INTENT(IN) :: mask
REAL(SP) :: swp
```

```
if (mask) then
   swp=a
   a=b
   b=swp
end if
END SUBROUTINE masked_swap_rs
SUBROUTINE masked_swap_rv(a,b,mask)
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(a)) :: swp
where (mask)
   swp=a
   a=b
   b=swp
end where
END SUBROUTINE masked_swap_rv
SUBROUTINE masked_swap_rm(a,b,mask)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a,b
LOGICAL(LGT), DIMENSION(:,:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(a,1),size(a,2)) :: swp
where (mask)
   swp=a
   a=b
   b=swp
end where
END SUBROUTINE masked_swap_rm
FUNCTION reallocate_rv(p,n)
   Reallocate a pointer to a new size, preserving its previous contents.
REAL(SP), DIMENSION(:), POINTER :: p, reallocate_rv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_rv(n), stat=ierr)
if (ierr /= 0) call &
   nrerror('reallocate_rv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_rv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_rv
FUNCTION reallocate_iv(p,n)
INTEGER(I4B), DIMENSION(:), POINTER :: p, reallocate_iv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_iv(n), stat=ierr)
if (ierr /= 0) call &
   nrerror('reallocate_iv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_iv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_iv
FUNCTION reallocate_hv(p,n)
CHARACTER(1), DIMENSION(:), POINTER :: p, reallocate_hv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_hv(n), stat=ierr)
if (ierr /= 0) call &
   nrerror('reallocate_hv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_hv(1:min(nold,n))=p(1:min(nold,n))
```

```
deallocate(p)
END FUNCTION reallocate_hv
FUNCTION reallocate_rm(p,n,m)
REAL(SP), DIMENSION(:,:), POINTER :: p, reallocate_rm
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_rm(n,m),stat=ierr)
if (ierr /= 0) call &
   nrerror('reallocate_rm: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p.1)
mold=size(p,2)
reallocate_rm(1:min(nold,n),1:min(mold,m))=&
   p(1:min(nold,n),1:min(mold,m))
deallocate(p)
END FUNCTION reallocate_rm
FUNCTION reallocate_im(p,n,m)
INTEGER(I4B), DIMENSION(:,:), POINTER :: p, reallocate_im
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_im(n,m),stat=ierr)
if (ierr /= 0) call &
   nrerror('reallocate_im: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p,1)
mold=size(p,2)
reallocate_im(1:min(nold,n),1:min(mold,m))=&
   p(1:min(nold,n),1:min(mold,m))
deallocate(p)
END FUNCTION reallocate_im
   Routines returning a location as an integer value:
FUNCTION ifirstloc(mask)
   Index of first occurrence of .true. in a logical vector.
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
INTEGER(I4B) :: ifirstloc
INTEGER(I4B), DIMENSION(1) :: loc
loc=maxloc(merge(1,0,mask))
ifirstloc=loc(1)
if (.not. mask(ifirstloc)) ifirstloc=size(mask)+1
END FUNCTION ifirstloc
FUNCTION imaxloc_r(arr)
   Index of maxloc on an array.
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B) :: imaxloc_r
INTEGER(I4B), DIMENSION(1) :: imax
imax=maxloc(arr(:))
imaxloc_r=imax(1)
END FUNCTION imaxloc r
FUNCTION imaxloc_i(iarr)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: iarr
INTEGER(I4B), DIMENSION(1) :: imax
INTEGER(I4B) :: imaxloc_i
imax=maxloc(iarr(:))
imaxloc i=imax(1)
END FUNCTION imaxloc_i
FUNCTION iminloc(arr)
   Index of minloc on an array.
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), DIMENSION(1) :: imin
INTEGER(I4B) :: iminloc
imin=minloc(arr(:))
```

```
iminloc=imin(1)
END FUNCTION iminloc
   Routines for argument checking and error handling:
SUBROUTINE assert1(n1,string)
   Report and die if any logical is false (used for arg range checking).
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1
if (.not. n1) then
   write (*,*) 'nrerror: an assertion failed with this tag:', &
       string
   STOP 'program terminated by assert1'
end if
END SUBROUTINE assert1
SUBROUTINE assert2(n1,n2,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2
if (.not. (n1 .and. n2)) then
   write (*,*) 'nrerror: an assertion failed with this tag:', &
       string
   STOP 'program terminated by assert2'
end if
END SUBROUTINE assert2
SUBROUTINE assert3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3
if (.not. (n1 .and. n2 .and. n3)) then
   write (*,*) 'nrerror: an assertion failed with this tag:', &
       string
   STOP 'program terminated by assert3'
end if
END SUBROUTINE assert3
SUBROUTINE assert4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3,n4
if (.not. (n1 .and. n2 .and. n3 .and. n4)) then
   write (*,*) 'nrerror: an assertion failed with this tag:', &
       string
   STOP 'program terminated by assert4'
end if
END SUBROUTINE assert4
SUBROUTINE assert_v(n,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, DIMENSION(:), INTENT(IN) :: n
if (.not. all(n)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
       string
   STOP 'program terminated by assert_v'
end if
END SUBROUTINE assert_v
FUNCTION assert_eq2(n1,n2,string)
   Report and die if integers not all equal (used for size checking).
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2
INTEGER :: assert_eq2
if (n1 == n2) then
   assert_eq2=n1
   write (*,*) 'nrerror: an assert_eq failed with this tag:', &
   STOP 'program terminated by assert_eq2'
end if
```

```
END FUNCTION assert_eq2
FUNCTION assert_eq3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3
INTEGER :: assert_eq3
if (n1 == n2 .and. n2 == n3) then
   assert_eq3=n1
else
   write (*,*) 'nrerror: an assert_eq failed with this tag:', &
   STOP 'program terminated by assert_eq3'
end if
END FUNCTION assert_eq3
FUNCTION assert_eq4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3,n4
INTEGER :: assert_eq4
if (n1 == n2 .and. n2 == n3 .and. n3 == n4) then
   assert_eq4=n1
else
   write (*,*) 'nrerror: an assert_eq failed with this tag:', &
   STOP 'program terminated by assert_eq4'
END FUNCTION assert_eq4
FUNCTION assert_eqn(nn,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, DIMENSION(:), INTENT(IN) :: nn
INTEGER :: assert_eqn
if (all(nn(2:) == nn(1))) then
   assert_eqn=nn(1)
else
   write (*,*) 'nrerror: an assert_eq failed with this tag:', &
       string
   STOP 'program terminated by assert_eqn'
end if
END FUNCTION assert_eqn
SUBROUTINE nrerror(string)
   Report a message, then die.
CHARACTER(LEN=*), INTENT(IN) :: string
write (*,*) 'nrerror: ',string
STOP 'program terminated by nrerror'
END SUBROUTINE nrerror
   Routines relating to polynomials and recurrences:
FUNCTION arth_r(first,increment,n)
   Array function returning an arithmetic progression.
REAL(SP), INTENT(IN) :: first,increment
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: arth_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) arth_r(1)=first
if (n <= NPAR_ARTH) then
   do k=2.n
       arth_r(k) = arth_r(k-1) + increment
   end do
else
   do k=2,NPAR2_ARTH
       arth_r(k)=arth_r(k-1)+increment
   end do
   temp=increment*NPAR2_ARTH
```

k=NPAR2\_ARTH

```
do
        if (k \ge n) exit
        k2=k+k
        arth_r(k+1:min(k2,n))=temp+arth_r(1:min(k,n-k))
        temp=temp+temp
        k=k2
    end do
end if
END FUNCTION arth_r
FUNCTION arth_d(first,increment,n)
REAL(DP), INTENT(IN) :: first,increment INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: arth_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) arth_d(1)=first
if (n <= NPAR_ARTH) then
        arth_d(k)=arth_d(k-1)+increment
    end do
else
   do k=2,NPAR2_ARTH
        arth_d(k) = arth_d(k-1) + increment
    end do
    temp=increment*NPAR2_ARTH
   k=NPAR2_ARTH
   do
        if (k \ge n) exit
        k2=k+k
        arth_d(k+1:min(k2,n))=temp+arth_d(1:min(k,n-k))
        temp=temp+temp
        k=k2
    end do
end if
END FUNCTION arth_d
FUNCTION arth_i(first,increment,n)
INTEGER(I4B), INTENT(IN) :: first,increment,n
INTEGER(I4B), DIMENSION(n) :: arth_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) arth_i(1)=first
if (n <= NPAR_ARTH) then
        arth_i(k)=arth_i(k-1)+increment
    end do
else
    do k=2,NPAR2_ARTH
        arth_i(k)=arth_i(k-1)+increment
    end do
    temp=increment*NPAR2_ARTH
   k=NPAR2_ARTH
    do
        if (k \ge n) exit
        k2=k+k
        arth_i(k+1:min(k2,n))=temp+arth_i(1:min(k,n-k))
        temp=temp+temp
        k=k2
    end do
end if
END FUNCTION arth_i
FUNCTION geop_r(first,factor,n)
   Array function returning a geometric progression.
REAL(SP), INTENT(IN) :: first,factor
```

```
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: geop_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) geop_r(1)=first
if (n <= NPAR_GEOP) then
   do k=2,n
       geop_r(k)=geop_r(k-1)*factor
   end do
else
   do k=2,NPAR2_GEOP
       geop_r(k)=geop_r(k-1)*factor
   end do
   temp=factor**NPAR2_GEOP
   k=NPAR2_GEOP
       if (k \ge n) exit
       k2=k+k
       geop_r(k+1:min(k2,n))=temp*geop_r(1:min(k,n-k))
       temp=temp*temp
       k=k2
   end do
end if
END FUNCTION geop_r
FUNCTION geop_d(first,factor,n)
REAL(DP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: geop_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) geop_d(1)=first
if (n <= NPAR_GEOP) then
   do k=2.n
       geop_d(k)=geop_d(k-1)*factor
   end do
else
   do k=2,NPAR2_GEOP
       geop_d(k)=geop_d(k-1)*factor
   end do
   temp=factor**NPAR2_GEOP
   k=NPAR2_GEOP
   do
       if (k \ge n) exit
       k2=k+k
       geop_d(k+1:min(k2,n))=temp*geop_d(1:min(k,n-k))
       temp=temp*temp
       k=k2
   end do
end if
END FUNCTION geop_d
FUNCTION geop_i(first,factor,n)
INTEGER(I4B), INTENT(IN) :: first,factor,n
INTEGER(I4B), DIMENSION(n) :: geop_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) geop_i(1)=first
if (n <= NPAR_GEOP) then
   do k=2,n
       geop_i(k)=geop_i(k-1)*factor
   end do
else
   do k=2,NPAR2_GEOP
       geop_i(k)=geop_i(k-1)*factor
   end do
```

```
temp=factor**NPAR2_GEOP
   k=NPAR2_GEOP
   dо
       if (k \ge n) exit
       k2=k+k
       geop_i(k+1:min(k2,n))=temp*geop_i(1:min(k,n-k))
       temp=temp*temp
       k=k2
   end do
end if
END FUNCTION geop_i
FUNCTION geop_c(first,factor,n)
COMPLEX(SP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
COMPLEX(SP), DIMENSION(n) :: geop_c
INTEGER(I4B) :: k,k2
COMPLEX(SP) :: temp
if (n > 0) geop_c(1)=first
if (n <= NPAR_GEOP) then
   do k=2,n
       geop_c(k)=geop_c(k-1)*factor
   end do
else
   do k=2.NPAR2 GEOP
       geop_c(k)=geop_c(k-1)*factor
   end do
   temp=factor**NPAR2_GEOP
   k=NPAR2_GEOP
   dο
       if (k \ge n) exit
       geop_c(k+1:min(k2,n))=temp*geop_c(1:min(k,n-k))
       temp=temp*temp
       k=k2
   end do
end if
END FUNCTION geop_c
FUNCTION geop_dv(first,factor,n)
REAL(DP), DIMENSION(:), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(size(first),n) :: geop_dv
INTEGER(I4B) :: k,k2
REAL(DP), DIMENSION(size(first)) :: temp
if (n > 0) geop_dv(:,1)=first(:)
if (n <= NPAR_GEOP) then
   do k=2,n
       geop_dv(:,k)=geop_dv(:,k-1)*factor(:)
   end do
else
   do k=2,NPAR2_GEOP
       geop_dv(:,k)=geop_dv(:,k-1)*factor(:)
   end do
   temp=factor**NPAR2 GEOP
   k=NPAR2_GEOP
   do
       if (k \ge n) exit
       k2=k+k
       geop_dv(:,k+1:min(k2,n))=geop_dv(:,1:min(k,n-k))*&
           spread(temp,2,size(geop_dv(:,1:min(k,n-k)),2))
       temp=temp*temp
       k=k2
   end do
end if
```

```
END FUNCTION geop_dv
RECURSIVE FUNCTION cumsum_r(arr,seed) RESULT(ans)
   Cumulative sum on an array, with optional additive seed.
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
REAL(SP), OPTIONAL, INTENT(IN) :: seed
REAL(SP), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j
REAL(SP) :: sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0.0_sp
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
    do j=2,n
        ans(j)=ans(j-1)+arr(j)
    end do
else
    ans(2:n:2) = cumsum_r(arr(2:n:2) + arr(1:n-1:2), sd)
    ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
END FUNCTION cumsum_r
RECURSIVE FUNCTION cumsum_i(arr,seed) RESULT(ans)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), OPTIONAL, INTENT(IN) :: seed
INTEGER(I4B), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j,sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0_i4b
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
    do j=2,n
        ans(j)=ans(j-1)+arr(j)
else
    ans(2:n:2) = cumsum_i(arr(2:n:2) + arr(1:n-1:2), sd)
    ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
END FUNCTION cumsum_i
RECURSIVE FUNCTION cumprod(arr, seed) RESULT(ans)
   Cumulative product on an array, with optional multiplicative seed.
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
REAL(SP), OPTIONAL, INTENT(IN) :: seed
REAL(SP), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j
REAL(SP) :: sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=1.0_sp
if (present(seed)) sd=seed
ans(1)=arr(1)*sd
if (n < NPAR_CUMPROD) then
    do j=2,n
        ans(j)=ans(j-1)*arr(j)
    end do
else
    ans(2:n:2) = cumprod(arr(2:n:2)*arr(1:n-1:2),sd)
    ans(3:n:2)=ans(2:n-1:2)*arr(3:n:2)
END FUNCTION cumprod
```

```
FUNCTION poly_rr(x,coeffs)
   Polynomial evaluation.
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
REAL(SP) :: poly_rr
REAL(SP) :: pow
REAL(SP), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n \le 0) then
   poly_rr=0.0_sp
else if (n < NPAR_POLY) then
   poly_rr=coeffs(n)
   do i=n-1,1,-1
       poly_rr=x*poly_rr+coeffs(i)
   end do
else
   allocate(vec(n+1))
   pow=x
   vec(1:n)=coeffs
       vec(n+1)=0.0_{sp}
       nn=ishft(n+1,-1)
       vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
       if (nn == 1) exit
       pow=pow*pow
       n=nn
   end do
   poly_rr=vec(1)
   deallocate(vec)
end if
END FUNCTION poly_rr
FUNCTION poly_dd(x,coeffs)
REAL(DP), INTENT(IN) :: x
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs
REAL(DP) :: poly_dd
REAL(DP) :: pow
REAL(DP), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n \le 0) then
   poly_dd=0.0_dp
else if (n < NPAR_POLY) then
   poly_dd=coeffs(n)
    do i=n-1,1,-1
       poly_dd=x*poly_dd+coeffs(i)
   end do
else
   allocate(vec(n+1))
   pow=x
   vec(1:n)=coeffs
   do
       vec(n+1)=0.0_dp
       nn=ishft(n+1,-1)
       vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
       if (nn == 1) exit
       pow=pow*pow
       n=nn
   end do
   poly_dd=vec(1)
    deallocate(vec)
end if
END FUNCTION poly_dd
```

```
FUNCTION poly_rc(x,coeffs)
COMPLEX(SPC), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
COMPLEX(SPC) :: poly_rc
COMPLEX(SPC) :: pow
COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n \le 0) then
    poly_rc=0.0_sp
else if (n < NPAR_POLY) then
    poly_rc=coeffs(n)
    do i=n-1,1,-1
       poly_rc=x*poly_rc+coeffs(i)
    end do
else
    allocate(vec(n+1))
    pow=x
    vec(1:n)=coeffs
   do
        vec(n+1)=0.0_sp
       nn=ishft(n+1,-1)
       vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
       if (nn == 1) exit
       pow=pow*pow
       n=nn
    end do
    poly_rc=vec(1)
    deallocate(vec)
end if
END FUNCTION poly_rc
FUNCTION poly_cc(x,coeffs)
COMPLEX(SPC), INTENT(IN) :: x
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: coeffs
COMPLEX(SPC) :: poly_cc
COMPLEX(SPC) :: pow
COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n \le 0) then
   poly_cc=0.0_sp
else if (n < NPAR_POLY) then
   poly_cc=coeffs(n)
    do i=n-1,1,-1
        poly_cc=x*poly_cc+coeffs(i)
    end do
else
    allocate(vec(n+1))
   pow=x
    vec(1:n)=coeffs
        vec(n+1)=0.0_sp
       nn=ishft(n+1,-1)
        vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
       if (nn == 1) exit
       pow=pow*pow
       n=nn
    end do
    poly_cc=vec(1)
    deallocate(vec)
end if
END FUNCTION poly_cc
FUNCTION poly_rrv(x,coeffs)
```

```
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(SP), DIMENSION(size(x)) :: poly_rrv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m \le 0) then
   poly_rrv=0.0_sp
else if (m < n .or. m < NPAR_POLY) then
   poly_rrv=coeffs(m)
    do i=m-1,1,-1
       poly_rrv=x*poly_rrv+coeffs(i)
    end do
else
        poly_rrv(i)=poly_rr(x(i),coeffs)
    end do
end if
END FUNCTION poly_rrv
FUNCTION poly_ddv(x,coeffs)
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(DP), DIMENSION(size(x)) :: poly_ddv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m \le 0) then
   poly_ddv=0.0_dp
else if (m < n .or. m < NPAR_POLY) then
    poly_ddv=coeffs(m)
    do i=m-1,1,-1
       poly_ddv=x*poly_ddv+coeffs(i)
    end do
else
       poly_ddv(i)=poly_dd(x(i),coeffs)
    end do
end if
END FUNCTION poly_ddv
FUNCTION poly_msk_rrv(x,coeffs,mask)
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask REAL(SP), DIMENSION(size(x)) :: poly_msk_rrv
poly_msk_rrv=unpack(poly_rrv(pack(x,mask),coeffs),mask,0.0_sp)
END FUNCTION poly_msk_rrv
FUNCTION poly_msk_ddv(x,coeffs,mask)
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(DP), DIMENSION(size(x)) :: poly_msk_ddv
poly_msk_ddv=unpack(poly_ddv(pack(x,mask),coeffs),mask,0.0_dp)
END FUNCTION poly_msk_ddv
RECURSIVE FUNCTION poly_term_rr(a,b) RESULT(u)
   Tabulate cumulants of a polynomial.
REAL(SP), DIMENSION(:), INTENT(IN) :: a
REAL(SP), INTENT(IN) :: b
REAL(SP), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)
if (n < NPAR_POLYTERM) then
    do j=2,n
       u(j)=a(j)+b*u(j-1)
    end do
```

```
else
    u(2:n:2) = poly_term_rr(a(2:n:2) + a(1:n-1:2)*b,b*b)
   u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
end if
END FUNCTION poly_term_rr
RECURSIVE FUNCTION poly_term_cc(a,b) RESULT(u)
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
COMPLEX(SPC), INTENT(IN) :: b
COMPLEX(SPC), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)
if (n < NPAR_POLYTERM) then
    do j=2,n
       u(j)=a(j)+b*u(j-1)
    end do
else
    u(2:n:2) = poly_term_cc(a(2:n:2)+a(1:n-1:2)*b,b*b)
    u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
end if
END FUNCTION poly_term_cc
FUNCTION zroots_unity(n,nn)
   Complex function returning nn powers of the nth root of unity.
INTEGER(I4B), INTENT(IN) :: n,nn
COMPLEX(SPC), DIMENSION(nn) :: zroots_unity
INTEGER(I4B) :: k
REAL(SP) :: theta
zroots_unity(1)=1.0
theta=TWOPI/n
k=1
do
    if (k \ge nn) exit
    zroots_unity(k+1)=cmplx(cos(k*theta),sin(k*theta),SPC)
    zroots_unity(k+2:min(2*k,nn))=zroots_unity(k+1)*&
        zroots_unity(2:min(k,nn-k))
   k=2*k
end do
END FUNCTION zroots_unity
   Routines for "outer" operations on vectors. The order convention is: result(i,j) = first\_operand(i)
   (op) second_operand(j).
FUNCTION outerprod_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerprod_r
outerprod_r = spread(a,dim=2,ncopies=size(b)) * &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_r
FUNCTION outerprod_d(a,b)
REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerprod_d
outerprod_d = spread(a,dim=2,ncopies=size(b)) * &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_d
FUNCTION outerdiv(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiv
outerdiv = spread(a,dim=2,ncopies=size(b)) / &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiv
FUNCTION outersum(a,b)
```

REAL(SP), DIMENSION(:), INTENT(IN) :: a,b

```
REAL(SP), DIMENSION(size(a), size(b)) :: outersum
outersum = spread(a,dim=2,ncopies=size(b)) + &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outersum
FUNCTION outerdiff_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a.b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiff_r
outerdiff_r = spread(a,dim=2,ncopies=size(b)) - &
   spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_r
FUNCTION outerdiff_d(a,b)
REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerdiff_d
outerdiff_d = spread(a,dim=2,ncopies=size(b)) - &
   spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_d
FUNCTION outerdiff_i(a,b)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: a,b
INTEGER(I4B), DIMENSION(size(a),size(b)) :: outerdiff_i
outerdiff_i = spread(a,dim=2,ncopies=size(b)) - &
   spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_i
FUNCTION outerand(a,b)
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: a,b
LOGICAL(LGT), DIMENSION(size(a), size(b)) :: outerand
outerand = spread(a,dim=2,ncopies=size(b)) .and. &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerand
   Routines for scatter-with-combine.
SUBROUTINE scatter_add_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source), size(dest_index), 'scatter_add_r')
m=size(dest)
do j=1,n
   i=dest_index(j)
    if (i > 0 .and. i \le m) dest(i)=dest(i)+source(j)
END SUBROUTINE scatter_add_r
SUBROUTINE scatter_add_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source), size(dest_index), 'scatter_add_d')
m=size(dest)
do j=1,n
    i=dest_index(j)
    if (i > 0 .and. i \le m) dest(i)=dest(i)+source(j)
end do
END SUBROUTINE scatter_add_d
SUBROUTINE scatter_max_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source), size(dest_index), 'scatter_max_r')
m=size(dest)
do j=1,n
   i=dest_index(j)
```

```
if (i > 0 .and. i \le m) dest(i)=max(dest(i), source(j))
end do
END SUBROUTINE scatter_max_r
SUBROUTINE scatter_max_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source), size(dest_index), 'scatter_max_d')
m=size(dest)
do j=1,n
    i=dest_index(j)
    if (i > 0 .and. i \le m) dest(i)=max(dest(i),source(j))
END SUBROUTINE scatter_max_d
   Routines for skew operations on matrices:
SUBROUTINE diagadd_rv(mat,diag)
   Adds vector or scalar diag to the diagonal of matrix mat.
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagadd_rv')
do j=1,n
   mat(j,j)=mat(j,j)+diag(j)
end do
END SUBROUTINE diagadd_rv
SUBROUTINE diagadd_r(mat,diag)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
   mat(j,j)=mat(j,j)+diag
end do
END SUBROUTINE diagadd_r
SUBROUTINE diagmult_rv(mat,diag)
   Multiplies vector or scalar diag into the diagonal of matrix mat.
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagmult_rv')
do j=1,n
    mat(j,j)=mat(j,j)*diag(j)
end do
END SUBROUTINE diagmult_rv
SUBROUTINE diagmult_r(mat,diag)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
\mathtt{REAL}(\mathtt{SP}), \mathtt{INTENT}(\mathtt{IN}) :: \mathtt{diag}
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
    mat(j,j)=mat(j,j)*diag
end do
END SUBROUTINE diagmult_r
FUNCTION get_diag_rv(mat)
   Return as a vector the diagonal of matrix mat.
REAL(SP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(SP), DIMENSION(size(mat,1)) :: get_diag_rv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_rv')
do j=1,size(mat,1)
    get_diag_rv(j)=mat(j,j)
```

Other routines:

```
end do
END FUNCTION get_diag_rv
FUNCTION get_diag_dv(mat)
REAL(DP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(DP), DIMENSION(size(mat,1)) :: get_diag_dv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_dv')
do j=1,size(mat,1)
   get_diag_dv(j)=mat(j,j)
end do
END FUNCTION get_diag_dv
SUBROUTINE put_diag_rv(diagv,mat)
   Set the diagonal of matrix mat to the values of a vector or scalar.
REAL(SP), DIMENSION(:), INTENT(IN) :: diagv
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n=assert_eq2(size(diagv),min(size(mat,1),size(mat,2)),'put_diag_rv')
do j=1,n
   mat(j,j)=diagv(j)
end do
END SUBROUTINE put_diag_rv
SUBROUTINE put_diag_r(scal,mat)
REAL(SP), INTENT(IN) :: scal
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
   mat(j,j)=scal
end do
END SUBROUTINE put_diag_r
SUBROUTINE unit_matrix(mat)
   Set the matrix mat to be a unit matrix (if it is square).
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: mat
INTEGER(I4B) :: i,n
n=min(size(mat,1),size(mat,2))
mat(:,:)=0.0_sp
do i=1,n
   mat(i,i)=1.0_sp
END SUBROUTINE unit_matrix
FUNCTION upper_triangle(j,k,extra)
   Return an upper triangular logical mask.
INTEGER(I4B), INTENT(IN) :: j,k
INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
LOGICAL(LGT), DIMENSION(j,k) :: upper_triangle
INTEGER(I4B) :: n
if (present(extra)) n=extra
upper_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) < n)
END FUNCTION upper_triangle
FUNCTION lower_triangle(j,k,extra)
   Return a lower triangular logical mask.
INTEGER(I4B), INTENT(IN) :: j,k
INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
LOGICAL(LGT), DIMENSION(j,k) :: lower_triangle
INTEGER(I4B) :: n
n=0
if (present(extra)) n=extra
lower_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) > -n)
END FUNCTION lower_triangle
```

$$\label{eq:function_vabs} \begin{split} & \text{FUNCTION vabs}(\texttt{v}) \\ & \text{Return the length (ordinary $L2$ norm) of a vector.} \\ & \text{REAL}(\texttt{SP}), \; \texttt{DIMENSION}(:), \; \texttt{INTENT}(\texttt{IN}) :: \; \texttt{v} \\ & \text{REAL}(\texttt{SP}) :: \; \texttt{vabs} \\ & \text{vabs} = & \text{sqrt}(\texttt{dot\_product}(\texttt{v},\texttt{v})) \\ & \text{END FUNCTION vabs} \end{split}$$

END MODULE nrutil