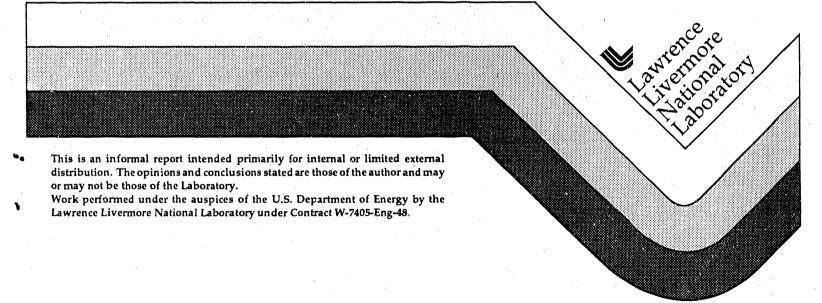
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APTBLIBE: Geometrical and Monte Carlo Sampling Routines for the Cray Computer

Arthur L. Edwards

April 1990



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Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

APTBLIBE: Geometrical and Monte Carlo Sampling Subroutines for the Cray Computers

Arthur L. Edwards.

UCRL-ID--103432

1990 April 4.

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AVAILABILITY

The latest revisions of the BUILD library APTBLIBE and the user document APTDOC are in the LIB library APTSLIBE, and may be obtained by executing the following on a Cray computer:

```
xport read .245100:aptslibe!end / t v
lib aptslibe!x aptdoc aptblibe!end / t v
```

where the exclamation character "!" represents the linefeed key.

Older versions of the LIB library APTSLIBE may be obtained by executing:

```
xport list .245100:altslibh / t v
read .245100:altslibh:yymmdd
end
```

where yymmdd is a copy of APTSLIBE saved in year "yy", month "mm", and day "dd".

Library APTBLIBE is a BUILD library of Cray-compiled binary modules. Individual or sets of modules may be extracted and added to other BUILD libraries by using the BUILD utility routine, or all of the modules may be made available by specifying the APTBLIBE library in the CIVIC, CFT, and/or LOD directives.

You may view the user document APTDOC on a TMDS screen by executing:

```
trix ac!o!aptdoc!tvnnnn!p1 / t v
```

where nnnn is your TMDS number. The document may be searched as you would any other ASCII test file. To send a printed copy of the document to your box, execute:

```
allout hsp aptdoc box ann aptdoc / t v
```

where ann is your box number.

The FORTRAN source files for any of the binary modules in APTBLIBE may be extracted from LIB file APTSLIBE by executing:

```
lib aptslibe / t v
list alwith. apt s.
x filelist
end
```

where filelist is a list of the desired files. These may also be viewed with TRIX, and/or printed copies obtained with ALLOUT.

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ABSTRACT

APTBLIBE is a new BUILD library of about 151 Cray-compiled binary subroutines for numerical geometry and Monte Carlo sampling, of which 93 are described here (the rest will be described in a revision). It is designed especially to support 2-D and 3-D codes that generate and track beams or particles of energy or matter (APT = All-Particle-Tracking). The LIB library APTSLIBE contains the FORTRAN source files, and the user document APTDOC, much of which can be updated directly from the source files. This document describes APTBLIBE and its subroutines, how to use them, and the features designed to simplify the development of new codes, and improve the speed, efficiency, reliability and ease of maintenance of any codes which make use of it.

INTRODUCTION

Many large-scale computer programs at LLNL and elsewhere require code modules for generating and tracking beams or particles of energy or matter in various types of spatial meshes and coordinate systems, in 1-D, 2-D and 3-D geometries. Some of these modules require Monte Carlo sampling of random variables from a variety of probability distributions. These and other codes may also have to solve difficult geometric problems in generating and rezoning the mesh. As a result, a large number of subroutines, functions, and algorithms have been developed over the years for geometric and Monte Carlo sampling applications, greatly varying in style, structure, readability, accessibility, modularity, and efficiency. A single large code may have the same function duplicated many times, in many forms, in different code modules.

Thus, there is a clear need for one or more standard libraries of numerical geometry and Monte Carlo sampling subroutines, both for use in developing new codes, especially those for 3-D geometries, and for gradual replacement of coding in existing codes as they are upgraded. The goals in designing such libraries include improving speed, efficiency, accuracy, reliability, accessibility, readability, generality, flexibility, ease of maintenance, and ease of use.

The APTBLIBE library is designed to meet this immediate need, and to provide a basis for expansion to meet future needs. APTBLIBE already contains geometric and Monte Carlo sampling subroutines used by many Monte Carlo particle-tracking codes, in addition to a comprehensive set of basic subroutines for geometrical applications in 1-D, 2-D and 3-D geometries, in Cartesian, cylindrical and spherical coordinate systems. The development and inclusion in the library of additional higher-level subroutines is simplified by the hierarchical nature of the set of subroutines, and is being done as needed.

The subroutines in APTBLIBE, how to use them, and the methods used to accomplish the design goals will be described below.

WHAT IS IN APTBLIBE

APTBLIBE currently contains about 93 subroutines, ranging from basic low-level procedures to the higher-level geometric and Monte Carlo sampling methods needed for Monte Carlo tracking of beams and particles of energy and matter in 3-D geometries. These subroutines can be subdivided into five groups, as follows:

The fundamental physical and chemical constants (2 subroutines). Mathematics and statistics (3 subroutines). Monte Carlo sampling (8+ subroutines). Precision and round-off error control (7 subroutines). Geometry (71+ subroutines).

A summary of the subroutines in each group follows. For a more detailed listing of subroutines by function, including the type of geometry and coordinate system, where applicable, see the appendix "SUBROUTINES BY FUNCTION" at the end of this document.

The latest self-consistent set of values of the fundamental constants of physics and chemistry are provided in two subroutines, aptconl (180 values in cm-g-sh-jerk-kev units), and aptconm (230 values in SI units). It is necessary to look at the source listing of each subroutine to find the index needed as an input argument to get the value of each constant.

The mathematics and statistics group consists of two subroutines for finding real roots of quadratic equations, aptqrts (scalar) and aptqrtv (vector), and one subroutine for finding the mean and standard deviation of an array of values, aptmean. Each has unique features for control of round-off errors.

The Monte Carlo sampling group consists of 8+ subroutines for random sampling from probability distributions, including aptslid and aptsliv for 1-D uniform and linear distributions (with no sampling in negative regions), apttloc and aptqloc for 2-D uniform spatial distributions over triangles and quadrangles, respectively, aptscat for 3-D uniform directional distributions, aptscap for 3-D cosine**power directional distributions, aptscad for uniform directional distributions in a plane in 3-D space, aptxnup for frequencies from Plank or Wien distributions, and others.

The precision and round-off error control group consists of 7 subroutines, including aptfdad (scalar) and aptfdav (vector) for adjusting values of a variable near 0.0 and 1.0, aptvlic (2-D) and aptvlim (3-D) for imposing lower limits on the magnitudes of vector components, aptvtoc (2-D) and aptvtol (3-D) for applying any of several limit or truncation options to the magnitudes of spatial point coordinates or vector components, and aptrnds for rounding off floating point numbers to any specified relative or absolute precision. See the section titled "FUZZY GEOMETRY" below.

The geometry group consists of 74+ subroutines for a broad range of applications. These include conversion between various coordinate systems; doing basic vector and matrix operations; finding angle relationships between lines and between vectors; testing for special geometric relationships; doing the basic symmetry group operations of translation, rotation, reflection, and inversion, and combinations of these; linear and global scaling; finding distances; finding the initial vector direction and distance between two points in any coordinate system; moving a point a specified distance in a specified initial direction in any coordinate system; finding the alternate geometric descriptions of lines and planes; finding vectors perpendicular to lines in a major plane, or planes in 3-D space;

finding the vertex areas of a triangle; finding the vertex areas and shape (convex, boomerang or bowtie) of a quadrangle; finding the local coordinates (fractional distances between opposite sides) of points in quadrangles; finding the intersections between straight lines or linear tracks and various boundaries in 2-D and 3-D.

HOW TO USE APTBLIBE

APTBLIBE is a BUILD library currently containing about 93 Cray-compiled binary subroutines. The "availability" section at the beginning of this document tells how to get APTBLIBE, the source file LIB library APTSLIBE, and the user document APTDOC.

The appendix "SUBROUTINES BY FUNCTION" in this document contains a detailed summary of the subroutines in APTBLIBE by function, including the number of spatial dimensions and type of coordinate system, when applicable. This should allow a user to find the name of the subroutine with the required function, if it is in APTBLIBE.

The section of this document titled "SUBROUTINE DESCRIPTIONS IN ALPHABETIC ORDER" contains the initial comment block from each of the subroutines in APTBLIBE, extracted directly from the source files. Each comment block contains the calling statement and argument list, the dates of origination and last update, the location of the needed libraries and source file, the purpose and general description of the subroutine, lists of input and output arguments, a list of calls to other APTBLIBE subroutines, a history of significant changes that might affect the user, and a list of detailed definitions of all arguments. In most cases, this information should be sufficient to allow proper use of the subroutine. If not, the source file may be obtained from LIB library file APTSLIBE and read to obtain additional information, including definitions of all internal variables, comments describing each step of the procedure, and the coding itself. Each source file is intended to be completely self-documented.

For efficiency, 1-D and 2-D analogues of 3-D geometric algorithms have been placed in separate subroutines, to eliminate unnecessary subroutine arguments and complexity. All strictly 2-D subroutines, in which all points and vectors are confined to a major plane, have names ending in the letter "c". Subroutines are provided for rotating any non-major plane into a major plane. The rotation operator may be saved to do the inverse rotation later, after major-plane calculations are done.

Most of the subroutines in APTBLIBE are vectorized, and some algorithms are offered in two or more subroutines, depending on whether certain arguments are scalar values or array values, or on how certain geometric objects are defined. For example, a line may be represented by two points, or a point and a directional vector, or a plane may be represented by three points or a point and a normal vector. Subroutines are provided to interconvert between these representations.

All communication between APTBLIBE subroutines and each other, and with the calling program, is through argument lists. There are no shared cliches or common blocks. Input and output arrays in each argument list are usually members of a single table, with the same index and same array size. It is up to the user to allocate memory for these arrays, and put the input data into the required form. All local variables in APTBLIBE subroutines are declared in local labelled common blocks, named by prefixing the subroutine name with the letter "I". When local temporary arrays are needed, array processing is done in blocks of 64 or less, so no local array is sized any greater than 64.

Most subroutines indicate an input data error, failure to find a a requested result, or the occurence of a special or limiting case, by returning a scalar and/or array integer flag, or a physically impossible value of an output argument. Integer flags may have several possible values. The most often used flag, "nerr", is usually returned with a value of 1 when a specified array size is non-positive. The calling program should test for any of these cases that can possible occur, and take appropriate action before errors propagate or a

crash occurs. Great care is taken to identify all special and extreme cases, and to indicate their occurence to the calling program by use of the special result flags.

SUBROUTINE DESIGN

The subroutines in the APTBLIBE library were designed with the following goals: speed, efficiency, accuracy, reliability, accessibility, readability, generality, flexibility, ease of maintenance, and ease of use.

Calculational speed is obtained primarily by making maximum use of vectorization of do-loops, by eliminating unnecessary calculations by using separate subroutines for 2-D analogues of 3-D procedures, and by using input options to eliminate do-loops not needed for a particular application.

Efficiency is obtained by using a hierarchy of subroutines, beginning with a set of basic operations, followed by increasingly higher-level subroutines, making maximum use of calls to lower-level subroutines to avoid repetition of coding. This also belps to insure uniformity of method, increases reliability, simplifies maintenance, and simplifies the addition of higher-level user applications to the library.

Accuracy is obtained by thorough testing to eliminate coding errors, and by the careful use of the techniques of "fuzzy geometry", to eliminate or control the effects of numerical round-off errors. See the section of this document titled "FUZZY GEOMETRY TECHNIQUES".

Reliability is obtained by thorough testing, including all possible extreme, special, and degenerate cases, and all possible types of input errors, to ensure that the expected results are obtained in all cases, and that sufficient information is returned to the calling program to allow appropriate action to be taken in all cases, whenever possible. The test program for a particular subroutine is run whenever that subroutine, or any subroutine it is dependent on, is changed.

Accessability is obtained by making all source files available in LIB library file APTSLIBE.

Readability is obtained by making each subroutine adhere to the same strict coding standard. The requirements include the inclusion of an initial block of comments containing certain required information (see the section of this document titled "SUBROUTINE DESCRIPTIONS IN ALPHABETIC ORDER") and liberal use of blank lines and comments. The coding standard also specifies the format of all FORTRAN statements, to ensure readability and uniformity in all subroutines. In general, the names of dummy arguments and local variables are chosen by a consistent set of rules in all subroutines, making is easier to remember their meanings.

Generality and flexibility are obtained by including all of the basic geometric and vector operations in separate subroutines, allowing a hierarchy of subroutines to be developed, ranging from low-level to high-level applications; by including separate subroutines for 1-D, 2-D and 3-D analogues of the same process, and for the same process carried out in different coordinate systems; and by including subroutines for conversion between different coordinate systems, and between different descriptions of the same geometric objects.

Ease of maintenance is obtained by a variety of methods, including use of a coding standard, use of a nomenclature standard, use of a hierarchical subroutine structure, and use of a number of computer tools for updating, compiling, loading, saving, and documenting, all of which are in place, and procedures for their use documented.

Ease of use is obtained by providing complete documentation, both here and in each source file, by allowing communication with the calling calling program only through the argument list, which eliminates any dependency on macros, cliches, or shared common blocks; by the use of a very basic set of FORTRAN statement types, minimizing or eliminating the need for changes to run on different computers; and by the general, flexible, and modular structure of the subroutines.

The average subroutine has 222 lines, of which 45 are blank, 75 are the initial comment block, 16 are other comments, 8 are dimension declarations for arguments, 13 are common block declarations for local variables, and the remaining 63 are other coding. Many of the latter have appended comments. (Note: appended comments are easily moved to a separate line by using trix ac with a simple alter file.)

FUZZY GEOMETRY TECHNIQUES

A unique feature of this library of subroutines is the inclusion and careful use of a number of techniques to control or eliminate the effects of round-off error due to the finite number of bits of precision available on the Crays and other computers.

These "fuzzy geometry" techniqes make it possible to get correct and unambiguous answers to important geometric questions such as whether geometric objects are coincident, congruent, colinear, coplanar, parallel, perpendicular or tangent, within the uncertainty due to round-off error, and to avoid producing meaningless results that may later require special handling and testing to prevent major errors or program crashes.

Most subroutines have an input argument specifying a relative precision "tol", and allow certain intermediate and final results to be truncated to zero, if their absolute values are less than the estimated error in their calculation, based on "tol" and the actual numerical procedures used.

Other subroutines (aptfdad, aptfdav, aptvtoc and aptvtol) provide a number of options to truncate or place limits on scalar values, spatial point coordinates, or vector components. Subroutine aptrnds may be used to round off any floating point number to a specified absolute or relative precision. These options may be tailored to the precision of the computer in use, and to the requirements of the particular application.

On the Crays, the value of "tol" should be approximately equal to 1.E-12**(1/n), when the tested value x is to be used in the form x**n. A larger value should be used (e.g., 1.E-11), when the input arguments are likely to have been affected previously by round-off error.

Whenever an expression contains a denominator which can legitimately have a value of zero, a fuzz factor "fuz", equal to 1.E-99, is added to the denominator, to avoid division by zero. The value 1.E-99 might have to be changed on some computers. Whenever this technique results in an incorrect value of an output argument, either a separate warning flag is returned, or the description or the output argument in the subroutine comment block contains a warning, allowing the calling program to test for such results.

CRAY MEMORY REQUIREMENTS

The APTBLIBE library currently requires 72,000 words of Cray memory. The binary modules in APTBLIBE require an average of about 1000 words of Cray memory each, including about 250 words for the local common block. Since a call to one APTBLIBE subroutine may initiate a chain of calls to other lower-level APTBLIBE subroutines, as well as subroutines in other system libraries, the total memory requirement may be larger. Currently, the longest call chain is four.

SUBROUTINE DESCRIPTIONS IN ALPHABETIC ORDER

SUBROUTINE APTBANC

call aptbanc (au, av, bu, bv, cu, cv, np, tol, bdu, bdv, du, dv, nerr)

Version: aptbanc Updated 1990 March 8 17:00. aptbanc Originated 1990 March 8 17:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptbanclend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the bisector bd = (bdu, bdy) of the angle "abc" formed by the points a = (au, ay), b = (bu, by), and c = (cu, cy) in the uv plane, and point d' (du, dv), the intercept of the bisector on the line "ca". If points "a", "b" and "c" are colinear,

vector "bd" will be zero, and point "d" will be point "b".

Input: au, av, bu, bv, cu, cv, np, tol.

Output: bdu, bdv, du, dv, nerr.

Calls: aptvdic, aptvuac (sources in aptslibe,

binaries in aptblibe).

Glossary:

The u and v coordinates of point "a". Size np. au, av Input

The u and v components of the vector "bd" which bisects angle "abc", and connects points "b" and "d". bdu, bdv Output

The u and v coordinates of point "b". Size np. bu. by Input

The u and v coordinates of point "c". Size np. Input cu, cv

The υ and v coordinates of point "d" on line "ca". du, dv Output The intercept of bisector "bd" on line "ca".

Size np.

Output Indicates an input error, if not 0. nerr

1 if np is not positive.

Size of arrays au, av, bu, bv, cu, cv, Input np

bdu, bdv, du, dv.

Input Numerical tolerance limit.

SUBROUTINE APTBANG

call aptbang (ax, ay, az, bx, by, bz, cx, cy, cz, np, tol, bdx, bdy, bdz, dx, dy, dz, nerr)

1990 March 8 17:40. Version: aptbang Updated 1990 March 8 17:40. aptbang Originated 1990 March 8 17:40.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptbanglend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the bisector bd = (bdx, bdy, bdz) of the angle "abc" formed by the points

a = (ax, ay, az), b = (bx, by, bz), and c = (cx, cy, cz),
and point d = (dx, dy, dz), the intercept of the bisector on
the line "ca". If points "a", "b" and "c" are colinear, vector "bd" will be zero, and point "d" will be point "b".

Input: ax, ay, az, bx, by, bz, cx, cy, cz, np, tol.

bdx, bdy, bdz, dx, dy, dz, nerr. Output:

Calls: aptvdis, aptvuna (sources in aptslibe,

binaries in aptblibe).

Glossary:

The x, y, z coordinates of point "a". Size np. ax, ay, az Input

The x, y, z components of the vector "bd" which bdx, y, z Output

bisects angle "abc", and connects points "b" and "d".

bx, by, bz Input The x, y, z coordinates of point "b". Size np.

The x, y, z coordinates of point "c". Size np. cx, cy, cz Input

The x, y, z coordinates of point "d" on line "ca".

The intercept of bisector "bd" on line "ca". dx, dy, dz Output

Size np.

Indicates an input error, if not 0. nerr Output

1 if np is not positive.

Size of arrays ax, ay, az, bx, by, bz, cx, cy, cz, пp Input

bdx, bdy, bdz, dx, dy, dz.

Numerical tolerance limit. tol Input

SUBROUTINE APTCINC

ra

rb

tol

Input

Input.

Input

call aptcinc (ra, au, av, rb, bu, bv, np, tol, cu, cv, du, dv, nint, nerr) Version: aptcinc Updated 1990 March 20 14:40. aptcinc Originated 1990 March 20 14:40. Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Source: xport read .245100:aptslibe / 1 1 lib aptslibelx aptblibe aptcinclend / 1 1. aptslibe is a LIB library of FORTRAN scurce files. aptblibe is a BUIID library of Cray-compiled binaries. Purpose: To find, for each of np sets of input data, the points of intersection c = (cu, cv) and d = (du, dv) of the circle of radius ra at point a = (au, av) and the circle of radius rb at point b = (bu, bv), if an intersection occurs. Flag nint indicates the number of intersection points. Flag nerr indicates any input error. Input: ra, au, av, rb, bu, bv, np, tol. Out put: cu, cv, du, dv, nint, nerr. Calls: aptvdic, aptvadc, aptvplc, aptvuac (sources in aptslibe, binaries in aptblibe). Glossary: Input ' The u and v coordinates of point "a" at the center au, av of the circle with radius ra, in the uv plane (2-D). bu, by Input The u and v coordinates of point "b" at the center of the circle with radius rb, in the uv plane (2-D). Output \cdot The u and v coordinates of point "c" at an intersection cu, cv of the two circles centered at points "a" and "b", if an intersection occurs (nint = 1 or 2). Size np. Same as "d" if nint = 1. Meaningless, but set to "a" If nint = 0 or 3. du, dv Output The u and v coordinates of point "d" at an intersection of the two circles centered at points "a" and "b", if an intersection occurs (nint = 1 or 2). Size np. Same as "c" if nint - 1. Meaningless, but set to "a" if nint = 0 or 3. nerr Output Indicates an input error, if not 0. 1 if np is not positive. nint Out put Indicates the number of intersection points: 0 if no intersection occurs. Ignore points "c", "d". 1 if the circles are tangent at the single point "c" = "d". 2 if the circles overlap, intersecting at the two points "c" and "d". 3 if the circles are congruent. The intersection includes each circle. Ignore points "c", "d". np Input Size of arrays.

The radius of the circle centered at point "a". Size np. The absolute value is used.

The radius of the circle centered at point "b". Size np. The absolute value is used.

On Cray computers, recommend 1.e-5 to 1.e-11.

Numerical tolerance limit.

SUBROUTINE APTCONL

call aptconl (ind, np, pgcon, nerr)

Version: aptconl Updated 1990 March 2 15:30. aptconl Originated 1989 March 2 15:30.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Refs:

- 1. "The 1986 Adjustment of the Fundamental Physical Constants", Codata Bulletin Number 63, November 1986, Pergamon Press.
- 2. "Metric Practice Guide E 380-72e", 1973, American Society for Testing and Materials, 1916 Race Street, Philadelphia, Pa 19103.
- 3. File physicons in LIB library physlibe. Execute:

xport read .245100:physlibelend / t v
lib physlibelx physconslend / t v
allout hsp physcons / t v
trix aclolphysconsitvNNNNip1 / t v

Source:

xport read .245100:aptslibe / 1 1
lib aptslibe(x aptblibe aptconlend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose:

To provide the best available values of the fundamental physical constants and conversion factors of physics and chemistry, in cm-g-shake-keV units. See aptronm for SI units. For each of np values of ind, the constant with local index ind is returned in array pocon. The local indices are tabulated below. For definitions of the constants, see the full listing of this subroutine, or reference 3 listed above. If any value of ind is not in the range from 1 to 180, the returned value of pocon will be -1.e99.

```
37 pgfrtoam
                            73 pgk.
                                         109 pgmsubmu 145 pgratde
 1 pga
  pgab185
              38 pgfrtog
                            74 pgketoam
                                         110 pgmsubn
                                                        146 pgratdp
              39 pgfrtojk
  pgalpha
                            75 pgketofr
                                                        147 pgratea
                                         111 pamsubo
              40 pofrtoke
                            76 pgketojk
  pgalphai
                                         112 pgmub
                                                        148 pgrated
  pgamtohz
                            77 paketoro
              41 pyfrtorc
                                                        149 pgratemu
                                         113 pgmube
              42 pgg
                            78 pgkevtog
 6 pgamtojk
                                         114 pgmubf
                                                        150 pgratep
              43 pggamma
  pgamtoke
                            79 pglamce
                                          115 pamubw
                                                        151 pgratmue
  pgamtorc
              44 pggamp
                            80 pglamceb
                                         116 pgmud
                                                        152 pgratne
              45 pggampb
                            81 polamon
  pgamu
                                         117 pgmudb
                                                        153 pgratnp
              46 pggampp
10 pgamud
                                         118 pgmudn
                            82 pglamonb
                                                        154 pgratpe
              47 pggamppb
11 pgamue
                            83 pglamcp
                                          119 pgmue
                                                        155 pgratpmu
12 pgamumu
              48 pggolden
                            84 pglamcpb
                                         120 pgmueb
                                                        156 pgrctoam
13 pgamun
              49 pggsube
                            85 pglosch
                                          121 pgmuen
                                                        157 pgrctofr
              50 pggsubmu
                            86 pgmagfq
14 pgamup
                                          122 pgmumu
                                                        158 pgrctog
15 pgamutog
              51 pggsubn
                            87 pgmdev
                                          123 pomumub
                                                        159 parctojk
16 pgastar
              52 pggtoamu
                            88 pgmdj
                                         124 pgmumun
                                                        160 pgrctoke
17 pgasube
              53 pagtofr
                            89 pameev
                                          125 pgmun
                                                        161 pgrmole
              54 pagtojk
18 pgasubmu
                            90 pomej
                                         126 pgmune
                                                        162 pgrydb
19 pgatm
              55 pagtokev
                            91 pgmmrde
                                          127 pamunf
                                                        163 pgrydbc
20 pgatomx
              56 pagtora
                            92 pgmmrdp
                                          128 pgmunt
                                                        164 pgrydbe
              57 pgh
21 pgbohr
                            93 pgmmremu
                                         129 pgmuntb
                                                        165 pgrydbev
22 pgc
                            94 pgmmrep
              58 pghart
                                          130 pgmuntn
                                                        166 pgsate
23 pacsub1
              59 pohartev
                            95 pommrmup
                                         131 pamunw
                                                        167 pgsatez
24 pgcsub2
              60 pghbar
                            96 pgmmrne
                                          132 pgmup
                                                        168 pgsb
25 pgcunit
              61 pghbarc
                            97 pgmmrnp
                                          133 pgmupb
                                                        169 pgsia
26 pgcuxun
              62 pghbarok
                            98 pammuev
                                          134 pgmupn
                                                        70 pgsid220
27 pgdrohm
              63 pghlen
                            99 pgmmuj
                                          135 pgmupp
                                                        171 pgsigw
28 pge
              64 pghmass
                           100 pgmnev
                                          136 pgmuppb
                                                        172 pgsivolm
29 pgebase
              65 pghok
                           101 pgmnj
                                          137 pgmuppn
                                                        173 pgtemp
30 pgec
              66 pghtime
                           102 pgmolh
                                          138 pgmuvac
                                                        174 pgthomx
31 pgeoh
              67 pgjfvr
                           103 pgmolhc
                                          139 pgnsuba
                                                        175 pgubb
32 paeome
              68 pgjktoam
                           104 pgmoxun
                                         140 pgombi85
                                                        176 pgv76bi
33 pgeomp
              69 pgjktofr
                           105 pgmpev
                                          141 pgqcirc
                                                        177 paymols
                                                        178 pgvmolz
34 pgepsvac
              70 pgjktog
                           106 pgmpj
                                          142 pgqcirch
                                         143 pagha
35 pgerad
              71 pgjktoke
                           107 pgmsubd
                                                        179 pgwien
36 pgfar
              72 pgjktorc
                          108 pgmsube
                                         144 paghr
                                                        180 pi
```

Input: ind, no. Output: pgcon, nerr. Calls: none (sources in aptslibe, binaries in aptblibe). Glossary: ind Indices of constants to be stored in array ogcon. Input Size no. Input Size of arrays ind, pgcon. np Constants. Value pocon(n) is constant with pacon Out put index ind(n). nerr Output Error flag. 1 if np is not positive. Definitions: SI UNIT AND CM-G-SHAKE UNIT CONVERSION FACTORS Definitions and conversion of base units Length or distance. 1 cm (centimeter) = 0.01 m (meter). Mass. 1 g (gram) = 0.001 kg (kilogram). Time. 1 sh (shake) = 1.0e-08 s (second). Electric current. 1 labA = 1 (jerk / cm) **0.5 = 1.0e+09 A (ampere). 1 A = 1 C / s = (1.0e-07 J / m) **0.5.Temperature. 1 keV = 1.160445e+07 K (Kelvin). 1 K = 1 / 273.16 of the thermodynamic temperature of the triple point of water. Note: 1988 NBS triple point of Gallium = 302.9169 K (1.7 ppm). Definitions and conversion of derived units Acceleration. 1 cm / $sh^{**}2 = 1.0e+14 m / s^{**}2$. Area. 1 cm**2 = 1.0e-04 m**2. Density. 1 g / cm**3 = 1.0e+03 kg / m**3. Electric capacitance. 1 labF = 1 sh**2 / cm = 1.0e-07 F (farad). 1 F = 1 A s / V = 1.0e-07 s**2 / m.Electric inductance. 1 labH = 1 cm = 1.0e-09 H (henry). 1 H = 1 V s / A = 1.0e+07 m. Electric resistance. 1 labohm = 1 cm / sh = 0.1 ohm. 1 ohm = 1 V / A = 1.0e+07 m / s. Electric voltage. 1 labV = 1 (jerk cm / sh**2) **0.5 = 1.0e+08 V (volt). 1 V = 1 W / A = (1.0e+07 J m / s**2) **0.5. Electrical charge. 1 labC = 1 (jerk sh^{**2} / cm) **0.5 = 10 C (coulomb). 1 C = 1 A s = (1.0e-07 J s^{**2} / m) **0.5. Electrical conductance. 1 labS = 1 sh / cm = 10 S (siemen). 1 S = 1 A / V = 1.0e-07 s / m. Electron volts. 1 keV (kiloelectron volts) = 1000 eV (electron volts). 1 eV = 1.60217733e-19 J. Energy or work. 1 jerk = 1.0a+09 J (joule). 1 J = 1 kg m**2 / s**2 = 1 N m (newton meter).Force. 1 g cm / $sh^{++}2 = 1$ jerk / cm = 1.0e+07 N (newton). 1 N = 1 Kg m / s**2 = 1 J / m.Magnetic flux. 1 labWb = 1 (jerk cm)**0.5 = 1 Wb (weber).

1 Wb 4 1 V s = (1.0e+07 J m) **0.5.

Magnetic flux density. 1 labT = 1 (jerk / cm**3)**0.5 = 10,000 T (tesla).

1 T = 1 Wb / m**2 = (1.0e+07 J / m**3)**0.5.

Power. 1 jerk / sh = 1.0e+17 W (watt). 1 W = 1 J / s = 1.0e-17 jerk / sh.

Pressure or energy density. 1 jerk / cm**3 = 1.0e15 Pa (pascal). 1 Pa = 1 N / m**2 = 1 J / m**3.

Specific heat. 1 jerk / (g keV) = 8.617385e+04 J / (kg K).

Thermal conductivity. 1 jerk / (sh cm keV) = 8.617385e+11 W / (m K).

Velocity. 1 cm / sh = 1.0e+06 m / s.

Volume. 1 cm**3 = 1.0e-06 m**3.

SUBROUTINE APTCONM

```
call aptconm (ind, np, pgcon, nerr)
```

Version: aptcomm Updated 1990 March 2 15:30. aptcomm Originated 1989 March 2 15:30,

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Refs: 1. "The 1986 Adjustment of the Fundamental Physical

Constants*, Codata Bulletin Number 63, November 1986, Pergamon Press.

- "Metric Fractice Guide E 380-72e", 1973, American Society for Testing and Materials, 1916 Race Street, Philadelphia, Pa 19103.
- 3. File physions in LIB library physlibe. Execute: xport read .245100:physlibelend / t v lib physlibelx physionslend / t v allout hsp physions / t v trix aciolphysionsltvNNNNlp1 / t v

Source

xport read .245100:aptslibe / 1 1
lib aptslibe!x aptblibe aptcommend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose

43 pgevtoj

44 pgevtok

87 pgjtohz

88 pgjtok

To provide the best available values of the fundamental physical constants and conversion factors of physics and chemistry, in SI units. See aptconl for cm-g-shake-keV units. For each of np values of ind, the constant with local index ind is returned in array pgcon. The local indices are tabulated below. For definitions of the constants, see the full listing of this subroutine, or reference 3 listed above. If any value of ind is not in the range from 1 to 217, the returned value of pgcon will be -1.e99.

```
45 paevtoka
                            89 pajtoka
 1 pga
                                         133 pgmpav
                                                        177 pgratea
 2 pgabi85
              46 pgevtorm
                            90 pgjtorm
                                         134 pgmpj
                                                        178 pgrated
 3 pgad
              47 pgfar
                            91 pgk
                                          135 pgmsubd
                                                        179 pgratemu
 4 pgalpha
              48 pgg
                            92 pgkd
                                          136 pgmsube
                                                        180 pgratep
 5 pgalphai
              49 pagamma
                                         137 pgmsubmu
                                                        181 pgratmue
                            93 pgkgtoam
                            94 pgkgtoev
 6 pgamtoev
              50 pggamp
                                         138 pgmsubn
                                                        182 pgratne
                            95 pakatoht
 7 pgamtoht
              51 pagampb
                                         139 pgmsubp
                                                        183 pgratnp
 8 pgamtohz
                            96 pakatohz
              52 pggampp
                                          140 pgmub
                                                        184 pgratpe
 9 pgamtoj
              53 pagamppb
                            97 pakatoj
                                                        185 pgratpmu
                                          141 pgmube
10 pgamtok
              54 pagolden
                            98 pgkgtok
                                          142 pgmubf
                                                        186 pgrmold
                                                        187 pgrmole
                            99 pgkgtorm
11 pgamtokg
              55 pggsube
                                         143 pgmubk
                           100 poktoam
12 pgamtorm
              56 pagsubmu
                                          144 pgmubw
                                                        188 pgrmtoam
13 pgamu
              57 pagsubn
                           101 paktoev
                                          145 pgmud
                                                        189 parmtoev
14 pgamud
              58 pgh
                           102 pgktoht
                                                        190 pgrmtoht
                                          146 pgmudb
15 pgamue
              59 pghart
                           103 paktohz
                                          147 pgmudn
                                                        191 pgrmtohz
16 pgamumu
              60 pghartev
                           104 pgktoj
                                          148 pgmue
                                                        192 pgrmtoj
17 pgamun
              61 pghbar
                           105 pgktokg
                                          149 pgmueb
                                                        193 pgrmtok
                                          150 pamuen
18 pgamup
              62 pohbarc
                           106 pgktorm
                                                        194 parmtoka
19 pgastar
              63 pghbarok
                           107 pglamce
                                          151 pamumu
                                                        195 parydb
20 pgasube
                                         152 pgmumub
                                                        196 parydbc
              64 pghlen
                           108 pglamceb
21 pgasubmu
              65 pghmass
                           109 pglamon
                                          153 pamumun
                                                        197 pgrydbe
22 pgatm
              66 pghok
                           110 pglamchb
                                         154 pomun
                                                        198 pgrydbev
                                                        199 posate
23 pgatomx
              67 pghtime
                           111 pglamcp
                                          155 pomune
                                          156 pgmunf
                                                        200 pgsatez
24 pgbohr
              68 pghttoam
                           112 pglamcpb
25 pgc
              69 pghttoev
                           113 pglosch
                                          157 pgmunk
                                                        201 pgsb
                           114 pgmagfq
                                          158 pgmunt
                                                        202 pgsbd
26 pgcsubl
              70 pghttohz
27 pgcsub2
              71 pghttoj
                           115 pomdev
                                          159 pgmuntb
                                                        203 pgsia
28 pgcsub2d
              72 pghttok
                           116 pamdj
                                          160 pgmuntn
                                                        204 pgs1d220
29 pgcunit
              73 pghttokg
                           117 pomeev
                                          161 pgmunw
                                                        205 pgsigw
                           118 pomej
30 pgcuxun
              74 pghttorm
                                          162 pamup
                                                        206 pgsivolm
31 pgdrohm
              75 pghyfsph
                           119 pommrde
                                          163 pgmupb
                                                        207 pgtemp
32 pge
                                          164 pgmupn
                                                        208 pgtempt
              76 pghzt.oam
                           120 pgmmrdp
33 pgebase
              77 pghztoev
                           121 pommremu
                                         165 panupp
                                                        209 pathomx
34 pgec
              78 pghztoht
                           122 pammrep
                                          166 pgmuppb
                                                        210 pgubb
35 pgeoh
              79 pghztoj
                           123 pommrmup
                                          167 pgmuppn
                                                        211 pgubbd
36 pgeome
              80 pghztok
                           124 pommrne
                                          168 pgmuvac
                                                        212 pgv76bi
37 pgeomp
              81 pghztokg
                           125 pgmmrnp
                                          169 pgnsuba
                                                        213 pgvmolt
                           126 pammuev
                                          170 pgomb185
38 pgepsvac
              82 pghztorm
                                                        214 paymoltz
39 pgerad
              83 pgjfvr
                           127 pammuj
                                          171 pageire
                                                        215 pgwlen
40 pgevtoam
              84 pgjtoamu
                           128 pomnev
                                          172 pageirch
                                                        216 pawlend
41 pgevtoht
              85 pgjtoev
                           129 pomnj
                                          173 pagha
42 pgevtohz
              86 pgjtoht
                           130 pgmolh
                                          174 paghr
```

131 pgmolhc

132 pomoxun

175 pgratde

176 pgratdp

```
Input:
            ind, np.
Output:
           pgcon, nerr.
            none
Calls:
            (sources in aptslibe, binaries in aptblibe).
Glossary:
            Input
                     Indices of constants to be stored in array pgcon.
1 nd
                       Size np.
                     Size of arrays ind, pgcon.
            Input
αn
                     Constants. Value pgcon(n) is constant with
pgaon
            Output
                        index ind(n).
            Output Error flag. 1 if no is not positive.
nerr
Definitions:
            SI UNIT AND CM-G-SHAKE UNIT CONVERSION FACTORS
                Definitions and conversion of base units
Length or distance. 1 cm (centimeter) = 0.01 m (meter).
Mass. 1 g (gram) = 0.001 \text{ kg (kilogram)}.
Time. 1 sh (shake) = 1.0e-08 s (second).
Electric current. 1 labA = 1 (jerk / cm) **0.5 = 1.0e+09 A (ampere). 1 A = 1 C / s = (1.0e-07 \text{ J/m}) **0.5.
Temperature. 1 keV = 1.160445e+07 K (Kelvin).
                1 K = 1 / 273.16 of the thermodynamic temperature of
               the triple point of water, Note: 1988 NBS triple point of Gallium = 302,9169 K (1.7 ppm),
            Definitions and conversion of derived units
Acceleration. 1 cm / sh^{**}2 = 1.0e+14 m / s^{**}2.
Area. 1 cm**2 = 1.0e-04 m**2.
Density. 1 g / cm**3 = 1.0e+03 kg / m**3.
Electric capacitance. 1 labF = 1 sh**2 / cm = 1.0e-07 F (farad).
                          1 F = 1 A s / V = 1,0e-07 s**2 / m.
Electric inductance. 1 labH = 1 cm = 1.0e-09 H (henry).
1 H = 1 V s / A = 1.0e+07 m.
Electric resistance. 1 labohm = 1 cm / sh = 0.1 ohm. 1 ohm = 1 V / A = 1.0e+07 m / s.
Electric voltage. 1 labV = 1 (jerk cm / sh^{**}2) **0.5 = 1.0e+08 V (volt).
                      1 V = 1 W / A = (1.0e+07 J m / s**2)**0.5.
Electrical charge. 1 labC = 1 (jerk sh**2 / cm) **0.5 = 10 C (coulomb).
                       1 C = 1 A s = (1.0e-07 J s**2 / m)**0.5.
Electrical conductance. 1 labS = 1 sh / cm = 10 S (siemen).
                            1 S = 1 A / V = 1.0e-07 s / m.
Electron volts. 1 keV (kiloelectron volts) = 1000 eV (electron volts). 1 eV = 1.60217733e-19 J.
Energy or work. 1 jerk = 1.0e+09 J (joule).
                   1 J = 1 kg m**2 / s**2 = 1 N m (newton meter).
Force. 1 g cm / sh**2 = 1 jerk / cm = 1.0e+07 N (newton). 1 N = 1 Kg m / s**2 = 1 J / m.
Magnetic flux. 1 labWb = 1 (jerk cm) **0.5 = 1 Wb (weber). 1 Wb = 1 V s = (1.0e+07 \text{ J m}) **0.5.
Magnetic flux density. 1 labT = 1 (jerk / cm**3)**0.5 = 10,000 T (tesla).
```

1 T = 1 Wb / m**2 = (1.0e+07 J / m**3)**0.5.

Power. 1 jerk / sh = 1.0e+17 W (watt)
1 W = 1 J / s = 1.0e-17 jerk / sh.

Pressure or energy density. 1 jerk / cm**3 = 1.0e15 Pa (pascal).
1 Pa = 1 N / m**2 = 1 J / m**3.

Specific heat. 1 jerk / (g keV) = 8.617385e+04 J / (kg K).

Thermal conductivity. 1 jerk / (sh cm keV) = 8.617385e+11 W / (m K).

Velocity. 1 cm / sh = 1.0e+06 m / s.

Volume. 1 cm**3 = 1.0e-06 m**3.

SUBROUTINE APTCSYS

call aptesys (n1, n2, lunit, u, v, w, np, tol, nerr)

Version: aptosys Updated 1990 March 14 10:40. aptosys Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read #245100;aptslibe / 1 1 lib aptslibelx aptblibe aptosyslend / 1 1. aptalibe is a LIB library of FORTRAN source files. apublibe is a BUILD library of Cray-compiled binaries.

Purpose: To transform the np points (u, v, w) from coordinate system nl to coordinate system n2. Allowed coordinate systems are cartesian, cylindrical, spherical, Angles may be in degrees (iunit = 0) or radians (iunit = 1). Results will be truncated to zero if less than the estimated error in their calculation, based on tol. Disallowed input values of n1, n2, iunit, or np are indicated by a nonzero value of nerr.

n1, n2, iunit, u, v, w, np, tol. Input:

Output: u. v. w. nerr.

Glossary:

u.v.w

In/Out

iunit Indicates unit to be used for angles; Input O if angles are in degrees.

1 if angles are in radians.

n1 Indicates initial coordinate system type: Input

0 for cartesian coordinates. u=x, v=y, w=z. 1 for cylindrical coordinates. u=radius from zaxis, v = angle in xy plane, counterclockwise from x axis, w = z.

2 for spherical coordinates. u = radius from origin, v = angle in xy plane, counterclockwise from x axis, w = angle from z axis.

n2 Input Indicates final coordinate system. See n1.

nerr Output Indicates an input error, if not 0,

1 if np is not positive. 2 if either nl or n2 is not 0, 1, or 2.

3 if n1 = n2.4 if iunit is not 0 or 1.

Input Number of points (u, v, w). np

Numerical tolerance limit. Any angle with a sine tol Input or cosine (absolute value) less than tol will be adjusted to make its sine or cosine = 0.

The coordinates of a point. Size np. See nl, n2. Will be truncated to zero, if luss than the estimated error in their calculation,

base on tol.

SUBROUTINE APTCSYV

call aptcsyv (nl, n2, iunit, u, v, w, au, av, aw, np, tol, nerr)

Version: aptcsyv Updated 1989 December 1 13:10. aptcsyv Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100; aptslibe / 1 1

lib aptslibe x aptblibe aptosyviend / 1 l. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To transform the np points (u, v, w) and

the associated bound vectors a = (au, av, aw) from coordinate system n1 to coordinate system n2. Allowed coordinate systems are cartesian, cylindrical, spherical. Note: if (u, v, w) is at the origin, then au and av are independent of the coordinate system, and aw changes sign between the spherical coordinate system and the other two. Angles may be in degrees (lunit = 0) or redians (lunit = 1). Results will be truncated to zero if less than the estimated error in their calculation, based on tol. Disallowed input values of n1, n2, lunit, or np are indicated by a nonzero value of nerr.

Input: n1, n2, iunit, u, v, w, au, av, aw, np, tol.

Output: u, v, w, au, av, aw, nerr.

Glossary:

au, av, aw In/Out The u, v, w components of a bound vector at (u, v, w).

Size np.

1 Input Indicates initial coordinate system type:

O for cartesian coordinates. u = x, v = y, w = z.

1 for cylindrical coordinates. u = radius from z
axis, v = angle in xy plane, counterclockwise from x axis, w = z.

2 for spherical coordinates. u = radius from origin, v = angle in xy piane, counterclockwise from x axis, w = angle from z axis.

n2 Input Indicates final coordinate system. See nl.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

2 if either n1 or n2 is not 0, 1, or 2.

3 if n1 = n2.

4 if lunit is not 0 or 1.

tol Input Numerical tolerance limit. Any angle with a sine or cosine (absolute value) less than tol will be

adjusted to make its sine or cosine = 0.

Any spatial coordinate or vector component with a final value less than the estimated error in its calculation, based on tol, will be truncated to

zero.

base on tol.

SUBROUTINE APTDIST

call aptdist (nsys, iunit, au, av, aw, bu, bv, bw, np, tol, cu, cv, cw, dab, nerr)

Version: aptdist Updated 1990 March 14 16:00. aptdist Originated 1989 November 27 16:50.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1 lib aptslibe!x aptblibe aptdist!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, the distance dab, and initial unit direction vector c = (cu, cv, cw), from the point a = (au, av, aw) to the point b = (bu, bv, bw). Option mays specifies the coordinate system:

0 for Cartesian, 1 for cylindrical, 2 for spherical. Option iunit indicates the units for angles: 0 for degrees, 1 for radians.

Any component of vector "c" less than the estimated error in its calculation, based on tol, will be truncated to zero. Vector "c" will be zero, if point "a" is coincident with point "b", based on tol.

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

Input: nsys, iunit, au, av, aw, bu, bv, bw, np, tol.

Output: cu, cv, cw, dab, nerr.

Calls: aptcsys, aptcsyv, aptvdis, aptvuna (sources in aptslibe, binaries in aptblibe).

Glossary:

au, av, aw Input The u, v, w coordinates of point "a". Size np.

bu, by, bw Input The u, v, w coordinates of point "b". Size np.

cu, cv, cw Output The u, v, w components of vector "c". Size np.

May be truncated to zero, if less than the estimated numerical error in their calculation based on tol.

dab Output The distance from point "a" to point "b". Size np.

nsys Input Indicates coordinate system rype:

0 for cartesian coordinates. u = x, v = y, w = z.
1 for cylindrical coordinates. u = radius from z
axis, v = angle in xy plane, counterclockwise from
x axis, w = z.

2 for spherical coordinates. u = radius from origin, v = angle in xy plane, counterclockwise from x axis, w = angle from z axis.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.
2 if nsys is not 1, 2, or 3.
3 if iunit is not 0 or 1.

np Input Size of arrays.

tol Input Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTFDAD

call aptidad (fd, noptid, tol, nlim, nerr).

aptfdad Updated 1990 January 18 16:40. aptfdad Originated 1989 November 2 14:10. Version: aptfdad Updated

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source: lib aptslibe(x aptblibe aptfdad(end / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To adjust the value of fd, relative to the limits 0 and 1, based on the option noptfd and the numerical tolerance limit tol. Values of fd initially in the range from -tol to 1 + tol may be adjusted to the range from tol to 1 - tol. Values of fd outside the range from 0 to 1 may be adjusted to that range. The flag nim indicates if and how fd was adjusted. Flag nerr indicates any error in noptfd.

Input: fd, noptfd, tol.

Output: fd, nlim, nerr.

Clossary:

fd Input Fractional distance.

fd Output Fractional distance, with range limited if noptfd

is 1 or 2.

Output Indicates an input error, if not 0. nerr 1 if noptfd is not between 0 and 2.

Output 0 if no limit imposed on fd, 1 if the limit of

noptfd = 1 is imposed, 2 if the limit of noptfd = 2

is imposed.

nopt fd Input Option to limit range of fd: 0 for no limit;

1 to increase fd to tol, if in the range from -tol to tol, and decrease fd to 1.0 - tol, if in the range from 1.0 - tol to 1.0 + tol; and 2 to impose the limits for noptfd = 1, and then

limit fd to the range from 0.0 to 1.0.

tol Input Numerical tolerance limit. Needed if noptfd = 1 or 2.

SUBROUTINE APTFDAV

call aptfdav (fd, np, noptfd, tol, nlim, nerr)

Version: aptfdav Updated 1990 January 18 14:20. aptfdav Originated 1989 November 2 14:10.

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptfdavlend / 1 1. aptalibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

To adjust the np values of fd, relative to the limits 0 and 1, based on the option noptfd and the numerical tolerance limit Purpose: tol. Values of fd initially in the range from -tol to 1 + tol may be adjusted to the range from tol to 1 - tol. Values of fd

outside the range from 0 to 1 may be adjusted to that range. The flag nlim indicates if and how fd was adjusted.

Flag nerr indicates any error in noptfd.

Input: fd, np, noptfd, tol.

Output: fd, nlim, nerr.

Glossary:

Fractional distance. Size np. fd(n) Input

fd(n) Fractional distance, with range limited if noptf Output

is 1 or 2. Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive. 2 if noptfd is not between 0 and 2.

nlim(n) Output

0 if no limit imposed on fd, 1 if the limit of noptfd = 1 is imposed, 2 if the limit of noptfd = 2 is imposed. Size np.

nopt fd Input Option to limit range of fd: O for no limit;

1 to increase fd to tol, if in the range from -tol to tol, and decrease fd to 1.0 - tol, if in the range from 1.0 - tol to 1.0 + tol; and 2 to impose the limits for noptfd = 1, and then

limit fd to the range from 0.0 to 1.0.

Input Size of arrays fd, nlim. np

tol Input Numerical tolerance limit. Needed if noptfd = 1 or 2.

SUBROUTINE APTFDQC

tol

Input

call aptfdqc (au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol, fdk, fdl, ngood, nerr) Version: aptfdqc Updated 1990 January 26 16:20. aptfdqc Originated 1990 January 26 16:20. Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Source: xport read .245100:aptslibe / 1 1 lib aptslibelx aptblibe aptfdqc|end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the fractional distances fdk and fdl o' the point p = (pu, pv), between the opposite edges "da" and "bc", and "ab" and "cd", respectively, of the 2-D quadrilateral in the uv plane with vertices a = (au, av), b = (bu, bv), c = (cu, cv), and d = (du, dv).Flag nerr indicates any input error. au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol. Input: Output: fdk. fdl. ngood, nerr. aptgrtv (source in aptslibe, binary in aptblibe). Calls: Glossarv: The u and v coordinates of point "a" in the uv plane. au, av Input Size np. bu, bv Input The u and v coordinates of point "b" in the uv plane. Size no. cu, cv Input The u and v coordinates of point "c" in the uv plane. du, dv Input The u and v coordinates of point "d" in the uv plane. Size np. £dk Output Fractional distance of point "p" from the line segment "da" to the line segment "bc". Size np. Values between -tol and tol will be adjusted to tol. Values between 1.0 - tol and 1.0 + tol will be adjusted to 1.0 - tol. See ngood. Output Fractional distance of point "p" from the line segment "ab" to the line segment "cd". Size np.
Values between -tol and tol will be adjusted to tol. fdl Values between 1.0 + tol and 1.0 + tol will be adjusted to 1.0 - tol. See ngood. Indicates range of fractional distances fdk and fdl: ngood Output O if either fdk or fdl is outside the range from -tol to 1.0 + tol. Also if both are. 1 if fdk and fdl are both between -tol and 1.0 + tol. This can be true even when point "p" is outside a boomeranged or bowtied quadrangle. 2 if fdk and fdl are both between -tol and 1.0 + tol, and two possible solutions exist. This can happen when the quadrangle is a boomerang or bowtie. Only one of the solutions is returned. Output Indicates an input error, if not 0. nerr 1 if np is not positive. Input Size of arrays pu, pv, au, uv, bu, bv, cu, cv, du, dv, np fdk, fdl. Input The u and v coordinates of point "p" in the uv plane. pu, pv Size np.

Numerical tolerance limit.

SUBROUTINE APTINVC

call aptinvo (au, av, pu, pv, np, tol, nerr)

aptinvo Updated 1990 March 13 11:30. aptinvo Originated 1990 January 4 13:20. Version: aptinvc Updated

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptinvolend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To invert the np points or vectors p = (pu, pv) through the point a = (au, av), all in the uv plane. If "p" are unbound vectors, point a = (au, av) should be at the origin. The new components of "p" will be truncated to zero if less than the estimated error in their calculation, based on tol. Flag herr indicates any input error.

Input: itype, au, av, pu, pv, np, tol.

Output: pu, pv, nerr.

Glossary:

au, av The u and v components of the inversion point "a". Input

Indicates an input error, if not 0. herr Output 1 if np is not positive.

Number of 2-D points or vectors (pu, pv). Input nρ

In/Out pu, pv The u and v coordinates of a 2-D point, or the u and v components of a 2-D vector. Size np. Truncated to zero if less than the estimated error

in their calculation. See tol.

tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTINVP

call aptinvp (ax, ay, az, px, py, pz, np, tol, rinv)

MELL TO ME

Version: aptinvp Updated 1990 March 13 11:30. aptinvp Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe x aptblibe aptinvp!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the matrix operator rinv for inversion through the origin, and to do an equivalent inversion through the point

p = (px, py, pz). If "p" are unbound vectors, point "a" must be at the origin. The new components of "p" will be truncated to zero if less than the estimated error in their calculation,

based on tol.

Input: itype, ax, ay, az, px, py, pz, np, tol.

Output: px, py, pz, rinv.

Glossary:

ax, ay, az Input The x, y, z coordinates of the inversion point "a".

Input Number of points or vectors (px, py, pz). May be 0.

px,py,pz In/Out The : y, z coordinates of a point, or the x, y, z components of a vector. Size np.

Truncated to zero if less than the estimated error in their calculation. See tol.

rinv Output Array rinv (3,3). Inversion operator. Diagonal elements are -1. Off-diagonal elements are 0.

tol Numerical tolerance limit. Used to test and adjust Input point components. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTINIC

rc

tol

Input

Input

call aptinic (au, av, bu, bv, rc, cu, cv, np, tol, du, dv, eu, ev, nint, nerr) Version: aptinic Updated 1990 March 21 13:40. aptinic Originated 1990 March 21 13:40. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibelx aptblibe aptlniclend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. To find, for each of np sets of input data, any intersection points $d=(du,\ dv)$ and $e=(eu,\ ev)$ of the line through points $a=(au,\ av)$ and $b=(bu,\ bv)$, and the circle centered at point $c=(cu,\ cv)$ with radius rc, all in the uv plane. Purpose: Flag nint indicates the number or type of intersection points. Flag nerr indicates any input error. Input: au, av, bu, bv, rc, cu, cv, np, tol. Output: du, dv, eu, ev, nint, nerr. Calls: apturty, aptvade, aptvdie, aptvdoe (sources in aptslibe, binaries in aptblibe). Glossary: The u and v coordinates of point "a" on the line "ab" 1 nout au, av in the uv plane. Size np. The u and v coordinates of point "b" on the line "ab" bu, by Input in the uv plane. Size np. The u and v coordinates of point "c" at the center of cu, cv Input the circle in the uv plane with radius rc. Size np. The u and v coordinates of point "d" at an intersection du, dv Output of the line "ab" and the circle of radius rc centered at point "c", if an intersection occurs (nint = 1 or nint = 2). Meaningless if nint = -1 or 0. Size np. The u and v coordinates of point "e" at an intersection of the line "ab" and the circle or radius rc centered Out put eu, ev at point "c", if an intersection occurs (nint = 2). Meaningless if nint = -1, 0 or 1. Size np. nerr Output Indicates an input error, if not 0. 1 if np is not positive. nint Output Indicates the type and number of intersection points:
 -1 if points "a" and "b" coincide, based on tol. Points "d" and "e" are meaningless. 0 if no intersection occurs. Points "d" and "e" are meaningless. 1 if the line and circle are tangent at the single point "d". Point "e" is meaningless.
2 if the line and circle intersect at the two distinct points "d" and "e". Input Size of arrays. np

The radius of the circle in the uv plane, centered at

On Cray computers, recommend 1.e-5 to 1.e-11.

point "c". The absolute value is used.

Numerical tolerance limit.

SUBROUTINE APTINLO

call aptinic (au, av, bu, bv, cu, cv, du, dv, np, tci, dpmin, fracab, fraccd, eu, ev, ipar, nerr)

Version: aptinic Updated 1990 January 18 16:40. aptinic Originated 1990 January 11 11:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe(x aptblibe aptinic) and / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the intersection e = (eu, ev), if any, between the straight line between points a = (au, av) and b = (bu, bv), and the straight line between points c = (cu, cv), and d = (du, dv), all in the uv plane, where u, v and w are orthogonal directions. The fractional distance fracab of point "e" along line "ab", and the fractional distance fraced of point "e" along line "cd" are also returned. If the lines are parallel, ipar = 1 will be returned, and the distance dpmin between the lines will be returned. If dpmin is smaller than the estimated error in its calculation, it will be truncated to zero. If a line segment is too short, ipar = 2, 3 or 4 will be returned. Flag nerr will be 1 if np is not positive.

Input: au, av, bu, bv, cu, cv, du, dv, np, tol.

Output: dpmin, fracab, fraccd, eu, ev, ipar, nerr.

Calls: aptvdic, aptaxc (sources in aptslibe, binaries in aptblibe).

Glossary:

au, av Input The u and v coordinates of the first point on line segment "ab" in the uv plane. Size np.

bu, by Input The u and v coordinates of the second point on line segment "ab" in the uv plane. Size np.

cu, cv Input The u and v coordinates of the first point on line segment "cd" in the uv plane. Size np.

du, dv Input The u and v coordinates of the second point on line segment "cd" in the uv plane. Size np.

eu, ev Output The u and v coordinates of the intersection of lines "ab" and "cd". Size np.

fracab Output Fractional distance of "e" along line "ab". Size np. Meaningless if ipar = 2 or 4.

fraccd Output Fractional distance of "e" along line "cd". Size np. Meaningless if ipar = 3 or 4.

lpar Output 0 if lines are not parallel, 1 if they are. Size np.
2 if line segment "ab" is too short,
3 if line segment "cd" is too short.

4 if "ab" and "cd" are both too short.

Indicates an input error, if not 0.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Input Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTININ

dall aptinin (ax, ay, az, bx, by, bz, cx, cy, dz, dx, dy, dz, np, tol, dpmin, fracab, fraced, ex, ey, ez, fx, fy, fz, itrun, ipar, nerr) 1990 March 14 16:00. Version! aptinin Updated aptinin Originated 1989 November 2 14:10. Authori Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Sources xport read .245100;aptslibe / 1 1 lib aptslibelx aptblibe aptininiend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUIID library of Gray-compiled binaries. To find, for each of np sets of input data, the minimum Purposet distance dpmin between the line through the points a = (ax, ay, az) and b = (bx, by, bz), and the line through the points c = (cx, cy, cz) and d = (dx, dy, dz), and the point e = (ex, ey, ez) on line "ab", and the point f = (fx, fy, fz) on line "dd", at which the minimum distance dpmin occurs. If dpmin is smaller than the estimated error in its calculation, it will be truncated to zero, and itrun = 1 will be returned. The fractional distance fracab of point "e" along line "ab", and the fractional distance fraced of point "f" along line "cd", are also returned. If the lines are parallel, ipar - 1 will be returned. If a line segment is too short, ipar = 2, 3 or 4 will be returned. History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes. ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, np, tol. Input: Out put : dpmin, fracab, fraced, ex, ey, ez, fx, fy, fz, itrun, ipar, nerr. Calls: aptvdis, aptvdot, aptvuna (sources in aptslibe, binaries in aptblibe). Glossary: The first point on line segment "ab". Size np. ax, ay, az Input bx, by, bz Input The second point on line segment "ab". Size np. The first point on line segment "cd". Size np. cx, cy, cz Input Minimum distance from line "ab" to line "cd". dpmin Output Distance from e = (ex, ey, ez) to f = (fx, fy, fz). Truncated to zero if less than the estimated error in its calculation. See tol. Size np. dx, dy, dz Input The second point on line segment "dd". Size np. The x, y, z coordinates of the point on line "ab" ex, ey, ez Out put nearest line "cd". Size np. fx, fy, fz Output The x, y, z coordinates of the point on line "cd" nearest line "ab". Size np. Fractional distance of "e" along line "ab". Size np. fracab Output Meaningless if ipar = 2 or 4. Fractional distance of "f" along line "cd". Size np. fraccd Output Meaningless if ipar = 3 or 4. ipar Output O if lines are not parallel. 1 if they are, and points "e" and "f" can be moved arbitrarily by equal distances along the lines. Size np. 2 if line segment "ab" is too short. 3 if line segment "cd" is too short. 4 if "ab" and "cd" are both too short, O if dpmin not truncated to zero, based on tol. itrun Cutput

1 if dpmin is truncated to zero, based on tol.

Size np.

nerr	dutput	Indicates an input error, if not 0, 1 if np is not positive.
np	Input	Size of arrays,
tol	Input	Numerical tolerance limit.

SUBROUTINE APTLNPL

call aptlppi (px, py, pz, sx, sy, sz, ax, ay, sz, vnx, vny, vnz, np, tol, dpmin, dint, fracps, qx, qy, qz, lpar, nerr)

Version: aptinpl Updated 1990 March 15 13:40, aptinpl Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe!x aptblibe aptlnplend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the point of intersection of the line through points p = (px, py, pz) and s = (sx, sy, sz), with the plane through the point a = (ax, ay, az) with normal vector vn = (vnx, vny, vnz). The point of intersection will be defined by its distance dint from point "p", its fractional distance fracps along the line from "p" to "s", and its coordinates q = (qx, qy, qz). The perpendicular distance dpmin from the plane to point "p" is also returned.

If point "p" coincides with point "s", based on tol, the result will be the same as if line "ps" is parallel to the plane. If vector "vn" is too short, based on tol, the result will be the same as if line "ps" lies in the plane. If line "ps" is parallel to the plane, ipar will be 1. If, in addition, dpmin is not zero, dint, fracps, and the coordinates of "q" will be very large. If the line is parallel to the plane and dpmin is zero, then the line is in the plane, and dint and fracps will be zero, and the coordinates of "q" will be (px, py, pz).

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.
1990 March 15. Changed results when vector "vn" is too short.
Now gives same results as if line "ps" ls in the plane.

Input: px, py, pz, sx, sy, sz, ax, ay, az, vnx, vny, vnz, np, tol.

Output: dint, dpmin, fracps, gx, qy, qz, ipar, nerr.

Calls: aptvadd, aptvdis, aptvdot, aptvuna, aptvunb (sources in aptslibe, binaries in aptblibe).

Glossary;

ax,ay,az Input The x, y, z coordinates of point "a" in the plane.
Size np.

dint Output The distance of the point of intersection "q" from
point "p". Positive if in the same direction as
that from "p" to "s". Size np.
Meaningless if ipar is not zero.

fracps Output Fractional distance of point "q" along the line segment from point "p" to point "s". Size np.
May be negative or greater than 1.
Meaningless if ipar is not zero.

ipar Output 0 if the line is not parallel to the plane. Size np.
1 if it is. See dpmin, dint, fracps, qx, qy, qz.
2 if line "ps" is too short, based on tol.
3 if vector "vn" is too short, based on tol.
4 if "ps" and "vn" are both too short, based on tol.

nerr	Output	Indicates an input error, if not 0. 1 %f np is not positive.
np	Input	Size of arrays.
px, py, pz	Input	The x, y, z coordinates of point "p" on the line. Must differ from "s", based on tol. Size np.
qx,qy,qz	Output	The x, y, z coordinates of the point of intersection of the line through "p" and "s" with the plane through point "a" with normal vector "vn". Meaningless if ipar is not zero.
sx, sy, sz	Input	The x, y, z coordinates of point "s" on the line. Must differ from "p", based on tol. Size np.
tol	Input	Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.
vnx,y,z	Input	The x, y, z components of vector "vn" normal to the plane. Magnitude must exceed tol. Size np.

SUBROUTINE APTMAXW

call aptmaxw (tgas, np, erest, beta, gamma, nerr)

Version: aptmaxw Updated 1990 January 31 16:30. aptmaxw Originated 1990 January 31 16:30.

Authors: Eugene H. Canfield, LLNL, L-298, Telephone (415) 422-4125, Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe:x aptblibe aptmaxwlend / 1 1,
aptslibe is a LIB library of FORTRAN source files,
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np specified temperatures tgas, the relativistic velocity functions beta and gamma, by sampling from a relativistic Maxwellian distribution of particles with a rest mass energy of erest (same units as tgas).

Flag nerr indicates any input error.

Input: tgas, np, erest.

Output: beta, gamma, nerr.

Glossary:

beta Output Ratio of particle velocity to the speed of light: beta = v / c (c = 2.99792458e+08 m / s). Range is from 0.0 to 1. Size = np.

erest Input The rest mass of the particles (same units as tgas).

gamma Output Ratio of relativistic mass to particle rest mass:

gamma = sqrt (1.0 - beta**2).

Range is from 0.0 to infinity. Size np.

nerr Output Indicates an input error, if not zero.

1 if np is not positive.

np Input Size of arrays tgas, beta, gamma.

tgas Input Average particle temperature (same units as erest),
Size np.

SUBROUTINE AFTMEAN

call aptmean (x, np, tol, xmean, xdev, nerr)

Version: aptmean Updated 1990 January 31 14:10. aptmean Originated 1990 January 31 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptsliberx aptblibe aptmeantend / 1 . aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

To find, for the np values of \mathbf{x} , the mean value xmean and the standard deviation xdev of \mathbf{x} from xmean. Flag nerr indicates any input error. Purpose:

Input: x, np, tol.

Output: xmean, xdev, nerr.

Glossary:

nerr Output If not 0, indicates an input error. 1 if np i not positive.

np Input Size of array x.

tol Input Truncation error limit.

On Cray computers, recommend 1.e-11.

Input · A scalar value. Size np.

xdev Output. Standard deviation of x from xmean.

sqrt (mean (x**2) - (mean (x))**2).

xmean Output Mean value of x. Sum (x) / np.

SUBROUTINE APTMOPV

call aptmopv (smat, inv, ax, ay, az, px, py, pz, np, tol, nerr)

Version: aptmopv Updated 1990 March 14 19:30. aptmopv Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe(x aptblibe aptmopy)end / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptiblibe is a BUILD library of Cray-compiled binaries.

Purpose: To transform the np points or vectors p = (px, py, pz) by subtracting a = (ax, ay, az), then operating on the result with the 3 x 3 matrix operator smat (inv = 0) or its transpose (inv = 1), then adding a = (ax, ay, az).

Components of "p" smaller than the estimated error in their calculation, based on tol, will be truncated to zero. If np is not positive, nerr = 1 will be returned. If inv is not 0 or 1, nerr = 2 will be returned.

(1) if smat is a rotation operator (unitary, orthogonal, the transpose = the inverse, and the the cosine of the station angle is (trace - 1) / 2), the rotation is around an axis through the point a = (ax, ay, az). Option inv = 0 rotates the 3 row vectors of smat to be parallel to the major axes, or rotates the major axes to be parallel to the 3 column vectors of smat. Option inv = 1 rotates the 3 column vectors of smat to be parallel to the major axes, or rotates the major axes to be parallel to the major axes, or rotates the major axes to be parallel to the 3 row vectors of smat.

(2) if smat is a reflection operator (unitary, symmetric, its own inverse, and the trace = 1) the reflection is in a plane through the point a=(ax, ay, az); inv has no effect. If the values p=(px, py, pz) are unbound vectors, then a=(ax, ay, az) must be (0, 0, 0, 0). The sequential application of two reflections is a rotation and a possible translation.

(3) if smat is an inversion operator (diagonals = -1, other elements = 0), the inversion is through the point a = (ax, ay, az).

History: 1990 March 13. Deleted truncation of components based on total magnitude of vector.

Input: smat, inv, ax, ay, az, px, py, pz, np, tol.

Output: px, py, pz, nerr.

Glossary:

ax, ay, az Input The x, y, z coordinates of an invariant point.

inv Input 0 to operate with the matrix smat, 1 to operate with its transpose.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.
2 if inv is not 0 or 1.

np Input Size of arrays px, py, pz. Must be positive.

smat Input Array smat (3,3). A matrix operator.

tol Input Numerical tolerance limit.

On Cray computers, recommend l.e-5 to l.e-11.

SUBROUTINE APTMOVE

call aptmove (hsys, iunit, au, av, aw, bu, bv, bw, dpmove, np, tol, cu, cv, cw, du, dv, dw, nerr) Version: aptmove Updated 1990 January 18 14:20. aptmove Originated 1989 November 22 17:10. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: *xport read .245100:aptslibe / 1 1 Source: lib aptslibelx aptblibe aptmovelend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the new point c = (cu, cv, cw) and unit direction vector d = (du, dv, dw), resulting from moving from the point a = (au, av, aw) in the direction of the unit vector b = (bu, bv, bw) for a distance dpmove. Option nsys specifies the coordinate system: O for Cartesian, 1 for cylindrical, 2 for spherical. Option junit indicates the units for angles: O for degrees, 1 for radians. Any component of point "c" or vector "d" less than the estimated error in its calculation, based on tol, will be truncated to zero. Flag nerr indicates any input error. Input: nsys, iunit, au, av, aw, bu, bv, bw, dpmove, np, tol. Outpv:: cu, cv, cw, du, dv, dw, nerr. Calls: aptcsyv, aptvadd (sources in aptslibe, binaries in aptblibe). Glossarv: The u, v, w coordinates of point "a". Size np. au, av, aw Input bu. by. bw Input The u, v, w components of unit vector "b". Size np. The u, v, w coordinates of point "c". Size np. cu.cv.cw Output May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. The distance from point "a" to point "c". Size np. domove Input (Assuming vector "b" is a unit vector.) du, dv, dw Output The u, v, w components of unit vector "d". Size np. May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. iunit Input Indicates unit to be used for angles: O if angles are in degrees. 1 if angles are in radians. nsvs Input Indicates coordinate system type: 0 for cartesian coordinates. u = x, v = y, w = z. 1 for cylindrical coordinates. u = radius from z axis, v = angle in xy plane, counterclockwise from x axis, w = z. 2 for spherical coordinates. u = radius from origin, v = angle in xy plane, counterclockwise from x axis, w = angle from z axis. nerr Output Indicates an input error, if not 0. 1 if np is not positive.

2 if nsys is not 1, 2, or 3. 3 if iunit is not 0 or 1.

Size of arrays. np Input

Numerical tolerance limit. tol Input On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE AND THEORYS

call aptmovs (rhos, cths, sths, cphs, sphs, usrh, usth, usph, dpmove, np, tol, rho, cth, sth, cph, sph, urh, uth, uph, nerr) 1990 March 14 16:00. Version: aptmovs Updated aptmovs Originated 1989 December 4 17:00. Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Source: xport read .245100:aptslibe / 1 1 lib aptslibeix aptblibe aptmovslend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the new point p = (rho, cth, sth, cph, sph) and unit direction vector u = (urh, uth, uph), resulting from moving from the point ps = (rhos, cths, sths, cphs, sphs) in the direction of the unit vector us = (usrh, usth, usph) for a distance dpmove, in spherical coordinates. Any component of point "p" or vector "u" less than the estimated error in its calculation, based on tol, will be truncated to zero. If tol = 0, no truncation tests are done. Flag nerr indicates any input error. History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes. Input: rhos, cths, sths, cphs, sphs, usrh, usth, usph, dpmove, np, tol. Output: rho, cth, sth, cph, sph, urh, uth, uph, nerr. Calls: aptvuna (source in aptslibe, binary in aptblibe). Glossary: Output The cosine of the final value of phi (angle from the z axis). May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np. cphs Input The cosine of the initial value of phi. See uph. Size np. cth Out put The cosine of the final value of theta (angle in the xy plane counterclockwise from x axis). May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np. cths Input The cosine of the initial value of theta. See cth. Size np. domove Input The distance from point "ps" to point "p". Size np. (Assuming vector "us" is a unit vector.) Indicates an input error, if not 0. nerr Output 1 if np is not positive. np Input Size of arrays. The spherical radial component of final point "p". rho Output May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. rhos Input the spherical radial component of initial point "ps". Size np. sphs Input The sine of the initial value of phi. See cph.

Size np.

Size ap.

Output

May be truncated to zero, if less than the estimated numerical error in their calculation based on tol.

The sine of the final value of phi. See cph.

sths	Input	The sine of the initial value of theta. See cth. Size np.
sth	Output	The sine of the final value of theta. See cth. May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np.
tol	Input	Numerical tolerance limit. If zero, no tests done. On Cray computers, recommend 1.e-5 to 1.e-11.
uph	Output	The phi component of final unit direction vector "u". May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. See cph. Size np.
urh	Output	The rho component of final unit direction vector "u". May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np.
usph	Input	The phi component of initial unit direction vector "us". See cph. Size np.
usrh	Input	The rho component of initial unit direction vector "us". Size np.
usth	Input	The theta component of initial init direction vector "us". See cth. Size np.
uth	Output	The theta component of final unit direction vector "u". May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. See cth. Size np.

SUBROUTINE APTMPRD

call aptmprd (nrows, smat1, smat2, to1, smat, nerr)

Version: aptmprd Updated 1989 December 29 11:40. aptmprd Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe:x aptblibe aptmprdiend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the matrix product smat of the two square matices

smatl and smat2. Each must be sized nrows by nrows.

Considered as operators, smat is equivalent to the sequential application of smat2, then smat1. Components of smat within

tol of 0, 1, or -1 will be adjusted to those values. If nrows is not positive, nerr = 1 will be returned.

Input: smat1, smat2.

Output: smat, nerr.

Glossary:

nerr Output Indicates an input error, if not 0.

1 if nrows is non-positive.

nrows Input Number of rows - number of columns in smat1, smat2, and smat.

matrix product of smatr, smatr.

smatl Input A square matrix, with size smatl(nrows,nrows).

smat2 Input A square matrix, with size smat2(nrows,nrows).

tol Input Numerical tolerance limit. Used to test and adjust matrix elements. If the row and column vectors of smatl and smat2 are unit vectors, then

SUBROUTINE APTMVCY

dpmove, np, tol, pz, pr, cth, sth, uz, ur, ut, nerr) aptmvcy Updated 1990 March 14 16:00. Version: aptmvcy Originated 1989 December 4 11:00. Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibelx aptblibe aptmvcylend / 1 1. aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the new point p = (pz, pr, cth, sth) and unit direction vector u = (uz, ur, ut), resulting from moving from the point ps = (psz, psr, oths, sths) in the direction of the unit vector us = (usz, usr, ust) for a distance dpmove, in cylindrical coordinates. If kth = 0, all cths = 1.0, all sths = 0.0, and cth and sth will not be calculated, and none need be dimensioned. Any component of point "p" or vector "u" less than the estimated error in its calculation, based on tol, will be truncated to zero. If tol = 0, no truncation tests are done. Flag nerr indicates any input error. History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes. Input: kth, psz, psr, cths, sths, usz, usr, ust, domove, np, tol. Out out : pz, pr, cth, sth, uz, ur, ut, nerr, Calls: aptyuna (source in aptslibe, binary in aptblibe). Glossarv: Size np. The cosine of the final value of theta (angle in the cth Output xy plane counterclockwise from x axis). May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np, if kth = 1. Otherwise, not calculated. cths Input The cosine of the initial value of theta. See cth. Size np, if kth = 1. Otherwise, scalar 1.0. The distance from point "ps" to point "p". Size np. domove Input (Assuming vector "us" is a unit vector.) kth Input Indicates size of arrays cth, cths, sth, sths: 0 if array size is 1, with cths = 1.0, sths = 0.0, and cth and sth are not to be calculated. 1 if array size is np, input values of cths and sths will be used, and cth and sth will be calculated. Output Indicates an input error, if not 0. 1 if np is not positive. 2 if kth is not 0 or 1. Input Size of arrays. pr, pz Out put The r and z components of final point "p". Size np. May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. psr, psz Input The r and z coordinates of initial point "ps", Size np. The sine of the initial value of theta. See cth. sths Input Size np, if kth = 1. Otherwise, scalar 0.0. sth Output The sine of the final value of theta. See cth. May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size np, if kth = 1. Otherwise, not calculated.

call aptmvcy (kth, psz, psr, cths, sths, usz, usr, ust,

tol	Input	Numerical tolerance limit. If zero, no tests done. On Cray computers, recommend 1.e-5 to 1.e-11.
ur	Output	The r component of final unit direction vector "u". May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. size np.
usr	Input	The r component of initial unit direction vector "us". Size np.
ust	Input	The theta component of initial unit direction vector "us". See oth. Size np.
usz	Input	The z component of initial unit direction vector "us".
ut	Output	The theta component of final unit direction vector "u". May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. See cth. Size np.
uz	Output	The z component of final unit direction vector "u". Size np.

SUBROUTINE APTPLPL

dall aptplpl (ax, ay, az, bx, by, bz, dx, dy, dz, dx, dy, dz, np, tol, ex, ey, ez, fx, fy, fz, ux, uy, uz, ipar, dpmin, itrun, nerr)

Version: aptplp1 Updated 1990 March 15 15:10, aptplp1 Originated 1989 November 9 10:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe:x aptblibe aptplpliend / 1 1,
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of a set of input data, the line of intersection of the plane through point a = (ax, ay, az) with normal vector b = (bx, by, bz), and the plane through point c = (cx, cy, cz) with normal vector d = (dx, dy, dz), if any. Otherwise, if the planes are parallel, to find the distance between them. For nonparallel planes, the points e = (ex, ey, ez) and f = (fx, fy, fz) will be the points on the line of intersection nearest points "a" and "c", respectively, unit vector u = (ux, uy, uz) will be the direction of the line of intersection, and ipar will be zero.

If the planes are parallel, based on tol, ipar will be 1, and dpmin will be the the distance between the planes. If the planes are coincident, dpmin will be zero, itrun will be 1, and unit vector "u" will be in the direction of the line "ac".

Flag nerr indicates any input error, such as np not positive. Flag ipar will be 2, 3, or 4 if vector "b" or "d", or both, are too short, based on tol. If so, "e", "f" and "u" will be meaningless.

Method: The line of intersection "ef" lies in both planes, therefore is perpendicular to both normal vectors, thus parallel to b x d. The line "ae" is perpendicular to line "ef" and "b", thus parallel to b x (b x d). The line "cf" is perpendicular to line "ef" and "d", thus parallel to d x (b x d). The vector path "ac" equals the vector path "aefc". Taking components parallel to "ae", "ef", and "cf" provides equations for the unknown distances "ae", "ef", and "cf". If the planes are parallel, b x d is zero, and dpmin is the component of "ac" in the direction of the normal vector "b".

Note: Subroutine aptvpln may be used to find the vector normal to a plane for which at least 3 points are known.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

1990 March 15. Changed points "e" and "f" to "a" and "b", resp. when either vector "b" or "d" is too small. No effect when input data is good.

Input: ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, np, tol.

Output: ex, ey, ez, fx, fy, fz, ux, uy, uz, ipar, dpmin, itrun, nerr.

Calls: aptvadd, aptvdis, aptvdot, aptvuna, aptvunb, aptvxun (sources in aptslibe, binaries in aptblibe).

Glossarv:

ax, ay, az Input A point in plane "a". Size np.

cx,cy,cz Input A point in plane "c". Size np.

ex,ey,ez Output The x, y, z coordinates of the point on the line of intersection of planes "a" and "c" nearest point "a".

Meaningless, but point "a", if ipar is not 0.

fx, fy, fz	Output	The x, y, z coordinates of the point on the line of intersection of planes "a" and "c" nearest point "c". Meaningless, but point "c", if ipar is not 0.
dpmin	Out put	The distance between planes "a" and "o", if ipar = 1. Otherwise, zero. Size np.
ipar	Output	Indicates relative orientation of planes "a" and "c": 0 if the planes intersect. 1 if the planes are parallel, based on tol. 2 if vector "b" is too short, based on tol. 3 if vector "d" is too short, based on tol. 4 if vectors "b" and "d" are both too short. 0 orientation is indeterminate if ipar = 2, 3 or 4. Size np.
itrun	Output	If 1, indicates planes are parallel and coincident. Size np.
nerr .	Output	Indicates an input error, if not 0. 1 if np is not positive.
tol	Input	Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.
ux, uy, uz	Output	The x, y, z components of the unit vector parallel to the line of intersection of planes "a" and "c", if ipar = 0. Meaningless, but parallel to the line "ac" if ipar is not zero. Size np.

SUBROUTINE APTPLSP

call aptplap (raph, px, py, pz, ax, ay, az, bx, by, bz, np, tol, dpmin, roir, cx, cy, cz, itrun, narr)

1990 March 16 14:10. Version: aptblsp Updated aptplsp Originated 1990 March 16 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Authors

Sources xport read ,245100;aptslibe / 1 1 lib aptslibelx aptblibe aptplsplend / 1 1. aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

To find, for each of np sets of input data, the minimum distance dpmin to the point p = (px, py, pz), from the plane through the point a = (ax, ay, az) with normal vector b = (bx, by, bz) and the doordinates o = (ox, cy, cz) of the point in the plane nearest point "p". In addition, to find the radius roir of any circle of intersection of the plane with the sphere centered at point "p" with radius raph. Flag itrun indicates truncation of dpmin to zero (1) or

too small a magnitude of vector "b" (2). Flag nerr indicates any input error.

Input: raph, px, py, pz, ax, ay, az, bx, by, bz, np, tol.

Out put 1 dpmin, roir, ox, oy, oz, itrun, nerr.

Calls: aptptpl (source in aptslibe, binary in aptblibe).

Glossarv:

The x, y, z coordinates of point "a" in the plane. ax. av. az Input Size no.

The M, y, z components of vector "b" normal to the plane. Magnitude must exceed tol. Size np. bx, by, bz Input

cx, cy, cz Output The x, y, z coordinates of the point in the plane nearest point "p". Size np. The center of any circle of intersection. Returned as point "p" if normal vector "b" is too short, based on tol (itrun = 2).

dpmin Output The perpendicular distance to point "p" from the plane through point "a" with normal vector "b". Positive if point "p" is in the same direction from the plane as the normal vector "b". Truncated to zero if less than the estimated error in its calculation, based on tol (itrun = 1), Returned as zero if normal vector "b" is too short, based on tol (itrun = 2).

itrun Output Indicates a special result for one data set:

O if dpmin is not zero, and no input errors occur. 1 if the value of dpmin is truncated to zero, when less than the estimated error in its calculation, based on tol.

2 if normal vector "b" is too short, based on tol. The orientation of the plane is unknown, and dpmin and point "c" cannot be calculated.

nerr Output Indicates an input error, if not 0. 1 if np is not positive.

Size of arrava. np Input

px, py, pz Input The x, y, z coordinates of point "p". Size np. The center of the sphere with radius rsph.

rcir Output The radius of any circle of intersection centered at point "c". Size np. Positive if intersection occurs, zero if tangency occurs, negative if no intersection or tangency occurs, or if itrun = 2 or 3.

rsph Input The radius of the sphere centered at point "p".
Size np. The absolute value is used.

tol Input Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTETIC

dall aptitio (pu, pv, au, av, bu, bv, np, tol, noptid, dpmin, fdmin, nlim, itrun, nerr)

Version: aptptlo Updated 1990 February 14 13:00. aptptlo Originated 1989 December 29 16:40. 1990 February 14 13:00.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Authori

xport read .245100;aphalibe / 1 1 Sources lib aptalibers aptbl/be aptpticiend / 1 1. aptalibe is a LIB library of FORTRAN source files. apublibe is a BUILD 1 brary of Cray-compiled binaries.

To find, for each of up sets of input data, the minimum distance Purposes dpmin from the point p = (pu, pv) to the straight line through the points a = (au, av) and b = (bu, bv). All points are in the uv plane. Directions u, v and w are orthogonal.

> Option noptfd allows the fractional distance fdmin of the proximal point along line "ab" to be calculated, and allows the range of fdmin to be limited. Flag nl 4 indicates when such limitation has beem imposed. If alim = 2, dpmin is the distance from point "p" to the nearest end of line secment "ab".

> The value of dpmin will be truncated to zero if less than the estimated error in its calculation, based on tol, and if so, itrun = 1 will be returned.

If the points "a" and "b" coincide, based on tol, dpmin will be the distance from point "a" to point "p", and if dpmin is not zero, itrun will be -1.

Flag nerr indicates any input error.

History: 1990 February 12 15:20. Added input argument noptfd, optional output arguments fdmin, nlim.

Input: pu, pv, au, av, bu, bv, np, tol, noptfd.

Out put : dpmin, fdmin, nlim, itrun, nerr.

Calla: aptfdav, aptvaxo, aptvdio, aptvdoo (sources in aptslibe, binaries in aptblibe).

Glossarvi

au, av Input The u and v coordinates of point "a" on line "ab", Size np. All points are in the uv plane.

bu, by Input The u and v coordinates of point "b" on line "ab". Size np.

Distance from point "p" to the line "ab". Size np. domin **Out put** Truncated to zero if less than the estimated error in its calculation, based on tol, and if so, itrun = 1 will be returned.

If points "a" and "b" are coincident, dpmin is the distance from point "p" to point "a", and itrun = -1 is returned, unless dpmin = 0.0. If noptfd is 2, and fdmin is initially not in the range from 0.0 to 1.0, dpmin is the distance from point "p" to the nearest of points "a" and "b", and nlim = 2 is returned.

The value of dpmin is positive, if point "p" is to the left of the vector "ab" in the uv plane.

fdmin Out put Fractional distance between point "a" and point "b" of the point nearest point "p". See noptfd. Size np, if noptfd is not -1.

1t.run Output 0 if dpmin is not truncated to zero. Size np. 1 if dpmin is truncated to zero, when less than its estimated error, based on tol. -1 if dpmin is not zero, and points "a" and "b"

coincide, based on tol.

nerr	Output	Indicates an input error, if not 0. 1 if np is not positive. 2 if noptfd is not -1, 0, 1, or 2.
nlim	Output	O if no limit imposed on fdmin, 1 if the limit of noptfd = 1 is imposed, 2 if the limit of noptfd = 2 is imposed. Size np, if noptfd is not ~1. If 2, dpmin is the distance from point "p" to the nearest end of line segment "ab".
nopt fd	Input	Option to limit range of fdmin: 0 for no limit; -1 to not calculate fdmin or nlim. 0 to find fdmin, but impose no limits. 1 to increase fdmin to tol, if in the range from -tol to tol, and decrease fdmin to 1.0 - tol, if in the range from 1.0 - tol to 1.0 + tol. 2 to impose the limits for noptfd = 1, and then limit fdmin to the range from 0.0 to 1.0, and adjust the magnitude, but not the sign of dpmin if the later limit is imposed.
np	Input	Size of arrays pu, pv, au, av, bu, bv, itrun. If noptfd is not -1, the size of arrays fdmin, nlim.
pu, pv	Input	The u and v coordinates of point "p". Size np.
tol	Input	Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTPTLN

call aptptin (px, py, pz, ax, ay, az, bx, by, bz, np, tol,
noptfd, dpmin, fdmin, cx, cy, cz, nlim, itrun, nerr)

Version: aptptin Updated 1990 February 14 10:00. aptptin Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100;aptslibe / 1 1
lib aptslibe!x aptblibe aptptln!end / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the minimum distance dpmin from the point p = (pu, py, pz) to the straight line through the points a = (ax, ay, az) and b = (bx, by, bz), to find the coordinates c = (cx, cy, cz) of the proximate point on line "ab", and to find the fractional distance fdmin of that point along the line segment "ab". The value of dpmin will be truncated to zero if less than the estimated error in its calculation, based on to1, and if so itrun = 1 will be returned. Flag nerr indicates any input error.

Option noptid allows the line "ab" to be treated as a finite segment, by limiting the range of fdmin. Flag nlim indicates when such limitation has beem imposed.

If the points "a" and "b" coincide, based on tol, domin will be the distance from point "a" to point "p", and if domin is not zero, itrun will be -1.

History: 1990 February 12 16:00. Fixed bug affecting fdmin when np is greater than 64.

Input: px, py, pz, ax, ay, az, bx, by, bz, np, tol, noptfd.

Output: dpmin, fdmin, cx, cy, cz, nlim, itrun, nerr.

Calls: aptfdav, aptvadd, aptvdis, aptvdot (sources in aptslibe, binaries in aptblibe).

Glossary:

ax,ay,az Input The x, y, z coordinates of point "a" on line "ab". Size np.

cx,cy,cz Output The x, y, z coordinates of the point on the line "ab" nearest point "p". Point "p" if dpmin = 0. Size np.

fdmin Output Fractional distance between point "a" and point "b" of the point "c". Size np.

itrum Output 0 if dpmin is not truncated to zero.

1 if dpmin is truncated to zero, when less than its estimated error, based on tol. Size np.

-1 if dpmin is not zero, and points "a" and "b" coincide, based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.
2 if noptfd is not 0, 1, or 2.

nlim Output 0 if no limit imposed on fdmin, 1 if the limit of noptfd = 1 is imposed, 2 if the limit of noptfd = 2 is imposed. Size np.

If the latter limit is imposed, dpmin will be the distance from point "p" to the nearest end of the line segment.

noptfd Input Option to limit range of fdmin: 0 for no limit;

1 to increase fdmin to tol, if in the range from
-tol to tol, and decrease fdmin to 1.0 - tol, if
in the range from 1.0 - tol to 1.0 + tol; and
2 to impose the limits for noptfd = 1, and then
limit fdmin to the range from 0.0 to 1.0.

np Input Size of arrays px, py, pz, ax, ay, az, bx, by, bz,
cx, cy, cz, fdmin, itrun.

px,py,pz Input The x, y, z coordinates of point "p". Size np.

tol

Input

Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTPTPL

call aptptpl (px, py, pz, ax, ay, az, bx, by, bz, np, tol, dpmin, cx, cy, cz, itrun, nerr)

Version: aptptpl Updated 1990 March 15 11:50. aptptpl Originated 1989 November 2 14:10. 1990 March 15 11:50

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe!x aptblibe aptptpl!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the minimum distance

dpmin to the point p = (px, py, pz), from the plane through the point a = (ax, ay, az) with normal vector b = (bx, by, bz), and the coordinates c = (cx, cy, cz) of the point in the plane

nearest point "p".

Flag itrum indicates truncation of domin to zero (1) or too small a magnitude of vector "b" (2).

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

px, py, pz, ax, ay, az, bx, by, bz, np, tol. Input:

dpmin, cx, cy, cz, itrun, nerr. Output:

Calls: aptvadd, aptvdis, aptvdot, aptvunb (sources in aptslibe,

binaries in aptblibe).

Glossarv:

ax, ay, az Input The x, y, z coordinates of point "a" in the plane.

Size np.

The x, y, z components of vector "b" normal to the bx, by, bz Input

plane. Magnitude must exceed tol. Size np.

cx, cy, c2 Output The x, y, z coordinates of the point in the plane

nearest point "p". Size np.
Returned as point "p" if normal vector "b" is too short, based on tol (itrun = 2).

The perpendicular distance to point "p" from the domin Output

plane through point "a" with normal vector "b". Positive if point "p" is in the same direction

from the plane as the normal vector "b".

Truncated to zero if less than the estimated error

in its calculation, based on tol (itrun = 1).
Returned as zero if normal vector "b" is too short,

based on tol (itrun = 2).

itrun Output Indicates a special result for one data set:

1 if the value of dpmin is truncated to zero, when less than the estimated error in its calculation,

based on tol.

2 if normal vector "b" is too short, based on tol. The orientation of the plane is unknown, and dpmin and point "c" cannot be calculated.

Indicates an input error, if not 0. nerr Output

1 if np is not positive.

Size of arrays. Input np

px, py, pz Input The x, y, z coordinates of point "p". Size np.

tol Input Numerical tolerance limit.

SUBROUTINE APTODIC

call aptqdic (au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol, pab, pbc, pcd, pda, dpmin, nerr) aptodic Updated 1990 February 21 11:00. Version: aptqdic Originated 1990 February 21 11:00. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibe(x aptblibe aptqdic(end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the distances pab, pbc, pcd and pda from the point p = (pu, pv) to the sides of the quadrangle with vertices a = (au, av), b = (bu, bv), c = (cu, cv), and d = (du, dv), in counterclockwise order in the uv plans, and the minimum dpmin of pab, pbc, pcd and pda. The values of pab, pbc, pcd and pda will be truncated to zero, if less than the estimated error in their calculation, based on tol: Flag nerr indicates any input error. au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol. Input: Output: pab, pbc, pcd, pda, domin, nerr. Calls: aptptlc (source in aptslibe, binary in aptblibe). Glossary: Input The u, v coordinates of vertex "a" of the quadrangle. au, av Size np. bu, by The u, v coordinates of vertex "b" of the guadrangle. Input Size np. cu, cv Input The u, v coordinates of vertex "c" of the guadrangle. Size np. Minimum of absolute values of distances domin Output pab, pbc, pcd and pda. Size np. du, dv Input The u, v coordinates of vertex "d" of the quadrangle. Size np. Indicates an input error, if not 0. nerr Output 1 if np is not positive. Size of arrays pu, pv, au, av, bu, bv, cu, cv, du, dv, np Input pab, pbc, pcd, pda. Distance from point "p" to quadrangle side "ab".

Truncated to zero, if less than the estimated error pab Output in its calculation, based on tol. Absolute value. Distance from point "p" to quadrangle side "bc".

Truncated to zero, if less than the estimated error pbc Output in its calculation, based on tol. Absolute value, Distance from point "p" to quadrangle side "cd".

Truncated to zero, if less than the estimated error pcd Output in its calculation, based on tol. Absolute value. Distance from point "p" to quadrangle side "da".

Truncated to zero, if less than the estimated error pda Out put in its calculation, based on tol. Absolute value. pu, pv Input The u and v coordinates of point "p" in the uv plane. Size np. tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTOFDC

call aptqfdc (au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol, fdk, fdl, ngood, nerr)

Version: aptqfdc Updated 1990 February 14 16:00.

aptqfdc Originated 1990 February 14 16:00.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibeix aptblibe aptqfdclend / 1 1
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np points p = (pu, pv), the fractional distances fdk and fdl of point "p" between the opposite edges "da" and "bo", aid "ab" and "cd", respectively, of the 2-D quadrilateral in the uv plane with vertices a = (au, av), b = (bu, bv), c = (cu, cv), and d = (du, dv). Flag nerr indicates any input error.

Input: au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol.

Output: fdk, fdl, ngood, nerr.

Calls: aptqrtv (source in aptslibe, binary in aptblibe).

Glossary:

au, av Input The u and v coordinates of point "a" in the uv plane. bu, bv Input The u and v coordinates of point "b" in the uv plane. The u and v coordinates of point "c" in the uv plane. Input du, dv Input The u and v coordinates of point "d" in the uv plane. fdk Output Fractional distance of point "p" from the line segment "da" to the line segment "bc". Size np. Values between -tol and tol will be adjusted to tol. Values between 1.0 - tol and 1.0 + tol will be

fdl Output Fractional distance of point "p" from the line segment "ab" to the line segment "cd". Size np.

Values between -tol and tol will be adjusted to tol.

Values between 1.0 - tol and 1.0 + tol will be adjusted to 1.0 - tol. See ngood.

adjusted to 1.0 - tol. See ngood.

ngood Output Indicates range of fractional distances fdk and fdl:

0 if either fdk or fdl is outside the range from
-tol to 1.0 + tol. Also if both are.

1 if fdk and fdl are both between -tol and 1.0 + tol.
This can be true even when point "p" is outside
a boomeranged or bowtied quadrangle.

2 if fdk and fdl are both between -tol and 1.0 + tol,
and two possible solutions exist. This can happen
when the quadrangle is a boomerang or bowtie.
Only one of the solutions is returned.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input Size of arrays pu, pv, fdk, fdl.

pu, pv Input The u and v coordinates of point "p" in the uv plane. Size np.

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTOINC call aptqinc (ktype, ntype, au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol, pab, pbc, pcd, pda, dpmin, nloc, nerr) 1990 February 21 16:40. Version: aptqinc Updated aptqinc Originated 1990 February 21 16:40. Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Source: xport read .245100:aptslibe / 1 1 lib aptslibe(x aptblibe aptqinclend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of the np sets of input data, the distances pab, pbc, pcd and pda from the point $p=(pu,\ pv)$ to the sides of the quadrangle with vertices $a=(au,\ av),\ b=(bu,\ bv),$ c = (cu, cv), and d = (du, dv), in counterclockwise order in the uv plane, the minimum dpmin of pab, pbc, pcd and pda, and whether point "p" is inside the quadrangle or not (flag nloc). Option kflag allows the quadrangle shape type to be ignored, output, or input, and boomerangs and bowties to be tested. The values of pab, pbc, pcd and pda will be truncated to zero, if less than the estimated error in their calculation, based on tol. Flag nerr indicates any input error. Input: ktype, ntype, au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol. Output: pab, pbc, pcd, pda, dpmin, nloc, nerr. aptptlc, aptqvac (sources in aptslibe, binaries in aptblibe). Glossary: au, av Input The u, v coordinates of vertex "a" of the quadrangle. Size np. bu, by Input The u, v coordinates of vertex "b" of the quadrangle. The u, v coordinates of vertex "c" of the quadrangle. cu, cv Input Size np. dpmin Minimum of distances pab, pbc, pcd, pda. Size np. Output Minimum of absolute values of pab, pbc, pcd, pda, if point "p" is in a boomerang or bowtie, and ktype = 0, 1 or 2. Negative if nloc = 0. The u, v coordinates of vertex "d" of the quadrangle. du, dv Input Size np. ktype Input Indicates whether ntype is input or output, and whether or not cases for which nloc is initially zero will be tested to see if the point is actually inside a boomerang or bowtie. -1 if ntype is not input, and is not to be returned. No tests will be made for boomerangs or bowties. O if ntype is not input, and is not to be returned.

Tests will be made for boomerangs and bowties. 1 if ntype is not input, but will be returned. Tests will be made for boomerangs and bowties.

2 if ntype is input. Tests will be made for boomerangs and bowties.

nerr Output Indicates an input error, if not 0. 1 if np is not positive.

2 if ktype is not -1, 0, 1 or 2.

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nloc	Output	<pre>Indicates the location of point "p" relative to the quadrangle "abcd": -1 if all quadrangle vertices coincide. 0 if point "p" is outside the quadrangle "abcd", or is inside, but the quadrangle vertices were</pre>
		specified in clockwise order, or if ktype = -1, is inside a bowtie or in certain areas inside a boomerang. 1 if point "p" is inside the quadrangle "abcd", and either all four distances pab, pbc, pcd and pda are non-negative, or if ktype = 0, 1 or 2,
		the quadrangle is a boomerang or bowtle and the distances pass specific tests.
np	Input	Size of arrays pu, pv, au, av, bu, bv, cu, cv, du, dv, pab, pbc, pcd, pda.
ntype	1/0?	Shape type of quadrangle. Input if ktype = 2. Output if ktype = 1. Size np if ktype = 1 or 2. 0 if quadrangle is convex.
T.		11-14 if quadrangle has just one concave vertex at point "a", "b", "c", or "d", resp. (a boomerang). 21-24 if quadrangle has just two adjacent concave vertices at ends of sides "cd", "da", "ab", or
		"bc", respectively (a bowtie).
pab	Output	Distance from point "p" to quadrangle side "ab". Truncated to zero, if less than the estimated error in its calculation, based on tol.
pbc	Output	Distance from point "p" to quadrangle side "bc". Truncated to zero, if less than the estimated error in its calculation, based on tol.
pcd	Output	Distance from point "p" to quadrangle side "cd". Truncated to zero, if less than the estimated error in its calculation, based on tol.
pda	Output	Distance from point "p" to quadrangle side "da". Truncated to zero, if less than the estimated error in its calculation, based on tol.
pu, pv	Input	The u and v coordinates of point "p" in the uv plane. Size np.
tol	Input	Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTOLOC call aptqloc (au, av, bu, bv, cu, cv, du, dv, np, tol, fdk, fdl, pu, pv, nerr) Version: aptqloc Updated 1990 February 14 17:30. aptqloc Originated 1990 February 8 14:30. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibe(x aptblibe aptqloc!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find np points p = (pu, pv), by sampling from a uniform distribution over the planar quadrangle in the uv plane, with vertices a = (au, av), b = (bu, bv), c = (cu, cv), d = (du, dv), in counterclockwise order around the quadrangle. For a triangle, make du = au, dv = av, or call apttlod. If the quadrangle has a non-positive area, no points will be sampled. Variables fdk and fdl are the local coordinates in the quadrangle. For any point p = (pu, pv) in the quadrangle: pu = au + fdk * (bu - au) + fdl * (du - au) + fdk * fdl * (au - bu + cu - du) pv = av + fdk * (bv - av) + fdl * (dv - av) + fdk * fdl * (av - bv + cv - dv) Given p = (pu, pv), fdk and fdl may be found by calling subroutine aptqfdc. Flag nerr indicates any input error. History: 1990 February 14 17:30. Added capability to sample from boomerangs and bowties. Input: au, av, bu, bv, cu, cv, du, dv, np, tol. Output: fdk, fdl, pu, pv, nerr. Calls: aptqfdc, aptqvac, aptslid, aptsliv, apttloc (sources in aptslibe, binaries in aptblibe). Glossary: The u and v coordinates of vertex "a" of quadrangle. au, av Input The u and v coordinates of vertex "b" of quadrangle. bu, by Input The u and v coordinates of vertex "c" of quadrangle. cu, cv Input The u and v coordinates of vertex "d" of quadrangle. du, dv Input Indicates an input error, if not 0. nerr Output 1 if np is not positive. 2 if quadrangle area is not positive (no sampling). Size of arrays fdk, fdl, pu, pv. np Input Number of points "p" to sample. Fractional distance of point "p" between the quadrangle sides "da" and "bc". Range 0.0 to 1.0. Size np. Range may be less in a boomerang or bowtie. fdk Output Fractional distance of point "p" between the quadrangle sides "ab" and "cd". Range 0.0 to 1.0. Size np. Range may be less in a boomerang or bowtie. fdl

Numerical tolerance limit.

Sampled points. Size np.

Output

Input

Output

tol

pu, pv

SUBROUTINE APTORTS

call aptqrts (noptq, aa, bb, cc, qq, tol, nroots, root1, root2, itrun)

Version: aptqrts Updated 1990 March 21 14:00.

aptqrts Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptgrtslend / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find any real roots of the quadratic equation:

aa * x**2 + bb * x + cc = 0.

The method minimizes truncation error, and indicates when truncation error may still be significant, based on tol. Option noptq allows the user to specify the value of qq \sim bb**2 - 4.0 * aa *cc, instead of using the value calculated here.

Not.e: aptorty is a vectorized version of aptorts.

History: 1990 March 21 14:00. Changed to truncate small positive values

of qq to zero.

Input: noptq, aa, bb, cc, qq, tol.

Out put: qq, nroots, root1, root2, itrun.

Glossary:

qq

Coefficient of x**2 in a quadratic equation. Input

Input Coefficient of x in a quadratic equation.

Input Coefficient of 1 in a quadratic equation.

itrun Output Truncation error indicator. O if insignificant.

1 if the magnitude of qq is less than the estimated truncation error, based on tol. This indicates that the roots are near a minimum or maximum, or that the quadratic is almost the square of a linear function. The value of qq is truncated to zero.

2 if the input value of qq (noptq = 1) differs from the calculated value by more than the estimated

truncation error, based on tol.

noptq Input Option for getting value of qq = bb**2 - 4.0 * aa * cc:

O to not use input qq, but calculate from aa, bb, cc. 1 to use the input value of qq (more accurate). A nonzero value of tol must be used with this

option, for comparision of the input with the calculated value.

nroots Output Number of real roots:

-1 if ((aa .eq. 0.0) .and. (bb .eq. 0.0)).

Equation is null (cc .eq. 0.) or bad (cc .ne. 0.). 0 if (bb**2 .lt. 4.0 * aa * cc).

Roots are complex. 1 if equation is linear:

(aa .eq. 0.0) .and. (bb .ne. 0.0),

or if qq = 0.0.

2 if (bb**2 .gt. 4.0 * aa * cc).

If noptq = 1. Equal to qq = bb**2 - 4.0 * aa * cc, but Input.

calculated more accurately, due to cancellation of terms resulting from the composite nature of aa, bb,

and/or cc.

If noptq = 0. Equal to qq = bb**2 - 4.0 * aa * cc,
calculated locally. Output qq

root1 Output The first or only real root, if (nroots .ge. 1).

root2 Output The second real root, if (nroots .eq. 2).

to1 Input Numerical tolerance limit.

Must not be zero if noptq = 1.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTORTV

call aptqrtv (noptq, aa, bb, cc, qq, np, tol, nroots, root1, root2, itrun) Version: aptqrtv Updated 1990 March 21 14:00, aptorty Originated 1989 November 2 14:10. Author: Arthur L. Edwards, LLNL, L-298, Telephone (413) 422-4123. Sources xport read .245100:aptslibe / 1 1 lib aptalibe(x aptblibe aptqrtv|end / 1 1. aptalibe is a LIB library of FORTRAN source files, aptblibe is a BUIID library of Cray-compiled binaries. Purpose: To find any real roots of the quadratic equation: aa * x**2 + bb * x + cc = 0.for np sets of coefficients aa, bb, cc.
The solution is vectorized over the sets of coefficients, which are calculated in sections of 64 (or less, for the final section). The method minimizes truncation error, and indicates when truncation error may still be significant, based on tol. Option noptq allows the user to specify the value of qq - bb**2 - 4.0 * aa *cc, instead of using the value calculated here. Note: aptqrts is a scalar version of aptqrtv. History: 1990 January 19 15:00. Fixed bug for a = 0.0 or b = 0.0. 1990 March 21 14:00. Changed to allow truncation of small positive qq to zero. Input: noptq, aa, bb, cc, qq, np, tol. Output: qq, nroots, root1, root2, itrun. Glossary: aa Coefficients of x**2 in a quadratic equation. Size np. Input bb Input. Coefficients of x in a quadratic equation. Size np. cc Input Coefficients of 1 in a quadratic equation. Size np. itrun Output Truncation error indicator. O if insignificant. 1 if the magnitude of qq is less than the estimated truncation error, based on tol. This Indicates that the roots are near a minimum or maximum, or that the quadratic is almost the square of a linear function. The value of qq is truncated to zero. 2 If the input value of qq (noptq = 1) differs from the calculated value by more than the estimated truncation error, based on tol. Size np. nerr Output Indicates an input error, if not 0. i if np is not positive. noptq Option for getting value of qq = bb**2 - 4.0 * aa * cc: Input O to not use input qq, but calculate from aa, bb, cc. 1 to use the input value of qq (more accurate). A nonzero value of tol must be used with this option, for comparision of the input with the calculated value. nroots Output Number of real roots: -1 If ((aa .eq. 0.0) .and. (bb .eq. 0.0)). Equation is null (cc .eq. 0.) or bad (cc .ne. 0.). 0 if (bb**2 .lt. 4.0 * aa * cc). Roots are complex. 1 if equation is linear; (aa .eq. 0.0) .and. (bb .ne. 0.0),

Input Number of sets of input data aa, bb, cc, noptq, qq,

2 if (bb**2 .gt. 4.0 * aa * cc).

or 1f qq = 0.0.

qq Input If noptq = 1. Equal to qq = bb**2 - 4.0 * aa * co, but calculated more accurately, due to cancellation of terms resulting from the composite nature of aa, bb, and/or co. Size np.

qq Output If noptq = 0. Equal to qq = bb**2 - 4.0 * aa * co, calculated locally. Size np.

root1 Output The first or only real root, if (nroots .ge. 1). Size np. root2 Output The second real root, if (nroots .eq. 2). Size np.

tol Input Numerical tolerance limit. Must not be zero if noptq = 1. On Gray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTQUAD

oall aptquad (px, py, pz, ax, ay, az, bx, by, bz, ox, oy, oz, dx, dy, dz, noptfd, tol, dpmin, fdkq, fdlq, qx, qy, qz, nlimk, nlimi, itrun, nsida, ndon, nerr)

Version: aptquad Updated 1989 November 29 16:10. aptquad Criginated 1989 November 2 14:10.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: Mport read .245100:aptslibe / 1 1

lib aptuliber aptulibe aptquadlend / 1 1.

aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the minimum distance dpmin from the external point p = (px, py, pz), to the surface bounded by a 3-D quadrangle with vertices (ax,ay,az), (bx,by,bz), (cx,cy,cz), (dx,dy,dz); to find the point q = (qx, qy, qz) on the surface nearest the external point; and to find the fractional distances fdkq and fdlq of that point between opposite sides of the quadrangle. Option noptfd allows the ranges of fdkq and fdlq to be limited. Result and error flags are returned.

The equation of the surface (r, a, b, c, d are vectors) is:

r = a + (b - a) + fdk + (d - a) + fdl + (a - b + c - d) + fdk + fdl

r = a * (1 - fdk)*(1 - fdi) + b * fdk*(1 - fdi) + c * fdk*fdi + d * (1 - fdk)*fdi

where r is a vector (x, y, z), and fdk, fdl are fractional distances between opposite edges.

Method: Uses functional iteration, tangent plane approximation, and acceleration. The rate of convergence depends on the problem. For 2 initial values of fdk, iteratively find fdl nearest the external point, the best fdk for that fdl, etc. If two minima are found, use the least value of dpmin.

Input: px, py, pz, ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, tol.

Output: dpmin, fdkq, fdlq, qx, qy, qz, nlimk, nliml, itrun, nside, ncon, nerr.

Calls: aptfdad, aptptln, aptptpl, aptvdis, aptvpln (sources in aptslibe, binaries in aptblibe).

Glossary:

ax, ay, az Input The x, y, z coordinates of quadrangle vertex "a".

bx, by, bz Input The x, y, z coordinates of quadrangle vertex "b".

cx, cy, cz Input The x, y, z coordinates of quadrangle vertex "c".

dx, dy, dz Input The x, y, z coordinates of quadrangle vertex "d".

fdkq Ontput Fractional distance of the point q = (qx, qy, qz)
between opposite edges of the quadrangle,
from the edge bounded by (ax, ay, az) and
(dx, dy, dz). A value of exactly 0.0 or 1.0 may
indicate actual minimum point outside quadrangle,
Values within tol of 0.0 or 1.0 may be shifted
alightly inside quadrangle. See nlimk.

tqjd	Output	Fractional distance of the point q = (qx, qy, qz) between opposite edges of the quadrangle, from the edge bounded by (ax, ay, az) and (bx, by, bz). A value of exactly 0.0 or 1.0 may indicate actual minimum point outside quadrangle. Values within tol of 0.0 or 1.0 may be shifted slightly inside quadrangle. See nlimi.
itrun	Output	O if no change is made in the calculated value of dpmin, 1 if dpmin is changed to zero, when less than the estimated error in its calculation.
ncon	Output	Error flag. 1 or 2 if first two guesses fail to converge. 3 for total failure to find solution.
nerr	Output	Indicates an input error, if not 0. 1 is added if noptfd is not between 0 and 2.
nlimk	Output	0 if fdkq not adjusted. 1 if near 0.0 or 1.0, shifted inside quadrangle. 2 if outside range 0.0 to 1.0, shifted to 0.0 or 1.0.
nliml	Output	0 if fdlq not adjusted. 1 if near 0.0 or 1.0, shifted inside quadrangle. 2 if outside range 0.0 to 1.0, shifted to 0.0 or 1.0.
nopt fd	Input	Option to limit the ranges of fdkq, fdlq: 0 for no limit, 1 to increase to tol, if in the range from -tol to tol, and decrease to 1.0 - tol, if in the range from 1.0 - tol to 1.0 + tol (move a point near an edge slightly inside the quadrangle), and 2 to limit to the range from 0.0 to 1.0 (move a point outside the triangle to an edge).
nside	Output	<pre>1 if the point nearest p = (px, py, pz) in the extended surface through the quadrangle is actually q = (qx, qy, qz), within tolerance tol. 0 if q = (qx, qy, qz) is only the point on the edges of the quadrangle nearest (px, py, pz), but the vector connecting "p" to "q" is not normal to the surface.</pre>
px,py,pz	Input	The x, y, z coordinates of the external point "p",
dx, dy, dz	Output	The x, y, z coordinates of the point "q" nearest to $p = (px, py, pz)$ on the biquadratic surface.
t.ol	Input	Numerical tolerance limit. Convergence criterion for dpmin. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTOVAC

call aptqvac (au, av, bu, bv, cu, cv, dv, dv, np, tol, nopt, arpa, arpb, arpc, arpd, ntype, qu, qv, nerr)

Version: aptqvac Updated 1990 February 13 13:00. aptqvac Originated 1990 February 8 14:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibeix aptblibe aptqvactend / 1 1,
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the shape and size of np quadrangles in the uv plane, with vertices a = (au, av), b = (bu, bv), c = (cu, cv) and d = (du, dv) counterclockwise around the quadrangle.

Optionally (nopt = 0 or 2), the vertex parallelogram areas arpa, arpb, arpc and arpd will be returned, and (nopt = 1 or 2) the number and location of any concave (negative area) vertices will be returned, encoded in ntype, and if the quadrangle is a bowtie, the intersection of the sides q = (qu, qv), will be returned. The net area of the quadrangle is

0.25 * (arpa + arpb + arpc + arpd).

Flag nerr indicates any input error.

Input: au, av, bu, bv, cu, cv, du, dv, np, tol, nopt.

Output: ntype, arpa, arpb, arpc, arpd, nerr.

Calls: aptvdic, aptvaxc (sources in aptslibe, binaries in aptblibe).

Glossary:

arpb Output Parallelogram area at vertex "b" (nopt = 0 or 2). Size np.

arpc Output Parallelogram area at vertex "c" (nopt = 0 or 2). Size np.

arpd Output Parallelogram area at vertex *d (nopt = 0 or 2). Size np.

au, av Input The u and v coordinates of vertex "a" of quadrangle.
Size np.

bu, by Input The u and v coordinates of vertex "b" of quadrangle.
Size np.

cu, cv Input The u and v coordinates of vertex "o" of quadrangle. Size np.

du, dv Input The u and v coordinates of vertex "d" of quadrangle. Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.
2 if nopt is not 0, 1 or 2.

nopt Input Output option:

O or 2 to return vertax parallelogram areas.

1 or 2 to return shape type code ntype.

2 to return areas, ntype, and bowtle intersections.

```
ntype
Output
Shape type of quadrangle (nopt = 1 or 2).

O if all vertices are convex. Regular.

11 if only vertex "a" is concave. Boomerang.

12 if only vertex "b" is concave. Boomerang.

13 if only vertex "d" is concave. Boomerang.

14 if only vertices "c" and "d" are concave. Bowtie.

22 if only vertices "d" and "b" are concave. Bowtie.

23 if only vertices "a" and "b" are concave. Bowtie.

24 if only vertices "b" and "c" are concave. Bowtie.

31 if only vertex "b" is convex. Inverted boomerang.

32 if only vertex "b" is convex. Inverted boomerang.

33 if only vertex "d" is convex. Inverted boomerang.

34 if only vertex "d" is convex. Inverted boomerang.

40 if all vertices are concave. Inverted boomerang.

40 if all vertices are concave. Inverted regular.

The u and v coordinates of the intersection "q" of two opposite sides of a bowtied quadrangle.

Returned only if nopt = 1 or 2, and ntype = 21 to 24.

tol Input Numerical tolerance limit.
```

SUBROUTINE APTREFC

call aptrefc (pu, pv, au; av, bu, bv, np, tol, qu, qv, nerr)

Version: aptrefc Updated 1990 March 13 11:30. aptrefc Originated 1990 January 10 13:50.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe(x aptblibe aptrefclend / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the 2-D vector

q = (qu, qv) resulting from the reflection of the 2-D vector p = (pu, pv) from the line through the points a = (au, av)

and b = (bu, bv), all in the uv plane.
When point "a" coincides with point "b", based on tol,

no reflection takes place, and vector "q" equals vector "p". Coordinates u and v may be any orthogonal coordinates.

Flag nerr indicates any input error.

Method: The vector "sn" normal to the reflecting surface is the cross

product of the vector normal to the uv plane, (0, 0, 1), and the vector parallel to the line "ab". From simple geometry, "q" = "p" - 2.0 * ("p" dot "u"), where "u" is the

unit vector parallel to "sn".

Input: pu, pv, au, av, bu, bv, np, tol.

Output: qu, qv, nerr.

Glossary:

The u and v coordinates of point "a" in the uv plane. au, av Input Must differ from "b", based on tol. Size np.

bu, bv The u and v coordinates of point "b" in the uv plane. Input

Must differ from "a", based on tol. Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Size of arrays. Input np

The u and v components of the incident vector "p". pu, pv Input

Size np.

The u and v components of the reflected vector "q". au, av Output Components of "q" less than the estimated error in

their calculation, based on tol, will be truncated

to zero. Size no.

Numerical tolerance limit. tol Input

SUBROUTINE APTREFL

call aptrefl (pu, pv, pw, au, av, bu, bv, np, tol, qu, qv, qw, nerr)

Version: aptrefl Updated 1990 March 13 11:30. aptrefl Originated 1990 January 10 13:50.

Arthur L. Edwards, L%NL, L-298, Telephone (415) 422-4123, Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe(x aptblibe aptreflend / 1 1, aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the vector q = (qu, qv, qw) resulting from the reflection of vector
p = (pu, pv, pw) from the surface perpendicular to the uv plane
and through the points a = (au, av, 0), and b = (bu, bv, 0), when incident on the surface on the line "ab".

When point "a" coincides with point "b", based on tol, no reflection takes place, and vector "q" equals vector "p". Coordinates u, v and w may be any orthogonal coordinates.

Flag nerr indicates any input error.

The vector "sn" normal to the reflecting surface is the cross Method:

product of the vector normal to the uv plane, (0, 0, 1), and the vector parallel to the line "ab". From simple geometry, "q" = "p" - 2.0 * ("p" dot "u"), where "u" is the unit vector parallel to "sn".

Input: pu, pv, pw, au, av, bu, bv, np, tol.

qu, qv, qw, nerr. Output:

Glossarv:

The u and v coordinates of point "a" in the uv plane. au, av Input Must differ from "b", based on tol. Size np.

The u and v coordinates of point "b" in the uv plane.

Must differ from "a", based on tol. Size np. bu, bv Input

Indicates an input error, if not 0. nerr Output 1 if np is not positive.

np Input Size of arrays.

pu, pv, pw Input The u, v, w components of incident vector "p". Size np.

The u, v, w components of reflected vector "q". qu, qv, qw Output Components of "q" less than the estimated error in their calculation, based on tol, will be truncated to zero. Note that qw = pw. Size np.

tol Numerical tolerance limit. Input On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTREFS

call aptrefs (itype, ax, ay, az, bx, by, bz, cx, cy, cz, px, py, pz, np, tol, refm, nerr)

Version: aptrefs Updated 1990 March 14 16:00. aptrefs Originated 1990 January 10 13:50.

Author: . Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptrefslend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the matrix operator refm for reflection from a plane: itype = 0: the plane contains point a = (ax, ay, az), and

has normal vector b = (bx, by, bz). itype = 1: the reflection exchanges the points a = (ax, ay, az)

and (bx, by, bz).

itype = 2: the plane contains the 3 points a = (ax, ay, az),
b = (bx, by, bz), and c = (cx, cy, cz).

To do the reflection operation on the np points or vectors $\mathbf{p} = (\mathbf{px}, \mathbf{py}, \mathbf{pz})$. If $\mathbf{p} = (\mathbf{px}, \mathbf{py}, \mathbf{pz})$ are unbound vectors, either use module aptmopv, or make sure the reflection plane contains the origin. Size np may be 0. The new values of (px, py, pz) will be truncated to zero if less than the estimated error in their calculation,

based on tol.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: itype, ax, ay, az, bx, by, bz, cx, cy, cz, px, py, pz, np, tol.

Output: px, py, pz, refm, nerr.

Calls: aptvxun, aptvunb (sources in aptslibe,

binaries in aptblibe).

Glossary:

ax, ay, az Input The x, y, z coordinates or components of a point or

vector.

bx, by, bz Input The x, y, z coordinates or components of a point or

vector.

The x, y, z coordinates of a point. cx, cy, cz Input

Defines option for describing reflection plane: itype Input

0 if plane contains point a = (ax, ay, az), and and has normal vector b = (bx, by, bz).

1 if reflection exchanges (ax, ay, az), (bx, by, bz).

2 if plane contains points (ax, ay, az), (bx, by, bz)

and (cx, cy, cz).

Output Indicates an input error, if not 0. nerr

1 if the magnitude of any input vector is too small, 2 if any 2 of the points (a, b, c) are congruent, or if the points (a, b, c) are colinear, and

itype = 3.

3 if itype is not 0, 1 or 2.

Input Number of points or vectors (px, py, pz). May be 0. np

px,py,pz In/Out The x, y, z coordinates of a point, or

the x, y, z components of a vector. Size np. Will be truncated to zero, if less than the estimated

error in their calculation, based on tol.

Output Reflection operator (a unitary 3 x 3 matrix).

Must be sized refm(3,3).

Input Numerical tolerance limit. Used to test and adjust

unit vector and point components.

SUBROUTINE APTRKCL

call aptrkel (pr, ur, ut, uz, sr, dr, dintmn, dintmx, np, tol, nint, dint, nerr)

Version: aptrkcl Updated 1990 January 24 13:40. aptrkcl Originated 1990 January 19 16:20.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe/x aptblibe aptrkcliend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, any exit intersection of the linear track through point p = (pr) with unit direction vector u = (ur, ut, uz), with the cylindrical surface with fixed radius sr, for which (1) the distance dint from point "p" to the intersection is between the limits dintmn and dintmx, and (2) the radial component ur of the direction vector "u" at the intersection has the same sign as dr. Flag nerr indicates any input error.

Input: pr, ur, ut, uz, sr, dr, dintmn, dintmx, np, tol.

Output: nint, dint, nerr.

Input

Calls: aptqrtv, aptvlim (aptfdav optional) (sources in aptslibe, binaries in aptblibe).

Glossary:

dr '

dint Output Distance from point "p" to intersection at radius sr along track (not radial distance).

dintmn Input Minimum allowed value of distance to intersection.
Size np.

dintmx Input Maximum allowed value of distance to intersection. Size np.

Sign of exit direction through surface at sr. Size np.

nerr Output If not 0, indicates an input error.

1 if np is not positive.

nint Output O if no exit intersection was found.

1 if an exit intersection was found at the surface at radius sr, with a distance to intersection dint between dintmn and dintmx. Size np.

np Input Size of arrays pr, ur, ut, uz, sr, dr, dintmn, dintmx, nint.

pr Input Cylindrical radial coordinate of initial point on track. Size np.

sr Input Cylindrical radial coordinate of surface. Size np.

ur Input Initial cylindrical radial component of unit direction vector along track. Size np.

ut Input Initial theta component of unit direction vector along track. Theta is angle in x-y plane counterclockwise from x axis. Size np.

uz Input Initial axial z component of unit direction vector along track. Size np.

tol Input Truncation error limit.

Used to test for intersection being nearly tangent, and for accuracy of intersection.

Must not be zero.

On Cray computers, recommend 1.e-11.

SUBROUTINE APTRKCY

call aptrkcy (pz, pr, uz, ur, ut, az, ar, bz, br,
dintmn, dintmx, np, noptd, tolf, tols,
nint, pinz, pinr, dint, nerr)

Version: aptrkcy Updated 1990 January 23 16:30. aptrkcy Originated 1989 December 7 16:40.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100;aptslibe / 1 1
lib aptslibe!x aptblibe aptrkcy!end / 1 1.
aptslibe is a LIB library of FORTRAN source file

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, any acceptable exit intersection (pinz, pinr) of the linear track through point p = (pz, pr) with unit direction vector u = (uz, ur, ut), with the cylindrical axisymmetric surface through points a = (az, ar) and b = (bz, br), for which (1) the distance from point "p" to pin = (pinz, pinr) is between the limits dintmn and dintmx, (2) the intersection is between a = (az, ar) and b = (bz, br), and (3) the crossing at the intersection is from left to right in the zr plane (right to left in the rz plane).

This is a zone exit if the points (az, ar) and (bz, br) are the vertices of a zone edge, counterclockwise around the zone in the

the zr plane (clockwise in the rz plane).

History: 1990 January 23 10:10. Implemented use of aptfdav to adjust values of fintl and fint2 near 0.0 or 1.0. Vectorized

intersection test loop.

Input: pz, pr, uz, ur, ut, az, ar, bz, br, dintmn, dintmx, np,

noptd, tolf, tols.

Output: nint, pinz, pinr, dint, nerr.

Calls: aptqrtv, aptvlim, aptfdav.

(cources in aptslibe, binaries in aptblibe).

Glossary:

ar Input Cylindrical radial coordinate of beginning of cylindrical axisymmetric surface. Size np.

Theta ranges from 0 to 360 degrees.

az Input Cylindrical axial z coordinate of beginning of cylindrical axisymmetric surface. Size np.

br Input Cylindrical radial coordinate of end of cylindrical axisymmetric surface. Size np.

bz Input Cylindrical axial z coordinate of end of cylindrical axisymmetric surface. Size np.

dint Output Distance from (pz, pr) to intersection at (pinz, pinr), along track (not distance in zr plane).

 $\begin{array}{ll} \mbox{dintmn} & \mbox{Input} & \mbox{Minimum allowed value of distance to intersection.} \\ & \mbox{Size np.} \end{array}$

dintmx Input Maximum allowed value of distance to intersection. Size np.

nerr Output If not 0, indicates an input error.

1 if np is not positive.

nint Output O if no acceptable exit intersection was found.

1 if an acceptable exit intersection was found on the surface segment between (az, ar) and (bz, br), with a distance to the intersection dint between dintmn and dintmx. Size np.

noptd Input Option to limit the minimum magnitude of the components of the direction vector u = (uz, ur, ut). The method used here will fail if uz or ut is zero.

0 for no magnitude test. Must be done elsewhere.
1 to limit the minimum magnitudes of ut and uz to no less than tols.

np	Input	Size of arrays pz, pr, uz, ur, ut, az, ar, bz, br, dintmn, dintmx, nint, pinz, pinr.
pinr	Output	Cylindrical radial r coordinate of intersection point. Size np.
pinz	Output	Cylindrical axial z coordinate of intersection point. Size np.
pr	Input	Cylindrical radial r coordinate of the initial point on the track. Size np.
pz	Input	Axial z coordinate of the initial point on the track. Size np.
ur	Input	Initial cylindrical radial component of the unit direction vector along the track. Size np.
ut	Input	Initial theta component of the unit direction vector along the track. Theta is the angle in the xy plane counterclockwise from x axis. Size np.
uz	Input	Initial saial z component of unit direction vector along track. Size np.
tolf	Input	Truncation error limit to be imposed on the fractional distance of the intersection (pinz, pinr) along the line segment from (az, ar) to (bz, br). Values less than -tolf or greater than 1.0 + tolf will not be accepted. Values from -tolf to tolf will be changed to tolf. Values from 1.0 - tolf to 1.0 + tolf will be changed to 1.0 - tolf. Also used to test for the intersection being nearly tangent, and for the accuracy of the intersection. Must not be zero. On Cray computers, recommend 1.e-11.
tols	Input	Truncation error limit to be imposed on uz, ut and pinr. Magnitudes of ut and uz less than tols will be increased to tols. Values of pinr less than tols * pr will be increased to tols * pr. On Cray computers, recommend 1.e-5. A value of zero may produce unpredictable results.

SUBROUTINE APTRKIS

qx,qy,qz Output

call aptrkis (px, py, pz, vx, vy, vz, ac, ax, ay, az, axy, ayz, azx, axx, ayy, azz, dintmn, dintmx, np, tol, nint, qx, qy, qz, dint, nerr) 1990 March 14 16:00. Version: aptrkis Updated aptrkis Originated 1990 February 23 10:00. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibelx aptblibe aptrkislend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find, for each of np sets of input data, the distance distinct to the intersection $q=(qx,\ qy,\ qz)$ of the linear track through point $p=(px,\ py,\ pz)$ with direction vector $v=(vx,\ vy,\ vz)$, and the general second order surface for which the equation is and for which dint is between dintmn and dintmx. If two such intersections occur, the one with the smaller magnitude of dint will be returned. If no such intersection is found, nint will be 0, and dint and the coordinates of point "q" will be very large. Flag nerr indicates any input error. The vector normal to the surface is s = (df/dx, df/dy, df/dz). The sign of the direction of the intersection is determined by the dot product v * s. 1990 March 14. Changed tol to 0.0 in call to unit vector History: subroutine. Allows small magnitudes. Input: px, py, pz, vx, vy, vz, ac, ax, ay, az, axy, ayz, azx, axx, ayy, azz, dintmn, dintmx, np, tol. Out put: nint, qx, qy, qz, dint, nerr. Calls: aptqrtv, aptvadd, aptvunb (sources in aptslibe, binaries in aptblibe). Glossary: Input Coefficients of the implicit equation of a second-order surface in xyz space (ac, ax, ay, az, axy, ayz, azx, axx, ayy, azz). dint Out put. The distance of the point of intersection "q" from point "p", if nint = 1. Size np. Positive If in the same direction as vector "v". Acceptable only if between dintmn and dintmx. dintmn Input The minimum allowable value of dint. dintmx Input The maximum allowable value of dint. nerr Output Indicates an input error, if not 0. 1 if np is not positive. 1 if the track through point "p" in direction "v" intersects the surface at a distance dint between dintmn and dintmx. 0 if no such intersection was found. -1 if vector "v" is too short, based on tol. Input Size of arrays. px, py, pz Input The x, y, z coordinates of point "p".

The x, y, z coordinates of the point of intersection

of the line through point "p" with unit direction vector "v", and the surface, if nint = 1.

vx,vy,vz Input The $x,\ y,\ z$ components of direction vector "v". If the magnitude is too small, nint will be -1.

tol Input Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTRKLC call aptrkic (au, av, abu, abv, cu, cv, du, dv, dintmn, dintmx, np, tol, nint, eu, ev, dint, nerr) Version: aptrklo Updated 1990 March 14 16:00. aptrklo Originated 1990 January 11 15:10. 1990 March 14 16:00. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Sourcet lib aptslibelx apublibe aptrklolend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. To find, for each of the np sets of input data, any Purpose: intersection point e = (eu, ev) of the linear track through point a = (au, av) with the direction vector ab = (abu, abv), and the line segment from point c = (cu, cv) to point d = (du, dv), all in the uv plane of uvw space, for which (1) the distance from point "a" to point "a" is between the limits dintmn and dintmx, (2) point "e" is between point "c" and "d", and (3) the track crosses line "cd" from left to right and "d", and (3) the track crosses the current left to light in the uv plane. This is a zone exit if the points "c" and "d" are the vertices of a zone edge, counterclockwise around the zone in the uv plane. Flag mint indicates the type of intersection found. The distance dint of the intersection from point "a" is also returned. Flag nerr indicates any input error. History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes. Input: au, av, abu, abv, cu, cv, du, dv, dintmn, dintmx, np, tol. Output: nint, eu, ev, dint, nerr, Calls: aptfdav, aptvadc, aptvaxc, aptvdic, aptvubc (sources in aptslibe, binaries in aptblibe). Glossary: Input The u and v coordinates of point "a". Size np. au, av In the uv plane. abu, abv The u and v components of 2-D direction vector "ab". Input Must not both be zero. Size np. The u and v coordinates of point "c" in the uv plane.

Must differ from "d", based on tol. Size np. cu, cv Input du, dv Input The u and v coordinates of point "d" in the uv plane, Must differ from "c", based on tol. Size np. The distance of the point of intersection "e" from dint Output point "a". Positive if in the same direction as vector "ab". Size np. dintmn Input Minimum allowed value of distance to intersection. Size no. dintmx Input Maximum allowed value of distance to intersection. Size no. The u and v coordinates of the point of intersection of the line through point "a" with direction vector "ab", and line "cd", all in the uv plane. Output eu, ev nerr Output Indicates an input error, if not 0. 1 if np is not positive. nint Output Number of acceptable intersections found. 0 if none. 1 if an acceptable intersection was found.

2 if the track coincides with part of line "cd".

On Cray computers, recommend 1.e-5 to 1.e-11.

Input

Input

np tol Size of arrays.

Numerical tolerance limit.

SUBROUTINE APTRKPL

call aptrkpl (px, py, pz, vx, vy, vz, ax, ay, az, bx, by, bz, cx, cy, cz, np, tol, dpmin, dint, qx, qy, qz, ipar, nerr)

Version: aptrkpl Updated 1990 March 15 16:40. aptrkpl Originated 1989 November 30 15:50.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe(x aptblibe aptrkpl)end / 1 1.
aptslibe is a LIR library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the point of intersection q = (qx, qy, qz) of the linear track through point p = (px, py, pz) with direction vector v = (vx, vy, vz), and the plane through points a = (ax, ay, az), b = (bx, by, bz), and c = (cx, cy, cz), and the distance dint between points "p" and "q". The perpendicular distance dpmin from the plane to point "p" is also returned.

If the vector "v" is parallel to the plane, flag ipar will be 1. If so, and dpmin is not zero, dint and the coordinates of point "q" will be very large. Otherwise, if dpmin is zero, dint will be zero, and the coordinates of point "q" will be those of point "p".

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector sub-coutine. Allows small magnitudes.
1990 March 15. Changed the values of dpmin, dint, and point "q" when the plane "abo" is undefined (ipar = 3 or 4). No effect on problems with good input data.

Input: px, py, pz, vx, vy, vz, ax, ay, az, bx, by, bz, cx, cy, cz, ..., tol.

Output: dpmin, dint, qx, qy, qz, ipar, nerr.

Calls: aptvadd, aptvdis, aptvdot, aptvpin, aptvuna, aptvunb (sources in aptslibe, binaries in aptblibe).

Glossary:

ax,ay,az Input The x, y, z coordinates of point "a" in the plane.

Must differ from "b" and "c", based on tol. Size np.

bx,by,bz Input The x, y, z coordinates of point "b" in the plane.

Must differ from "a" and "c", based on tol. Size np.

cx,cy,cz Input The x, y, z coordinates of point "c" in the plane.

Must differ from "a" and "b", based on tol. Size np.

dint
Output The distance of the point of intersection "q" from point "p", if ipar = 0. Positive if in the same direction as vector "v". Size np.
Meaningless, but large if ipar = 1.
Meaningless, but zero if ipar = 2, 3, or 4.

dpmin Output The perpendicular distance to point "p" from the plane. Positive if point "p" is on the side of the plane for which points "a", "b", and "c" are counterclockwise. Meaningless if ipar = 2, 3, or 4. If less than the estimated error in its calculation, dpmin will be truncated to zero. Size np.

nerr Output Indicates an input error, if not 0.
1 if np is not positive.

np Input Size of arrays.

px, py, pz Input The x, y, z coordinates of point "p".

The M, y, z coordinates of the point of intersection of the line through point "p" with unit direction vector "v", and the plane through points "a", "b", and "c", if ipar = 0. Size np.

Meaningless, but large if ipar = 1.

Meaningless, but zero if ipar = 2, 3 or 4. qx,qy,qz Output

vx, vy, vz Input The x, y, z components of direction vector "v".

Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTRKAL

osil aptrkri (pr. ur. sr. dr. dintmn. dintmx, np. toi.
nint, dint, nerr)

Version: aptrkrl Updated 1990 January 24 15:50, aptrkrl Originated 1990 January 19 16:20,

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe:x aptblibe aptrkritend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, any exit intersection of the linear track through point p = (pr) with unit direction vector u = (ur, ut, up), with the spherical surface with fixed radius sr, for which (1) the distance dint from point "p" to the intersection is between the limits dintmn and dintmx, and (2) the radial component ur of the direction vector "u" at the intersection has the same sign as dr. Flag nerr indicates any input error.

Input: pr, ur, sr, dr, dintmn, dintmx, np, tol.

Output: nint, dint, nerr.

Calls: aptqrtv, aptvlim (aptfdav optional) (sources in aptslibe, binaries in aptblibe).

Glossary:

dint Output Distance from point "p" to intersection at radius sr along track (not radial distance).

dintmn Input Minimum allowed value of distance to intersection. Size np.

dintmx Input Maximum allowed value of distance to intersection. Size np.

dr Input Sign of exit direction through surface at sr. Size np.

nerr Output If not 0, indicates an input error.

1 if np is not positive.

nint Output O if no exit intersection was found.

1 if an exit intersection was found at the surface at radius sr, with a distance to intersection dint between dintmm and dintmx. Size np.

np Input Size of arrays pr, ur, sr, dr, dintmn, dintmx, nint.

pr Input Spherical radial coordinate of initial point on track, Size np.

sr Input Spherical radial coordinate of surface. Size np.

ur Input Initial spherical radial component of unit direction vector along track. Size np.

tol Input Truncation error limit.

Used to test for intersection being nearly tangent, and for accuracy of intersection. Must not be zero.

On Cray computers, recommend 1.e-11.

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SUBROUTINE APTRKSL

call aptrksl (au, abu, cu, du, dintmn, dintmx, np, tol, nint, ou, dint, nerr)

1990 January 24 16:00. Version; aptrksi Updated aptrksl Originated 1990 January 11 15:10.

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100;aptslibe / 1 1 lib aptalibelx apthlibe aptrkallend / 1 1. aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, any intersection of the linear track through point a = (au) in the direction of the unit vector ab = (abu, abv, abw), with the vw plane through the point a = (au), with the normal vector d = (du), for which (1) the distance dint from point "a" to the intersection is between the limits dintmn and dintmx, and (2) the direction vector abu has the same sign as du. This is equivalent to a zone exit in 1-D slab geometry, if du has the sign of the direction out of the zone at point ou. Flag ninc indicates the type of intersection found.

Flag nerr indicates any input error.

To find a zone exit in 1-D slab geometry.

Input: au, abu, cu, du, dintmn, dintmx, np, tol.

Out put: nint, dint, nerr.

aptvdil (source in aptslibe, binary in aptblibe). Calls:

Glossarv:

The u coordinate of point "a". The v and w coordinates au Input are zero. Directions u, v and w are orthogonal. Size np.

The u component of the unit direction vector "ab" along abu Input the track in uvw space. Size np. An acceptable intersection can only occur if abu has

the same sign as du.

The u coordinate of point "c". Size np. cu Input

dint Output The distance of the point of intersection of the track from point "a" to the uv plane through point "c". Positive if in the same direction as vector "ab".

du Input The u component of the outward normal vector of the vw plane at point "c". Size np. An acceptable intersection can only occur if abu has the same sign as du.

dintmn Input Minimum allowed value of distance to intersection dint. Size Do.

dintmx Input Maximum allowed value of distance to intersection dint. Size np.

nerr Output Indicates an input error, if not 0. 1 if np is not positive.

nint Output Number of acceptable intersections found. 0 if none. 1 if an acceptable intersection was found.

Size of arrays. np Input

tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTRNDS

call aptrnds (nopt, x, dx, nsig, np, tol, nerr)

aptrnds Updated 1990 February 2 10:40. aptrnds Originated 1990 February 2 10:40.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe!x aptblibe aptrndsiend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUJID library of Cray-compiled binaries.

To find, for each of np values of \mathbf{x} , the new value of \mathbf{x} after

rounding off to the nearest multiple of dx in the first nsig significant figures (nopt = 0), or in the absolute value

(nopt - 1).

Flag nerr indicates any input error.

nopt, x, dx, nsig, np. Input:

Output: x, nerr.

Glossary:

Precision of rounded result in significant figure dx Input nsig (nopt = 0), or in absolute value (nopt = 1). Must not be zero. Normally from 1.0 to 5.0.

Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive. 2 if nopt is not 0 or 1.

nopt Input Indicates type of rounding off to be done.

O to round off to the nearest multiple of dx in the first nsig significant figures of x.

1 to round off to the nearest multiple of dx in the

absolute value of x.

Input Size of arrays x, dx, and if nopt = 0, nsig. np

nsig Input Number of significant figures to be rounded off to the

nearest multiple of dx (nopt = 0).

Values less than 1 will be equivalent to 1.

Values greater than the machine limit will have

no effect.

Size np, if nopt = 0. Otherwise, undimensioned.

tol Input Precision of mixed integer and floating point

operations on machine. Recommend 1.e-11 on Cray.

Value to be rounded off, and rounded result. Size np. In/Out

SUBROUTINE APTROTA

call aptrota (theta, ku, vx, vy, vz, tol, rotm, nerr)

Version: aptrota Updated 1989 March 14 16:00. aptrota Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport_read .245100:aptslibe / 1 1 Source:

lib aptslibels aptblibe aptrotalend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the rotation matrix operator rotm, to do a

counterclockwise rotation by the angle theta, around the

axis parallel to the vector v = (vx, vy, vz).

(Counterclockwise: with the axis pointed at the observer.)
The angle may be in degrees (ku = 0) or radians (ku = 1). Flag nerr indicates any error in v (too small) or ku (not 0, 1).

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: theta, ku, vx, vy, vz.

Output: rotm, nerr.

Input

Calls: aptvunb (source in aptslibe, binary in aptblibe).

Glossary:

tol

ku Input Indicates theta units are degrees (0) or radians (1).

nerr Output Indicates an input error, if not 0.

1 if magnitude of (vx, vy, vz) too small. 2 if ku is not 0 or 1.

Output Rotation operator (a unitary 3 x 3 matrix). rotm

Must be sized rotm(3,3).

Angle of rotation around axis, counterclockwise when theta Input

rotation axis is pointed at observer. Units are degrees (ku = 0) or radians (ku = 1).

unit vector components and point coordinates.

Numerical tolerance limit. Used to test and adjust On Cray computers, recommend 1.e-5 to 1.e-11.

VΧ Input The x component of vector parallel to rotation axis.

Input The y component of vector parallel to rotation axis. vy

The z component of vector parallel to rotation axis. Input

SUBROUTINE APTROTC

call aptroto (au, av, bu, bv, cu, cv, np, tol, nerr)

Version: aptrotc Updated 1990 March 14 16:00. aptrotc Originated 1989 December 29 10:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptrotclend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To rotate the np 2-D vectors c = (cu, cv) around the w axis by the angle needed to make 2-D vector a = (au, av) parallel to 2-D vector b = (bu, bv). All are in the uv plane. Directions u, v and w are orthogonal. Any new components of c = (cu, cv) that are smaller than their estimated error, based on tol, will be truncated to zero. Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: au, av, bu, bv, cu, cv, tol.

Output: cu, cv, nerr.

Calls: aptvaxc, aptvdoc, aptvubc (sources in aptslibe,

binaries in aptblibe).

Glossary:

au, av Input The u and v components of the first vector.

The w components are zero.

bu, by Input The u and v components of the second vector.

The w components are zero.

cu, cv Input The u and v components of vector "c". Size np.

The w components are zero.

cu, cv Output The u and v components of vector "c", after

rotation. The w components are zero. Will be truncated to zero, if smaller than the estimated error in their calculation, based on tol. Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

2 if vector "a" is too short. 3 if vector "b" is too short.

np Input The size of arrays cu, cv.

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTROTP

call aptrotp (ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, tol, rotm, nerr)

Version: aptrotp Updated 1989 March 14 16:00. aptrotp Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibeix aptblibe aptrotpiend / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the rotation matrix operator rotm, for rotating the

plane containing the vectors $\mathbf{a}=(\mathbf{a}\mathbf{x},\ \mathbf{a}\mathbf{y},\ \mathbf{a}\mathbf{z})$ and $\mathbf{b}=(\mathbf{b}\mathbf{x},\ \mathbf{b}\mathbf{y},\ \mathbf{b}\mathbf{z})$ to be parallel to the plane containing the vectors $\mathbf{c}=(\mathbf{c}\mathbf{x},\ \mathbf{c}\mathbf{y},\ \mathbf{c}\mathbf{z})$ and $\mathbf{d}=(\mathbf{d}\mathbf{x},\ \mathbf{d}\mathbf{y},\ \mathbf{d}\mathbf{z})$, around an axis parallel to both planes. Any components of rotm within tol of -1.0, 0.0, or 1.0, will be truncated to those values.

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz. Input:

Output: rotm. nerr.

aptvaxb, aptvuna, aptvxun (sources in aptslibe, binaries in aptblibe). Calls:

Glossary:

ax, ay, az Input The x, y, z components of a vector.

bx, by, bz Input The x, v, z components of a vector.

cx, cy, cz Input The x, y, z components of a vector.

dx, dy, dz Input The x, y, z components of a vector.

Output Indicates an input error, if not 0. nerr

1 if the magnitude of any input vector is too small, or the two vectors in a plane are almost parallel.

Output Rotation operator (a unitary 3 x 3 matrix). rotm

Must be sized rotm(3,3).

tol Input Numerical tolerance limit. Used to test and adjust unit vector components and point coordinates.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTROTS

call aptrots (n1, th1, n2, th2, n3, th3, ku, to1, rotm, nerr)

Version: aptrots Updated 1989 November 13 15:20. aptrots Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe'x aptblibe aptrots'end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the rotation matrix operator rotm, to do a sequential rotation of angle th1 around axis n1, angle th2 around axis n2, and angle th3 around axis n3. All angles are measured counterclockwise, with the axis pointed at the observer.

The axes may be x (1), y (2), or z (3). Angles may be in degrees (ku = 0) or radians (ku = 1).

Flag nerr indicates any input error.

Input: n1, th1, n2, th2, n3, th3, ku, to1.

Output: rotm, nerr.

Glossary:

Glossary:	
ku Inp	t Indicates theta units are degrees (0) or radians (1).
n1 Inp	Indicates first axis is x (1), y (2), or z (3). May not be 0, but th1 may be 0.
n2 Inp	Indicates second axis is x (1), y (2), or z (3). May not be 0, but th2 may be 0.
n3 : Inp	Indicates third axis is x (1), y (2), or z (3). May not be 0, but th3 may be 0.
nerr Out	ut Indicates an input error, if not 0. 1 if n1, n2, or n3 not in range 1-3, or not unique. 2 if ku is nor 0 or 1.
rotm Out	ut Rotation operator (a unitary 3 x 3 matrix). Must be sized rotm(3,3).

thl Input Angle of rotation around axis nl, counterclockwise

when rotation axis is pointed at observer. Units are degrees (ku = 0) or radians (ku = 1).

th2 Input Angle of rotation around axis n2. See thl:

th3 Input Angle of rotation around axis n3. See th1.

tol Input Numerical tolerance limit. Used to test and adjust unit vector components and point coordinates.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTROTT

call aptrott (ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, tol, rotm, nerr)

Version: aptrott Updated 1990 March 14 16:00. aptrott Originated 1989 November 2 14:10.

Author: Arthur I. Edwards, LINL, 1-298, Telephone (415) 422-4123.

xport read /245/00:aptslibe / 1 1 Source:

aption is a Mill library of FORTRAN source files. aptiblibe is a MIB library of Cray-compiled binaries.

Purpose: To find the rotation matrix operator rotm, for rotating the vector a = (ax, ay, az) and the plane containing vectors "a" and b = (bx, by, bz), to be parallel to vector c = (cx, cy, cz) and the plane containing vectors "c" and d = (dx, dy, dz). Any components of rotm within tol of -1.0, 0.0, or 1.0, will be truncated to those values. Flag nerr indicates any input error.

> If vectors "a" and "b" are the first two vectors of the positive vector triple (a, b, a x b), and c and d are the first two vectors of the positive vector triple $(c, d, c \times d)$, then rotm rotates (a, b, a x b) onto (c, d, c x d), or equivalently, redefines the coordinate axes to be (a, b, c x d) instead of (c, d, c x d). (a x b indicates the vector product of a and b.)

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History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

Input: ax, ay, az, bx, by, bz, cx, cy, cz, dx, dy, dz, tol.

Output:

Calls: aptvxun, aptvunb (sources in aptslibe, binaries in aptblibe).

Glossarv:

ax, ay, az Input The x, y, z components of a vector.

bx, by, bz Input The x, y, z components of a vector.

dx, cy, cz Input The x, y, z components of a vector.

dx, dy, dz Input The x, y, z components of a vector.

nerr Output Indicates an input error, if not 0. 1 if the magnitude of any input vector is too small, or the two vectors in a plane are almost parallel.

rotm Output Rotation operator (a unitary 3 x 3 matrix). Must be sized rotm(3,3).

tol Input Numerical tolerance limit. Used to test and adjust unit vector components and point coordinates. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTROTV

call aptrotv (ax, ay, az, bx, by, bz, tol, rotm, nerr)

Version: aptroty Updated 1990 March 14 16:00. aptroty Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe!x aptblibe aptrotviend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the rotation matrix operator "rotm", for rotating the vector a = (ax, ay, az) to be parallel to the vector b = (bx, by, bz), around an axis perpendicular to both. Any components of "rotm" within tol of -1.0, 0.0, or 1.0, will be truncated to those values.
Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

Input: ax, ay, az, bx, by, bz, tol.

Output: rotm, nerr.

Calls: aptvxun, aptvdot, aptvunb (sources in aptslibe, binaries in aptblibe).

Glossary:

ax, ay, az Input The x, y, z components of vector "a".

bx, by, bz Input The x, y, z components of vector "b".

nerr Output Indicates an input error, if not 0.

1 if the magnitude of vector "a" or "b" is too small.

rotm Output Rotation operator (a unitary 3 x 3 matrix).

Must be sized rotm(3,3).

tol Input Numerical tolerance limit. Used to test and adjust unit vector components and point coordinates.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTSCAD

call aptiscad (np, au, av, aw, bu, bv, bw, nerr)

1990 February 27 10:20. aptscad Updated aptscad Originated 1990 February 27 10:20.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe(x aptblibe aptscad(end / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find up unit vectors b = (bu, bv, bw), representing random directions uniformly distributed in a plane

with the normal vector a = (au, av, aw) in 3-D space. Flag nerr indicates any input error (np not positive).

Calls: apticat, aptvxun

(sources in aptslibe, binaries in aptblibe).

Input: np, au, av, aw.

Output: bu, bv, bw, nerr.

Out.put

Glossary:

au, av, aw Input The u, v and w components of the vector normal to

the plane in which the vectors "b" are to be.

Output The u component of a unit vector representing a

direction chosen randomly from a uniform distribution in 3-D space, in the plane with normal

vector "a". Coordinates u, v and w may

be any 3 orthogonal coordinates. Size np.

The v component of a unit vector representing a direction chosen randomly from a uniform distribution in 3-D space, in the plane with normal

vector "a". Coordinates u, v and w may be any 3 orthogonal coordinates. Size np.

b₩ Output The w component of a unit vector representing a

direction chosen randomly from a uniform distribution in 3-D space, in the plane with normal vector "a". Coordinates u, v and w may be any 3 orthogonal coordinates. Size np.

nerr Output Indicates an input error, if not 0.

 λ if np is not positive.

np Input Size of arrays.

SUBROUTINE APTSCAP

call aptscap (np, au, av, aw, pm, bu, bv, bw, nerr)

Version: aptscap Updated 1990 January 10 10:30. aptscap Originated 1990 January 10 10:30.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptscaplend / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find np unit vectors b = (bu, bv, bw), representing random directions in a cosine**pm distribution in 3-D space, centered on an axis in the direction of vector a = (au, av, aw), with the restrictions that the magnitudes of the components be no smaller than the specified limits tolu, tolv, tolw, respectively. Flag nerr indicates any input error.

> If "ba" is the expected value of the component of vector "b" in the direction of vector "a", then:

Calls: aptmopv, aptrotv, aptvlim

(sources in aptslibe, binaries in aptblibe).

np, tolu, tolv, tolw, au, av, aw, pm. Input:

Output: bu, bv, bw, nerr.

Glossary:

The u, v and w components of a vector in the direction au, av, aw Input of the center of a cosine**pm distribution.

Out put The u component of a unit vector representing a direction chosen randomly from a cosine**pm distribution in 3-D space, centered in the direction of vector "a". Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolu;

The v component of a unit vector representing a Out put direction chosen randomly from a cosine**pm distribution in 3-D space, centered in the direction of vector "a". Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolv.

bw Output The w component of a unit vector representing a direction chosen randomly from a cosine ** pm distribution in 3-D space, centered in the direction of vector "a". Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolw.

nerr Output Indicates an input error, if not 0. 1 if np is not positive.

Size of irravs. np Input

Power used for the cosine**pm spatial distribution рm Input from which unit vector "b" is to be chosen.

Minimum magnitude of all bu components. tolu Input On Cray computers, recommend 1.e-5.

tolv Input Minimum magnitude of all by components. On Cray computers, recommend 1.e-5.

Minimum magnitude of all bw components. tolw Input On Cray computers, recommend 1.e-5.

SUBROUTINE APTSCAT

call aptscat (np, au, av, aw, nerr)

aptscat Updated 1990 January 10 10:40. aptscat Originated 1990 January 10 10:40. Version: aptscat Updated

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source: lib aptsilbelx aptblibe aptsoatlend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find np unit vectors a = (au, av, aw), representing random directions in 3-D space, with the restrictions that the magnitudes of the components be no smaller than the specified limits tolu, tolv, tolw, respectively.

Flag nerr indicates any input error (np not positive).

Input: np, tolu, tolv, tolw.

Output: au, av, aw, nerr.

aptvlim (source in aptalibe, binary in aptblibe). Calls:

Glossary:

Output The u component of a unit vector representing a random direction in 3-d space. Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolu.

Output The v component of a unit vector representing a random direction in 3-d space. Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolv.

Output The w component of a unit vector representing a random direction in 3-d space. Coordinates u, v and w may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolw.

Indicates an input error, if not 0. nerr Output 1 if np is not positive.

np Input Size of arrays.

Minimum magnitude of all au components. tolu Input. On Cray computers, recommend 1.e-5.

Minimum magnitude of all av components. tolv Input On Cray computers, recommend 1.e-5.

tolw Input Minimum magnitude of all aw components.

On Cray computers, recommend 1.e-5.

SUBROUTINE APTSCLC

call aptsclc (scale, au, av, bu, bv, pu, pv, np, tol, nerr)

Version: aptsolo Updated 1990 March 14 16:00. aptsolo Originated 1990 January 4 15:00.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibeix aptblibe aptsclolend / 1 1.

aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To linearly scale the np points or vectors p = (pu, pv) by the factor "scale", in the direction of the vector a = (au, av), with the point b = (bu, bv) invariant. All are in the uv plane. If $p=(pu,\,pv)$ are unbound vectors, invariant point "b" must be at the origin. This is the spatial part of a Lorentz transformation.

Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: scale, au, av, bu, bv, pu, pv, np, tol.

Output: pu, pv, nerr.

aptvubc (source in aptslibe, binary in aptblibe). Calls:

Glossary:

nerr

au, av Input The u and v components of the uv plane vector defining

the direction of linear scaling.

The u, v coordinates of the uv plane invariant point. bu, bv Input

> Indicates an input error, if not 0. Output. 1 if np is not positive.

2 if the magnitude of vector "a" is too small, relative to tol.

Size of arrays pu, pv. np : Input

pu, pv In/Out The u and v coordinates of a point, or components

of a vector in the uv plane. Size np.

Numerical tolerance limit. Used to test and adjust tol Input

unit vector, matrix element, and point

components.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTSCLL

call aptsoll (scale, ax, ay, az, bx, by, bz, px, py, pz, np, tol, refm, nerr)

Version: aptscll Updated 1990 March 14 16:00. aptscll Originated 1989 November 2 14:10,

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read ,245100;aptslibe / 1 1 Source: lib aptalibelx aptblibe aptaclilend / 1 1. aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the matrix operator refm for linear scaling with the factor scale, in the direction of the vector a = (ax, ay, az), with the point b = (bx, by, bz) invariant, and to do the scaling on the np points or vectors p = (px, py, pz). np may be 0. If p = (px, py, pz) are unbound vectors, make sure invariant point "b" is at the origin. This is the spatial part of a Lorentz transformation, Any components of refm within tol of -1.0, 0.0, or 1.0, will be truncated to those values,

flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

Input: scale, ax, ay, az, bx, by, bz, px, py, pz, np, tol.

Output: px, py, p:, refm, nerr.

Calls: aptvunb, aptmopv (sources in aptslibe, binarius in aptblibe).

Glossarva

ax, ay, az Input The x, y, z components of vector "a" in the direction of linear scaling.

The x, y, z coordinates of invariant point "b". bx, by, bz Input

Indicates an input error, if not 0. nerr Out put 1 if the magnitude of vector "a" is too small, relative to tol.

Number of points or vectors "p". May be 0. nn Input

The x, y, z coordinates or components of point or vector "p", before and after scaling. Size np. px,py,pz In/Out

reim Out put Linear scaling operator (a unitary 3 x 3 matrix). Must be sized refm(3.3).

Linear scaling factor. A negative value is equivalent to a positive linear scaling, followed by a reflection in the plane with the normal vector "a". scale Indut

Numerical tolerance limit. Used to test and adjust tol Input unit vector, matrix element, and point components. On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTSCLU

call aptsclu (scale, bx, by, bz, px, py, pz, np, tol, refm, nerr)

Version: aptsclu Updated 1990 March 13 16:00. aptsclu Originated 1990 March 13 16:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibeix aptblibe aptsclutend / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the matrix operator refm for uniform scaling by the factor "scale", with the point b = (bx, by, bz) invariant, and to do the scaling on the np points or vectors p = (px, py, pz). The array size np may be 0. If "p" are unbound vectors, invariant point "b" must be at the origin. Flag nerr indicates any input error.

Input: scale, bx, by, bz, px, py, pz, nr, tol.

Output: px, py, pz, refm, nerr.

Calls: aptvunb, aptmopv (sources in aptslibe, binaries in aptblibe).

Glossary:

bx, by, bz Input The x, y, z coordinates of invariant point "b".

nerr > Output Indicates an input error, if not 0. 1 if scale = 0.0.

np Input Number of points or vectors "p". May be 0.

px,py,pz-In/Out The x, y, z coordinates or components of point or vector "p", before and after scaling. Size np.

refm - Output Linear scaling operator (a unitary 3 x 3 matrix). Must be sized refm(3,3).

scale Input Scale factor for uniform scaling. A negative value is equivalent to a positive scaling, followed by an inversion. A value of 0.0 is treated as an error.

tol Input Numerical tolerance limit. Used to test and adjust unit vector, matrix element, and point components.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTSLID

```
call aptslid (xa, pa, xb, pb, np, xran, nerr)
                                   1990 February 7 14100.
Version: aptalid Updated
            aptalld Originated 1990 February 2 14:10.
Authori
           Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
Sourcet
            xport read .245100;aptslibe / 1 1
            lib aptslibelx aptblibe aptslidlend / 1 1.
            aptalibe is a LIB library of FORTRAN source files.
            aptblibe is a BUIID library of Cray-compiled binaries.
Purpose: To find np values of x, by sampling from a linear distribution
            function having probability pa at xa, and probability pb at xb.
            Flag nerr indicates any input error.
           If both pa and pb are non-negative, the expected value of x is <x> = fa * xa + fb * xb, where fa = (2.0 * pa + pb) / (3.0 * (pa + pb)) and fb = (pa + 2.0 * pb) / (3.0 * (pa + pb)).
            If pa is negative, and pb is positive, then nerr = 3,
           no values of x will be sampled between xa and xa' = (xa * pb - xb * pa) / (pb - pa), and <x> = fa' * xa + fb' * xb, where fa' = pb / (3.0 * (pb - pa)) and fb' = (2.0 * pb - 3.0 * pa) / (3.0 * (pb - pa)).
           If pa is positive, and pb is negative, then nerr = 3, no values of x will be sampled between xb and
           xb' = (xb * pa - xa * pb) / (pa - pb), and
<x> = fa' * xa + fb' * xb,
where fa' = (2.0 * pa - 3.0 * pb) / (3.0 * (pa - pb))
and fb' = pa / (3.0 * (pa - pb)).
            If both pa and pb are non-positive, then nerr = 2, and
            no values of x will be sampled.
History: 1990 February 5 13:20. Modified to eliminate sampling from
            any range of x with negative probability.
Input:
            xa, pa, xb, pb, np,
Output:
            xran, nerr.
Glossary:
nerr
            Output
                      Indicates an input error, if not 0.
                         1 if np is not positive.
                         2 if both pa and pb are non-positive.
                           No x values are sampled.
                         3 if either pa or pb is negative, and the other is
                           positive. Values of x are sampled only from the
                           positive part of the probability distribution.
            Input
                       Size of array xran.
            Input
                       Relative probabilities of random variables xa and xb,
pa, pb
                         respectively. Probability p(x) is linear in x.
                         The values of pa and pb need not be normalized.
                         If neither pa nor pb is positive (nerr = 2), no
                         values of x will be sampled. If either pa or pb is
                         negative, and the other is positive, (nerr = 3),
                         x values will only be sampled from the positive
                         part of the probability distribution.
                         To find pa and pb, when <x> is given:
                           xma = (2.0 * xa + xb) / 3.0,
                            xmb = (xa + 2.0 * xb) / 3.0.
                         For <x> between Xa and Xma, pb is negative, and:
                           pb = -((xma - (x>) / ((x> - xa)) * pa.
                         For <x> between kma and xmb:
                            (<x> - xma) * pa = (xmb - <x>) * pb.
                         For <x> between xmb and xb, pa is negative, and:
                           pa = -((\langle x \rangle - xmb) / (xb - \langle x \rangle)) \cdot pb.
xa, xb
            Input
                       Values of random variable x with relative probilities
                         pa and pb, respectively.
xran
            Out put
                       Randomly sampled value of x in range from xa to xb.
                         Size np.
```

SUBROUTINE APTSLIV

```
call aptsliv (xa, pa, xb, pb, np, xran, nerr)
                                      1990 February 7 14:00.
  Version: aptsliv Updated
              aptsliv Originated 1990 February 6 11:40.
              Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
  Author:
              xport read .245100:aptslibe / 1 1
  Source:
              lib aptslibe!x aptblibe aptsliv!end / 1 1.
              aptslibe is a LIB library of FORTRAN source files.
              aptblibe is a BUILD library of Cray-compiled binaries.
              To find np values of x, by sampling from np linear probability
  Purpose:
              distribution functions having probabilities pa at xa, and
              probabilities pb at xb.
              Flag nerr indicates any input error.
               If both pa and pb are non-negative, the expected value of x is
               \langle x \rangle = fa * xa + fb * xb,
              where fa = (2.0 * pa + pb) / (3.0 * (pa + pb))
and fb = (pa + 2.0 * pb) / (3.0 * (pa + pb)).
               If pa is negative, and pb is positive, then
               no values of x will be sampled between xa and
              xa' = (xa * pb - xb * pa) / (pb - pa), and <x> = fa' * xa + fb' * xb,
              where fa' = pb / (3.0 * (pb - pa))
and fb' = (2.0 * pb - 3.0 * pa) / (3.0 * (pb - pa)).
               If pa is positive, and pb is negative, then
               no values of x will be sampled between xb and
              xb' = (xb * pa - xa * pb) / (pa - pb), and
<x> = fa' * xa + fb' * xb,
where fa' = (2.0 * pa - 3.0 * pb) / (3.0 * (pa - pb))
and fb' = pa / (3.0 * (pa - pb)).
               If both pa and pb are non-positive, then the returned value
              will be -1.e99.
   Input:
               xa, pa, xb, pb, np.
  Output:
              xran, nerr.
   Glossary:
               Output
                          Indicates an input error, if not 0.
   nerr
                            1 if np is not positive.
                          Size of arrays xa, pa, xb, pb, xran.
   np
               Input
   pa, pb
               Input
                          Relative probabilities of random variables xa and xb,
                            respectively. Probability p(x) is linear in x.
                            The values of pa and pb need not be normalized.
                            A value of \boldsymbol{x} will be sampled only from the positive
                             range of each probability distribution function.
                            If neither pa nor pb is positive, the value of
                            xran will be -1.e99. Size np.
                            To find pa and pb, when <x> is given:

xma = (2.0 * xa + xb) / 3.0,

xmb = (xa + 2.0 * xb) / 3.0.
                            For \langle x \rangle between xa and xma, pb is negative, and:
pb = -(\langle xma - \langle x \rangle) / (\langle x \rangle - xa)) * pa.
                             For <x> between xma and xmb:
                               (<x> - xma) * pa = (xmb - <x>) * pb.
                            For <x> between xmb and xb, pa is negative, and:
pa = -(<x> - xmb) / (xb - <x>)) * pb.
                          Values of random variable \boldsymbol{x} with relative probilities
   xa, xb
               Input
                             pa and pb, respectivley. Size np.
                          Randomly sampled value of x in range from xa to xb.
   xran
               Output
                            Value returned is -1.e99 if neither pa nor pb
```

is positive. Size np.

SUBROUTINE APTSPSP

call aptspsp (ra, ax, ay, az, rb, bx, by, bz, np, tol, rc, cx, cy, cz, abx, aby, abz, nerr)

Version: aptspsp Updated 1990 March 20 14:00. aptspsp Originated 1990 March 20 14:00.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

Source:

xport read .245100;aptslibe / 1 1
lib aptslibe!x aptblibe aptspsp!end / 1 1.
aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np sets of input data, the radius rc and center c = (cx, cy, cz) of the circle of intersection of the sphere of radius ra at point a = (ax, ay, az) and the sphere of radius rb at point b = (bx, by, bz), if an intersection occurs. Vector ab = (abx, aby, abz) is normal to the plane of the

circle. Flag nerr indicates any input error.

Input: ra, ax, ay, az, rb, bx, by, bz, np, tol.

Output: rc, cx, cy, cz, abx, aby, abz, nerr.

Calls: aptvdis, aptvadd, aptvuna (sources in aptslibe,

binaries in aptblibe).

Glossarv:

The x, y, z components of the unit vector "ab", normal abx,y,z Output to any plane containing any circle of intersection of the two spheres. In the direction from point "a" to point "b". Zero if points "a" and "b" coincide,

within the limit of precision tol.

ax, ay, az Input The x, y, z coordinates of point "a" at the center of the sphere with radius ra. Size np.

bx, by, bz Input The x, y, z coordinates of point "b" at the center of the sphere with radius rb. Size np.

cx, cy, cz Output The x, y, z coordinates of point "c" at the center of the circle with radius rc, at the intersection of the two spheres, if an intersection occurs.

nerr Output Indicates an input error, if not 0. 1 if np is not positive.

Size of arrays. np Input

ra Input The radius of the sphere centered at point "a". Size np. Absolute value will be used.

The radius of the sphere centered at point "b". rb Input. Size np. Absolute value will be used.

The radius of the circle centered at point "c", at the Output rc intersection of the two spheres, if an intersection occurs. Size np. Positive if the spheres intersect. Zero if the spheres are tangent. Negative if the spheres do not intersect.

tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

pu, pv

tol

Input

Input

Size np.

Numerical tolerance limit.

SUBROUTINE APTTING call apttinc (au, av, bu, bv, cu, cv, pu, pv, np, tol, pab, pbc, pca, dpmin, nloc, nerr) 1990 February 21 15:20. Version: apttinc Updated apttinc Originated 1990 February 21 15:20. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibe!x aptblibe apttinc!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. To find, for each of the np sets of input data, the distances pab, pbc and pca from the point p = (pu, pv) to the sides of the triangle with vertices a = (au, av), b = (bu, bv) and c = (cu, cv), in counterclockwise order in the uv plane, the minimum dpmin of the distances pab, pbc and pca, and whether point "p" is inside the triangle or not (flag nloc). The values of pab, pbc and pca will be truncated to zero, if less than the estimated error in their calculation, based on tol. Flag nerr indicates any input error. Input: au, av, bu, bv, cu, cv, pu, pv, np, tol. Out put: pab, pbc, pca, dpmin, nloc, nerr, Calls: aptptlc (source in aptslibe, binary in aptblibe). Glossary: au, av Input The u, v coordinates of vertex "a" of the triangle. Size np. The u, v coordinates of vertex "b" of the triangle. by, by Input Size np. The u, v coordinates of vertex "c" of the triangle. cu, cv Input Size np. The minimum of the distances pab, pbc and pca. dpmin out put Size np. Indicates the location of point "p" relative to the nloc Output triangle "abc": -1 if all triangle vertices coincide.

O if point "p" is outside the triangle "abc" (one or two of pab, pbc, pca are negative), or is inside, but the triangle vertices were specified in clockwise order (pab, pbc and pca are all non-positive). 1 if point "p" is inside triangle "abc" (pab, pbc and pbc are all non-negative). Indicates an input error, if not 0. nerr Output 1 if np is not positive. Size of arrays pu, pv, au, av, bu, bv, cu, cv, Input np pab, pbc, pca. Distance from point "p" to triangle side "ab".
Truncated to zero, if less than the estimated error pab Output in its calculation, based on tol. Distance from point "p" to triangle side "bc".
Truncated to zero, if less than the estimated error Output pbc in its calculation, based on tol. Distance from point "p" to triangle side "ca".
Truncated to zero, if less than the estimated error Output pca in its calculation, based on tol.

The u and v coordinates of point "p" in the uv plane.

On Cray computers, recommend 1.e-5 to 1.e-11.

pu, pv

tol

Output

Input

```
SUBROUTINE APTTLOC
     call apttloc (au, av, bu, bv, cu, cv, np, tol,
                    fdk, fdl, pu, pv, nerr)
      Version: apttloc Updated 1990 February 8 14:30.
                apttloc Originated 1990 February 8 14:30.
      Author:
                Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
      Source:
                xport read .245100:aptslibe / 1 1
                lib aptslibe!x aptblibe apttloc!end / 1 1.
                aptslibe is a LIB library of FORTRAN source files.
                aptblibe is a BUILD library of Cray-compiled binaries.
      Purpose: To find np points p = (pu, pv), by sampling from a
                uniform distribution over the triangle in the uv plane with
                vertices a = (au, av), b = (bu, bv), c = (cu, cv), in any order around the triangle.
                Variables fdk and fdl are the local coordinates in the
                triangle. For any point p = (pu, pv) in the triangle:
                  pu = au + fdk * (bu - au) + fdk * fdl * (cu - bu)

pv = av + fdk * (bv - av) + fdk * fdl * (cv - bv)
                   fdk = ((p-a) \times (c-b)) / ((b-a) \times (c-b))
                  fdl = -((p - a) \times (b - a)) / ((p - a) \times (c - b)),
                where a, b, c and p are the position vectors, x indicates
                the vector product, and the scalar w components are used.
                The unnormalized probability distribution for fdk and fdl is:
                  prob(fdk,fdl) = fdk
                which is linear for fdk, uniform for fdl.
                Flag nerr indicates any input error.
      Input:
                au, av, bu, bv, cu, cv, np, tol.
      Output:
                fdk, fdl, pu, pv, nerr.
      Calls:
                aptslid (source in aptslibe, binary in aptblibe).
      Glossary:
      au, av
                Input
                          The u and v coordinates of vertex "a" of triangle.
                 Input
                          The u and v coordinates of vertex "b" of triangle.
      bu, by
                          The u and v coordinates of vertex "c" of triangle.
      cu, cv
                Input
                Output
                          Indicates an input error, if not 0.
      nerr
                            1 if np is not positive.
                Input
                          Size of arrays fdk, fdl, pu, pv.
                            Number of points "p" to sample.
      fdk
                Output
                          Fractional distance of p int "p" between vertex "a"
                            and side "bc", Range U.O to 1.0. Size np.
      fdl
                Output
                          Fractional distance of point "p" between the triangle
```

sides "ab" and "ca". Range 0.0 to 1.0. Size np.

On Cray computers, recommend 1.e-5 to 1.e-11.

Sampled point p. Size np.

Numerical tolerance limit.

SUBROUTINE APTTRAC

call apttrac (au, av, pu, pv, np, tol, nerr)

1990 March 13 11:30. Version: apttrac Updated apttrac Originated 1990 January 4 12:00.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe's aptblibe apttrac!end / 1 l. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To translate the origin to the 2-D point a = (au, av),

by subtracting the vector "a" from the np 2-D points

p = (pu, pv). New coordinates less than the estimated error in their calculation, based on tol, will be truncated to zero.

Flag nerr indicates any input error.

Input: au, av, pu, pv, np, tol.

Output: pu, pv, nerr.

Glossary:

nerr

Output Indicates an input error, if not 0.

1 if np is not positive.

2 if the magnitude of (au, av) is no greater than

tol.

np Input Number of 2-D points (pu, pv).

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

In/Out The u and v coordinates of 2-D point "p". pu, pv

Size np.

Truncated to zero if smaller than the estimated

error in their calculation, based on tol.

SUBROUTINE APTTRAN

call apttran (ax, ay, az, px, py, pz, np, tol, nerr)

1990 March 13 11:30. Version: apttran Updated apttran Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe!x aptblibe apttranlend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To translate the origin to the point a = (ax, ay, az),

by subtracting the vector "a" from the np points

p = (px, py, pz). New coordinates less than the estimated error in their calculation, based on tol, will be truncated to zero.

Flag nerr indicates any input error.

Input: ax, ay, az, px, py, pz, np, tol.

Output: px, py, pz, nerr.

Glossary:

nerr Output Indicates an input error, if not 0.

1 if np is not positive.
2 if the magnitude of (ax, ay, az) is no greater than

tol.

Number of points (px, py, pz). np Input

Numerical tolerance limit. tol Input

On Cray computers, recommend 1.e-5 to 1.e-11.

px,py,pz In/Out The x, y, z coordinates of point "p". Size np. Truncated to zero if smaller than the estimated

error in their calculation, based on tol.

SUBROUTINE APTTRIP

call apttrip (px, py, pz, ax, ay, az, bx, by, bz, cx, cy, cz, noptfd, tol, dpmin, fda, fdb, fdc, xmin, ymin, zmin, nlima, nlimb, nlimo, itrun, nside, nerr) Version: apttrip Updated 1990 January 18 14:20. apttrip Originated 1989 November 2 14:10. Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Source: xport read .245100:aptslibe / 1 1 lib aptslibe(x aptblibe apttrip(end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To find the distance dpmin from a point p = (px, py, pz)to a plane defined by the three points a = (ax, ay, az), b = (bx, by, bz), and c = (cx, cy, cz), and the point rmin = (xmin, ymin, zmin) nearest to point p, and in the plane, subject to constraints that may be imposed by option noptfd and the value of tol. Optionally, to find the fractional distances (fda, fdb, fdc) of point rmin along the triangle's altitudes. Flags niima, nlimb, nlimc indicate when fda, fdb, fdc have been restrained. Flag itrun indicates when dpmin has been truncated to zero. Flag nside indicates when the minimum point is inside the triangle. Flag nerr indicates any input error. ax, ay, az, bx, by, bz, cx, cy, cz, px, py, pz, tol. Input: Output: dpmin, fda, fdb, fdc, xmin, ymin, zmin, nlima, nlimb, nlimc, itrun, nside, nerr. Calls: aptfdad, aptptln, aptvdis, aptvpln (sources in aptslibe, binaries in aptblibe). Glossary: ax, ay, az Input The x, y, z coordinates of point "a". bx, by, bz Input The x, y, z coordinates of point "b". cx, cy, cz Input The x, y, z coordinates of point "c". dpmin Output Distance from point "p" to the nearest (constrained) point in the plane defined by points "a", "b", "c". a value less than the estimated error in its calculation is truncated to zero (itrun = 1). dpmin is positive when the external point is on the side of the plane for which the three points are in counterclockwise order. See noptfd. fda Output Fractional distance of point (xmin, ymin, zmin) from side "bc" to vertex "a". fdb Output Fractional distance of point (xmin, ymin, zmin) from side "ca" to vertex "b". fdc Output Fractional distance of point (xmin, ymin, zmin) from side "ab" to vertex "c". itrun Out put O if no change is made in the calculated value of dpmin, 1 if dpmin is changed to zero, when less than the estimated error in its calculation. nerr Output Indicates an input error, if not 0. 1 is added if noptfd is not between 0 and 2. 2 is added if 3 points representing triangle are colinear or congruent. nlima Output O if no limit imposed on fda, 1 if the limit of noptfd = 1 is imposed, 2 if the limit of noptfd = 2 is imposed. nlimb,c Output Like nlima, but for fdb, fdc, respectively.

nopt fd	Input	Option to limit range of fda, fdb, fdc: -1 for no limit, no calculation of fda, fdb, fdc, 0 for no limit, 1 to increase to tol, if in the range from -tol to tol, and decrease to 1.0 - tol, if in the range from 1.0 - tol to 1.0 + tol (move a point near an edge slightly inside the triangle), and 2 to limit to the range from 0.0 to 1.0 (move a
,		point outside the triangle to an edge).
nside	Output	0 if minimum point outside the triangle, 1 if inside 0 if moved to edge, when noptfd = 2.
px, py, pz	Input	The x, y, z coordinates of point "p".
tol	Input	Numerical tolerance limit for dpmin, fda, fdb, fdc. On Cray computers, recommend 1.e-5 to 1.e-11.
xmin .	Output	The x coordinate of pt in plane nearest point "p". May be constrained by option noptfd.
ymin	Output	The y coordinate of pt in plane nearest point "p". May be constrained by option noptfd.
zmin	Output	The z coordinate of pt in plane nearest point "p". May be constrained by option noptid.

SUBROUTINE APTVADC

call aptvade (au, av, bmult, b, cu, év, np, tol,. du, dv, vlen, nerr)

Version: aptvadc Updated 1990 February 22 9:30.

aptvadc Originated 1989 November 20 13:20.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvadclend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, the 2-D vector sum d(n) = a(n) + bmult * b(n) * c(n), where d = (du, dv), a = (au, av), and c = (cu, cv), and to find vien, the magnitude of vector "d", all in the uv plane..

Any component of vector "d" less than the estimated error in its calculation, based on tol, will be truncated to zero.

Flag nerr indicates any input error.

History: 1990 February 22. Delected truncation of vector components to

zero based on vector magnitude.

Input: au, av, bmult, b, cu, cv, np, tol.

Out.put: du, dv, vlen, nerr.

Glossary:

The u and v coordinates of point "a". Size np. au, av Input

The w components are zero. The directions u, v and w

are orthogonal.

Coefficient of vector "c", when multiplied by bmult.

bmult Multiplier of term b(n) * c(n). Not an array.

The u and v coordinates of point "c". Size np. cu, cv Input

The w components are zero.

du, dv Output The u and v components of vector "d". Size np.

The w components are zero.

Will be truncated to zero if less than the estimated

numerical error in their calculation based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

пp Input Size of arrays au, av, b, cu, cv, vlen, du, dv.

Numerical tolerance limit. Used to truncate tol Input

the components of 2-D vector d = (du, dv). On Cray computers, recommend 1.e-5 to 1.e-11.

Magnitude of vector "d". May be truncated to zero, vlen Output if less than the estimated error in its calculation.

See tol. Size np.

SUBROUTINE APTVADD

call aptvadd (ax, ay, az, bmult, b, cx, cy, cz, np, tol, dx, dy, dz, vlen, nerr)

Version: aptvadd Updated 1990 February 22 9:30. aptvadd Originated 1989 November 20 13:20.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe(x aptblibe aptvadd(end / 1 1.

aptslibe is a LIB library of FORTRAN source files, aptblibe in a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, the vector sum d(n) = a(n) + bmult * b(n) * c(n), where d = (dx, dy, dz),

a = (ax, ay, az), and c = (cx, cy, cz), and to find vien, the

magnitude of vector "d".

Any component of vector "d" less than the estimated error in

its calculation, based on tol, will be truncated to zero.

Flag nerr indicates any input error.

History: 1990 February 22. Deleted truncation of vector components to

zero based on vector magnitude.

Input: ax, ay, az, bmult, b, cx, cy, cz, np, tol.

Output: dx, dy, dz, vlen, nerr.

Glossary:

ax, ay, az Input The x, y, z components of vector "a". Size np.

b Input Coefficient of vector "c", when multiplied by bmult.

bmult Input Multiplier of term b(n) * c(n). Not an array.

cx, cy, cz Input The x, y, z components of vector "c". Size np.

numerical error in their calculation based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input Size of arrays.

tol Input Numerical tolerance limit. Used to truncate the components of vector d = (dx, dy, dz).

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen Output Magnitude of vector "d". May be truncated to zero, if less than the estimated error in its calculation.

See tol. Size np.

SUBROUTINE APTVANC

call aptvanc (au, av, bu, bv, np, tol, costh, sinth, nerr)

Version: aptvanc Updated 1990 March 14 16:00. aptvanc Originated 1990 January 8 16:40.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvanclend / 1 1.

aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries,

Purpose: To find the cosine costh and sine sinth of the angle between the pair of 2-D vectors a = (au, av) and b = (bu, bv), measured counterclockwise in the uv plane, from vector "a" to vector "b", for each of np sets of input data. The values of costh and sinth will be truncated to zero, if less than the estimated error in their calculation, based on tol. Flag nerr indicates

any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: au, av, bu, bv, np, tol.

Output: costh, sinth, nerr.

Calls: aptvaxc, aptvdoc, aptvubc

(sources in aptslibe, binaries in aptblibe).

Glossary:

au, av Input The u and v components of a 2-D vector. Size np.

bu, by Input The u and v components of a 2-D vector. Size np.

costh Output Cosine of the angle between the 2-D vectors "a" and "b". Will be truncated to zero, 1: less than the

estimated error in its calculation, based on tol.
Meaningless if the magnitude of "a" or "b" is zero.
The angle is measured counterclockwise in the uv

plane, from vector "a" to vector "b".

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input' Size of arrays au, av, bu, bv, costh, sinth.

sinth Output Sine of the angle between the 2-D vectors "a" and

"b". Will be truncated to zero, if less than the estimated error in its calculation, based on tol.

Meaningless if the magnitude of "a" or "b" is zero.

The angle is measured counterclockwise in the uv

plane, from vector "a" to vector "b".

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTVANG

call aptvang (ax, ay, az, bx, by, bz, np, tol, costh, nerr)

1990 March 14 16:00. Version: aptvang Updated aptvang Originated 1990 January 5 12:10.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvanglend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the cosine costh of the angle between the pair of vectors a = (ax, ay, az) and b = (bx, by, bz), for each of np sets of input data. The value of costh will be truncated to zero, if less than the estimated error in its calculation,

based on tol. Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector

subroutine. Allows small magnitudes.

Input: . ax, ay, az, bx, by, bz, np, tol.

costh, nerr. Out put :

Calls: aptvdoc, aptvunb (sources in aptslibe, binaries in aptblibe).

Glossary:

ax, ay, az Input The x, y, z components of a vector. Size np.

The x, y, z components of a vector. Size np. bx, by, bz Input

Cosine of the angle between the vectors "a" and "L". Will be truncated to zero, if less than the estimated costh Out put

error in its calculation, based on tol.

nerr Output. Indicates an input error, if not 0.

1 if np is not positive.

Input Size of arrays ax, ay, az, bx, by, bz, costh.

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

SUBROUTINE APTVAXB

call aptvaxb (ax, ay, az, bx, by, bz, np, tol, cx, cy, cz, vlen, nerr)

Version: aptvaxb Updated 1990 March 13 11:30.

aptvaxb Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptsilbe!x aptblibe aptvaxb!end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the vector products $c = \{cx, cy, cz\}$ of the np vector pairs $a = \{ax, ay, az\}$ and $b = \{bx, by, bz\}$, and the magnitudes vien of the vectors "c". Any components of vector "c" less than the estimated error in their calculation, based on tol, will be

truncated to zero.

Flag nerr indicates any input error.

With no truncation,

cx = ay * bz - az * by cy = az * bx - ax * bz

cz = ax * by - ay * bx.

Input: ax, ay, az, bx, by, bz, np, tol.

Output: cx, cy, cz, vlen, nerr.

Glossary:

ax, ay, az Input The x, y, z components of input vector "a". Size np.

The x, y, z components of input vector "b". Size np. bx, by, bz Input

cx, cy, cz Output

The x, y, z components of output vector "c". Size np. Vector (cross) product of vectors "a" and "b". Truncated to zero if less than the estimated error in

their calculation. See tol.

Indicates an input error, if not 0.
 1 if np is not positive. nerr Output

Size of arrays ax, ay, az, bx, by, bz, cx, cy, cz. Input np

Numerical tolerance limit. tol Input

On Cray computers, recommend 1.e-5 to 1.e-11.

Magnitude of the vector product "c". vlen(n) Output

SUBROUTINE APTVAXC

call aptvaxc (au, av, bu, bv, np, tol, cw, nerr)

Version: aptvaxc Updated 1990 January 18 16:40. aptvaxc Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe(x aptblibe aptvaxclend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the vector products cw of the np 2-D vector pairs a = (au, av) and b = (bu, bv). Vectors a and b are in the uv plane. The directions u, v, and w are orthogonal. Any values of cw less than the estimated error in their calculation, based on tol, will be truncated to zero. Flag nerr indicates any

input error.

With no truncation, cw = au * bv - av * bu.

Input: au, av, bu, bv, np, tol.

Output: cw, nerr.

Glossary:

au, av Input The u and v components of input vector "a". Size np.
The w components are zero. Directions u, v and w

are orthogonal.

The w components are zero.

Output The w component of output vector "c". Size np.

Vector (cross) product of vectors "a" and "b".

The u and v components are zero.

Equal to the area of the parallelogram with sides

"a" and "b".

Positive if the angle from "a" to "b", in the uv plane, is in the range from zero to 180 degrees.

Truncated to zero if less than the estimated error in

their calculation. See tol.

nerr itput Indicates an input error, if not 0.

1 if np is not positive.

np Input Size of arrays au, av, bu, bv, cw.

tol Input Numerical tolerance limit.

SUBROUTINE APTVDIC

call aptvdic (au, av, bu, bv, np, tol, du, dv, dab, nerr)

Version: aptvdic Updated 1990 March 7 17:00. aptvdic Originated 1989 December 29 15:50.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

Source: xport read .245100:aptslibe / 1 1

lib aptslibe:x aptblibe aptvdic!end / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, the 2-D vector

d = (du, dv) from point a = (au, av) to point b = (bu, bv),
and its magnitude dab, the distance from "a" to "b", all in the

uv plane. Directions u, v and w are orthogonal.
Any component of vector "d" less than the estimated error in

its calculation, based on tol, will be truncated to zero. Flag nerr indicates any input error.

With no truncation, (du, dv) = (bu, bv) - (au, av), and distance dab = sqrt (du**2 + dv**2).

Input: au, av, bu, bv, np, tol.

Output: du, dv, dab, nerr.

Glossary:

The u and v coordinates of point "a". Size np. au, av Input The w coordinates are zero. Directions u, v and w

are orthogonal.

The u and v coordinates of point "b". Size np. bu, bv Input

The w coordinates are zero.

Distance between points "a" and "b", equal to dab Output the length of 2-D vector d = (du, dv). May be

truncated to zero, if less than the estimated error

in its calculation. See tol. Size np.

du, dv Output The u and v components of 2-D vector "d". Size np.

The w coordinates are zero.

May be truncated to zero, if less than the estimated numerical error in their calculation based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Input The size of arrays au, av, bu, bv, dab, du, dv. пp

tol Input Numerical tolerance limit. Used to truncate the components of 2-D vector d = (du, dv).

SUBROUTINE APTVD1L

call artvdil (au, bu, np, tol, du, nerr)

1990 January 18 14:20. Version: aptvdis Updated aptvdis Originated 1990 January 17 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe!x aptblibe aptvdillend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of the np sets of input data, the distance

d = (du) from point a = (au) to point b = (bu), in the u

direction. Directions u, v and w are orthogonal.

If the magnitude of du is less than its estimated error, based

on tol, it will be truncated to zero. Flag nerr indicates any input error.

With no truncation, du = bu - au.

Input: au, bu, np, tol:

Output: du, nerr.

Glossary:

du

au Input The u coordinate of point "a". Size np. The v and w coordinates are zero. Directions u, v and w are orthogonal.

The u coordinate of point "b". Size np.

bu Input The v and w coordinates are zero.

Distance between points "a" and "b", in the u Output direction. May be truncated to zero, if less than the estimated error in its calculation. See tol.

Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

пp Input The size of arrays au, bu, du.

tol Input Numerical tolerance limit.

SUBROUTINE APTVDIS

call aptvdis (ax, ay, az, bx, hy, bz, np, tol, dx, dy, dz, dab, nerr)

Version: aptvdis Updated 1990 February 22 9:30.

aptvdis Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

Source: xport read .245100:aptslibe / .1 1

lib aptslibe(x aptblibe aptvdislend / 1 1, aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the np distance vectors d = (dx, dy, dz) from the

points a = (ax, ay, az) to the points b = (bx, by, bz), and their magnitudes, dab, the distances from "a" to "b".

Any component of vector "d" less than the estimated error in its carculation, based on tol, will be truncated to zero.

Flag nerr indicates any input error.

With no truncation, (dx, dy, dz) = (bx, by, bz) - (ax, ay, az), and distance dab = sqrt (dx**2 + dy**2 + dz**2).

1990 February 22. Deleted truncation of vector components to History: zero based on vector magnitude.

Input: ax, ay, az, bx, by, bz, np, tol.

dx, dy, dz, dab, nerr.

Output: Glossary:

ax, ay, az Input The x, y, z coordinates of point "a". Size np.

The x, y, z coordinates of point "b". Size np. bx, by, bz Input

Distance between points (ax, ay, az) and (bx, by, bz), the length of vector d = (dx, dy, dz). May be Output

truncated to zero, if less than the estimated error

in its calculation. See tol. Size np.

The x, y, z components of vector "d". Size np. dx, dy, dz Out put

May be truncated to zero, if less than the estimated numerical error in their calculation based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Input. The size of arrays ax, ay, az, bx, by, bz,

dab, dx, dy, dz.

tol Input Numerical tolerance limit. Used to truncate

the components of vector d = (dx, dy, dz).

SUBROUTINE APTVDOC

call aptvdoc (au, av, bu, bv, np, tol, spab, nerr)

Version: aptwdoc Updated 1990 January 18 14:20. aptvdoc Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvdoctend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUIID library of Cray-compiled binaries.

Purpose: To find the scalar (dot) product spab of the np 2-b vectors a = (au, av) and b = (bu, bv). The value of spab will be truncated to zero, if less than the estimated error in its

calculation, based on tol. Flag nerr indicates any input error.

With no truncation, spab = au * bu + av * bv.

Input: au, av, bu, bv, np, tol.

Output: spab, nerr.

Glossary:

au, av Input The u and v components of a 2-D vector. Size np.

bu, by Input The u and v components of a 2-D vector. Size np.

Indicates an input error, if not 0. nerr . Output

1 if np is not positive.

Input Size of arrays au, av, bu, bv, spab. пp

spab (n) Out put Scalar product of vectors "a" and "b". Will be

truncated to zero, if less than the estimated error

in its calculation, based on tol.

tol Input Numerical tolerance limit.

SUBROUTINE APTYDOT

call aptvdot (ax, ay, az, bx, by, bz, np, tol, spab, nerr)

1990 Uanuary 18 14:20. Version: aptvdot Updated aptvdot Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibels aptblibe aptvdotlend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the scalar (dot) product spab of the np vectors a = (ax, ay, az) and b = (bx, by, bz). The value of spab will be truncated to zero, if less than the estimated

erroi in its calculation, based on tol. Flag nerr indicates any input error.

With no truncation, spab = ax * bx + ay * by + az * bz.

ax, ay, az, bx, by, bz, np, tol. Input:

Output: spab, nerr.

Glossary:

ax, ay, az Input The x, y, z components of a vector. Size np.

bx, by, bz Input The x, y, z components of a vector. Size np.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Size of arrays ax, ay, az, bx, by, bz, spab. np Input

Scalar product of vectors "a" and "b". Will be spab (n) Out put

truncated to zero, if less than the estimated error in its calculation, based on tol.

tol Input Numerical tolerance limit.

SUBROUTINE APTVLIC

call aptivic (au, av, np, tolu, tolv, vien, nerr)

Version: aptvlic Updated 1990 January 18 14:20. aptvlic Originated 1990 January 3 13:40.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvliciend / 1 1.

aptalibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To adjust the np 2-D vectors a = (au, av), by imposing the lower

limits tolu and tolv on the magnitudes of the components au and av, respectively, while retaining the initial magnitude of the vector "a". If all are initially zero, the output vector "a" will be zero, and vien will be zero.

Flag nerr indicates any input error.

Input: au, av, np, tolu, tolv.

Output: au, av, vlen, nerr.

Glossary:

The u and v components of input vector "a". Size np. au, av Input Directions u, v and w are orthogonal.

The u and v components of output vector "a". Size np. au, av Output

Magnitudes will be at least tolu, tolv, respectively, subject to the requirement that the final magnitude of vector "a" be the same as the

initial magnitude.

Indicates an input error, it not 0. nerr Output 1 if np is not positive.

пp Input Size of arrays au, av, vien.

tolu Input Numerical tolerance limit for component au. On Cray computers, recommend 1.e-5 to 1.e-11.

tolv Input Numerical tolerance limit for component av. On Cray computers, recommend 1.e-5 to 1.e-11.

Magnitude of vector "a". vien(n) Output

SUBROUTINE APTVLIM

call aptvlim (au, av, aw, np, tolu, tolv, tolw, vien, nerr)

Version: aptvlim Updated 1990 January 18 16:40. aptvlim Originated 1989 December 19 13:40.

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe(x aptblibe aptvlimend / 1 1, aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries.

To adjust the np vectors a = (au, av, aw), by imposing the lower Purpose:

limits tolu, tolv, and tolw on the magnitudes of the components au, av, and aw, respectively, while retaining the initial magnitude of the vector "a". If all are initially zero, the output vector "a" will be zero, and vien will be zero.

Flag nerr indicates any input error.

Input: au, av, aw, hp, tolu, tolv, tolw.

Out put: au, av, aw, vlen, nerr.

Glossary:

tolv

The u, v, w components of input vector "a". Size np. au, av, aw Input

au, av, aw Output The u, v, w components of output vector "a". Size np. Magnitudes will be at least tolu, tolv, tolw, respectively, subject to the requirement that the

final magnitude of vector "a" be the same as the

initial magnitude.

nerr Output Indicates an input error, it not 0.

1 if np is not positive.

Input Size of arrays au, av, aw, vien.

tolu Input Numerical tolerance limit for component au. On Cray computers, recommend 1.e-5 to 1.e-11.

> Input Numerical tolerance limit for component av.

On Cray computers, recommend 1.e-5 to 1.e-11.

tolw Input Numerical tolerance limit for component aw.

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output Magnitude of vector "a".

SUBROUTINE APTVPLC

call aptypic (au, av, bu, bv, np, tol, cu, cv, vien, nerr)

Version: aptvplc Updated 1990 March 13 11:30, aptvplc Originated 1989 December 28 13:20.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibelx aptblibe aptvplc|end / 1 1, aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the vector c = (cu, cv) normal to the line defined by the two points a = (au, av), b = (bu, bv), and in the uv plane, for each of the np sets of points "a" and "b". The directions u, v, w are orthogonal. The magnitude vien of the normal vector "c" is equal to the length of the line segment "ab". If vien is zero, the points "a" and "b" are congruent. By convention, the direction of the normal vector is from right to left, relative to the direction from "a" to "b" in the uv plane. The components of "c" will be truncated to zero, if less than

the estimated numerical error in their calculation, based on

Input: au, av, bu, bv, np, tol.

Output: cu, cv, vlen; nerr.

Glossary:

au, av Input The u and v coordinates of point "a". Size np.

bu, by Input The u and v coordinates of point "b". Size np.

cu, cv Output The u and v components of normal vector "c".

May be truncated to zero, if less than the estimated numerical error in their calculation. See tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input The number of sets of points "a" and "b" for which the

normal vector "c" is to be calculated.

Must be positive.

tol Input Numerical tolerance limit for cu, cv.

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output The magnitude of the normal vector "c". Size np.

Zero if points "a" and "b" are congruent.

SUBROUTINE APTVPLN

call aptvpln (ax, ay, az, bx, by, bz, cx, cy, cz, np, tol, dx, dy, dz, vlen, nerr)

Version: aptvpln Updated 1990 March 14 11:00. aptvpln Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100;aptslibe / 1 1

lib aptslibe(x aptblibe aptvpln(end / 1).
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the vector d = (dx, dy, dz) normal to the plane defined by the three points a = (ax, ay, az), b = (bx, by, bz, and c = (cx, cy, cz), for each of the np sets of points (a, b, c). The magnitude vien of the normal vector "d" is equal to the area of the parallelopiped for which 3 of the vertices are (a, b, c). If vien = 0, the points (a, b, c) are congruent or colinear. The components of vector "d" will be truncated to zero, it less than the estimated numerical error in their calculation, based

History: 1990 February 22. Deleted truncation of vector components to

zero based on vector magnitude.

Input: ax, ay, az, bx, by, bz, cx, cy, cz, np, tol.

Output: dx, dy, dz, vlen, nerr.

on tol.

Glossary:

ax, ay, az Input The x, y, z coordinates of point "a". Size np.

bx,by,bz Input The x, y, z coordinates of point "b". Size np.

cx,cy,cz Input The x, y, z coordinates of point "c". Size np.

dx,dy,dz Output The x, y, z components of normal vector "d".

May be truncated to zero, if less than the estimated

numerical error in their calculation. See tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input The number of sets of points (a, b, c) for which the

normal vector "d" is to be calculated.

Must be positive.

tol Input Numerical tolerance limit for dx, dy, dz.

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output The magnitude of the normal vector "d". Size np.
Zero if points (a, b, c) are congruent or collnear.

SUBROUTINE APTVSUC

```
call aptvsuc (noptf, fa, au, av, fb, bu, bv, np, tol,
                 cu, cv, clen, nerr)
            aptvsuc Updated 1990 April 3 16:00, aptvsuc Originated 1989 April 3 16:00,
Version; aptvauc Updated
            Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
Aut.hor1
            xport read .245100:aptslibe / 1 1
Sources
            11b aptalibely aptblibe aptvauciend / 1 1.
            aptslibe is a LIB library of FORTRAN source files.
            aptblibe is a BUILD library of Cray-compiled binaries.
Purpose: To find, for each of the np sets of input data, the weighted
            sum c = .(cu, cv) of the vectors a = (au, av) and b = (bu, bv):

c(n) = fa * a(n) + fb * b(n), n = 1, np (noptf = 0), or

c(n) = fa(n) * a(n) + fb(n) * b(n), n = 1, np (noptf = 1),
             and to find clen, the magnitude of vector "c".
             Any component of vector "c" less than the estimated error in
             its calculation, based on tol, will be truncated to zero.
            Flag nerr indicates any input error.
            Special cases:
               sum: c + a + b (noptf = 0, fa = 1.0, fb = 1.0).

difference: c + a - b (noptf = 0, fa = 1.0, fb = -1.0).

bisector: c + 0.5 + (a + b) (noptf = 0, fa = fb = 0.5).

interpolation: c + fa + a + (1.0 - fa) + b (noptf = 0),

c + (1.0 - fb) + a + fb + b (noptf = 0).
Input:
            noptf, fa, au, av, fb, bu, bv, np, tol,
Out put :
            cu, cv, clen, nerr.
Glossary:
                       The u and v components of vector "a". Size np.
au, av
             Input
bu, by
             Input
                       The u and v components of vector "b". Size np.
clen
             Output
                       Magnitude of vector "c". May be truncated to zero,
                          if less than the estimated error in its calculation,
                          See tol. Size np.
                       The u and v components of vector "c". Size np.
cu, cv
             Output
                          Will be truncated to zero if less than the estimated
                          numerical error in their calculation based on tol.
                        Coefficient of vector "a". Size 1 (noptf = 0) or
             Input
                          np (nopt f = 1).
fb
             Input
                        Coefficient of vector "b". Size 1 (noptf = 0) or
                          np (noptf = 1).
nerr
             Output
                        Indicates an input error, if not 0.
                          1 if np is not positive.
                          2 if noptf is not 0 or 1.
nopt f
             Input
                        Size option for fa, fb:
                          0 If fa and fb are scalars.
                          1 if fa and fb are arrays with size np.
                        Size of arrays.
np
             Input
                        Numerical tolerance limit. Used to truncate the components of vector "c".
tol
             Input
                          On Cray computers, recommend 1.e-5 to 1.e-11.
```

SUBROUTINE APTVSUM

```
call aptvsum (noptf, fa, ax, ay, az, fb, bx, by, bz, np, tol,
                 ax, cy, az, alen, nori)
                                  1990 April 3 13:20.
Version:
            aptvsum Updated
            aptvsum Originated 1989 April 3 13:20.
            Arthur L. Edwards, LLNL, 1-298, Telephone (415) 422-4123.
Authori
            xport read .245100:aptslibe / 1 1
Sourcet
            lib aptslibelx aptblibe aptvsumlend / 1 1.
            aptslibe is a LIB library of FORTRAN source files.
            aptblibe is a BUILD library of Cray-compiled binaries.
           To find, for each of the np sets of input data, the weighted sum c = (cx, cy, cz) of the vectors a = (ax, ay, az) and
Purpose:
            b = (bx, by, bz):
   c(n) = fa * a(n) + fb * b(n), n = 1, np (noptf = 0), or
   c(n) = fa(n) * a(n) + fb(n) * b(n), n = 1, np (noptf = 1),
and to find clen, the magnitude of vector "c".
Any component of vector "c" less than the estimated error in
            its calculation, based on tol, will be truncated to zero.
            Flag nerr indicates any input error.
            Special cases:
                                  c = a + b (nopt f = 0, fa = 1.0, fb = 1.0).
               sum:
               difference:
                                  c = a - b (nopt f = 0, fa = 1.0, fb = -1.0).
               blsector: c = 0.5 * (a + b) (noptf = 0, fa = fb = 0.5).

Interpolation: c = fa * a + (1.0 - fa) * b (noptf = 0),

c = (1.0 - fb) * a + fb * b (noptf = 0).
Input:
            noptf, fa, ax, ay, az, fb, bx, by, bz, np, tol.
Output:
            cx, cy, cz, clen, nerr.
Glossary:
ax, ay, az
           Input
                       The x, y, z components of vector "a". Size np.
                       The x, y, z components of vector "b". Size np.
bx, by, bz
           Input
clen
            Output
                       Magnitude of vector "c". May be truncated to zero,
                          if less than the estimated error in its calculation.
                          See tol. Size np.
cx, cy, cz Output
                       The x, y, z components of vector "c". Size np.
                          Will be truncated to zero if less than the estimated
                          numerical error in their calculation based on tol.
f a
             Input
                       Coefficient of vector "a". Size 1 (noptf = 0) or
                          np (noptf = 1).
fb
             Input
                       Coefficient of vector "b". Size 1 (noptf = 0) or
                          np (nopt f = 1).
nerr
            Output
                        Indicates an input error, if not 0.
                          1 if np is not positive.
                          2 if noptf is not ( or 1.
nopt f
             Input
                        Size option for fa, fb:
                          O if fa and fb are scalars.
                          1 if fa and fb are arrays with size np.
пp
             Input
                        Size of arrays.
                       Numerical tolerance limit. Used to truncate the components of vector "c".
tol
             Input
                          On Cray computers, recommend 1.e-5 to 1.e-11.
```

SUBROUTINE APTVTOC

call aptvtoc (au, av, np, kadj, knorm, tolu, tolv, vlen, nerr)

Version: aptytoc Updated 1990 January 18 14:20. aptivtoc Originated 1989 November 15 16:40.

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100;aptslibe / 1 1 Source:

lib aptslibe(x aptblibe aptvtoclend / 1 1.

aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To adjust the values of the components of the np 2-D vectors

a = (au, av), according to the option kadj, and the numerical tolerance limits tolu and toly, and to renormalize to a unit vector if option knorm = 1. Flag nerr indicates any input error.

Input: au, av, np, kadj, knorm, tolu, tolv.

Output: au, av, vlen, nerr.

Glossary:

au, av Input The u and v components of input vector "a". Size np. Directions u, v and w are orthogonal.

au, av Out put The u and v components of output vector "a". Size np. May be adjusted, according to the option kadj, and

the numerical tolerance limits tolu and tolv.

Indicates an input error, it not 0. nerr Output

1 if np is not positive.

2 if kadj is not from 0 to 7.

3 if knorm is not 0 or 1.

kadj Option for adjusting the components (au, av). Input

Values from 0 to 7 are allowed:

O to use a limiting value equal to the tolerance

limit times the vector magnitude.

Add 1 to use a limiting value equal to the tolerance limit.

Add 0 to use the same tolerance limit, tolu, for

au and av.

Add 2 to use tolu for au, tolv for av.

Add 0 to truncate the component to zero if less than

the limiting value.

Add 4 to increase components less than the limiting value, to the limiting value, with the same sign.

knorm Input Option for normalizing the adjusted vector "a" to a

unit vector. 0 = no, 1 = yes.

np Input Size of arrays au, av, vlen.

tolu Input Numerical tolerance limit for component au, and for au and av, for kad j = 0, 1, 4, and 5.

On Cray computers, recommend 1.e-5 to 1.e-11.

tolv Input Numerical tolerance limit for component av, for kadj = 2, 3, 6, and 7.

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output Magnitude of the input vector "a", after any

adjustment of components has been done, but before any remormalization (knorm = 1).

Will be zero if all components of "a" are zero, or

are truncated to zero.

SUBROUTINE APTVTOL

call aptvtol (ax, ay, az, np, kadj, knorm, tolx, toly, tolz, vlen, nerr) Version: aptvtol Updated 1990 January 18 16:40. aptvtol Originated 1989 November 15 16:40. 1990 January 18 16:40. Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author: xport read .245100:aptslibe / 1 1 Source: lib aptslibe(x aptblibe aptvtol)end / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries. Purpose: To adjust the values of the components of the np vectors a = (ax, ay, az), according to the option kadj, and the numerical tolerance limits tolx, toly, tolz, and to renormalize to a unit vector if option knorm # 1. Flag nerr indicates any input error. Input: ax, ay, az, np, kadj, knorm, tolx, toly, tolz. Output: ax, ay, az, vlen, nerr. Glossary: ax, ay, az Input The x, y, z components of input vector "a". Size np. ax, ay, az Output The x, y, z components of output vector "a". Size np. May be adjusted, according to the option kadj, and the numerical tolerance limits tolx, toly, tolz. nerı Output Indicates an input error, it not 0. 1 if np is not positive. 2 if kadj is not from 0 to 7. 3 if knorm is not 0 or 1. Option for adjusting the components (ax, ay, az). kad j Values from 0 to 7 are allowed: O to use a limiting value equal to the tolerance limit times the vector magnitude. Add 1 to use a limiting value equal to the tolerance limit. Add 0 to use the same tolerance limit, tolx, for ax, ay, and az. Add 2 to use tolx for ax, toly for ay, and tolz for az. Add 0 to truncate the component to zero if less than the limiting value. Add 4 to increase components less than the limiting value, to the limiting value, with the same sign. knorm Input Option for normalizing the adjusted vector "a" to a unit vector. 0 = no, 1 = yes.Input Size of arrays ax, ay, az, vlen. np tolx Input Numerical tolerance limit for component ax, and for ax, ay and az, for kadj = 0, 1, 4, and 5. On Cray computers, recommend 1.e-5 to 1.e-11. toly Input Numerical tolerance limit for component ay, for kadj = 2, 3, 6, and 7. On Cray computers, recommend 1.e-5 to 1.e-11. tolz Input Numerical tolerance limit for component az, for kadj = 2, 3, 6, and 7. On Cray computers, recommend 1.e-5 to 1.e-11. vlen(n) Output Magnitude of the input vector "a", after any adjustment of components has been done, but before any remormalization (knorm = 1). Will be zero if all components of "a" are zero, or

are truncated to zero.

SUBROUTINE APTVUAC

call aptvuac (au, av, np, tol, vlen, nerr)

Version: aptvuac Updated 1990 March 14 17:30. aptvuac Originated 1989 November 2 14:10.

Author: Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe!x aptblibe aptvuac!end / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the np unit vectors a = (au, av) parallel to the np

initial vectors a = (au, av), all in the uv plane (2-D). Any components of the initial vector "a" no greater than tol, or no greater than tol times the initial length of "a", will be truncated to zero. If all are zero, or are truncated to zero,

vien will be zero.

Flag nerr indicates any input error.

With no truncation,

(au, av) = (au, av) / sqrt (au**2 + av**2)

History: 1990 March 14. Modified to always return a unit vector.

Input: au, av, np, tol.

Output: au, av, vlen, merr.

Glossary:

au, av Input The u and v components of initial vector "a" in the

uv plane. Size np.

Will be truncated to zero if initially no greater than tol, or no greater than tol times the initial

length of "a".

au, av Output. The u and v components of unit vector "a" in the

uv plane. Size np.

nerr Output Indicates an input error, it not 0.

1 if np is not positive.

np Input Size of arrays au, av, vlen.

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

vien(n) Output Magnitude of the input vector "a", after any

truncation of components has been done, but before division by vien to form a unit vector.

SUBROUTINE APTVUBC

call aptvubc (au, av, np, tol, bu, bv, vlen, nerr)

Version: aptvubc Updated 1950 March 14 17:30. aptvubc Originated 1989 November 29 10:00.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1

lib aptslibe'x aptblibe aptvubciend / 1 1.

aptslibe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries,

Purpose: To find the np unit vectors b = (bu, bv) parallel to the np vectors a = (au, av), all in the uv plane (2-D). If any components of the initial vector "a" are no greater than tol, or no greater than tol times the initial length of "a", then the corresponding component of "b" will be truncated to zero. If all are zero, or are truncated to zero, vien will be zero.

Flag nerr indicates any input error.

With no truncation, (bu, bv) = (au, av) / sqrt (au**2 + av**2)

History: 1990 March 14. Modified to always return a unit vector.

Input: au, av, np, tol.

Output: bu, bv, vlen, nerr.

Glossary:

au, av Input The u and v components of vector "a" in the uv plane.

Size np.

bu, by Output The u and v components of vector "b" in the uv plane.

Size np.

A component will be zero if the corresponding component of vector "a" is no greater than tol, or no greater than tol times the length of "a".

nerr Output Indicates an input error, it not 0.

1 if np is not positive.

np Input Size of arrays au, av, bu, bv, vlen.

tol Input Numerical tolerance limit.

On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output Magnitude of vector "b", after any truncation of components has been done, but before division by

vien to form a unit vector.

SUBROUTINE APTVUNA

call aptvuna (ax, ay, az, np, tol, vien, nerr)

Version: aptvuna Updated 1990 March 14 17:30. aptvuna Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptvunalend / 1 1. aptslibe is a LIB library of FORTRAN source files.

aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the np unit vectors a = (ax, ay, az) parallel to the np initial vectors a = (ax, ay, az). Any components of the initial vector "a" no greater than tol, or no greater than tol times the initial length of "a", will be truncated to zero. If a.l are zero, or are truncated to zero, vlen will be zero. Flar nerr indicates any input error.

> With no truncation, (ax, ay, az) = (ax, ay, az) / sqrt (ax**2 + ay**2 + az**2).

History: 1990 March 14. Modified to always return a unit vector.

Input: ax, ay, az, np, tol.

Output: ax, ay, az, vlen, nerr.

Glossary:

The x, y, z components of input vector "a". Size np. Will be truncated to zero if initially no greater ax, ay, az Input than tol, or no greater than tol times the initial length of "a".

The x, y, z components of unit vector "a". Size np. ax, ay, az Output

nerr Output Indicates an input error, it not 0. 1 if np is not positive.

Input Size of arrays ax, ay, az, vlen.

tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

vlen(n) Output Magnitude of the input vector "a", after any truncation of components has been done, but before division by vien to form a unit vector.

SUBROUTINE APTVUNB

call aptvumb (ax, ay, az, mp, tol, ux, uy, uz, vlen, merr)

1990 March 21 15:50. Version: aptvunb Updated aptvunb Originated 1989 November 2 14:10.

Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibe(x aptblibe aptvumblend / 1 1. aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUIID library of Cray-compiled binaries.

Purpose: To find the np unit vectors u = (ux, uy, uz) parallel to the np vectors a = (ax, ay, az). If any component of vector "a" is no greater than tol, or no greater than tol times the length of "a", then the corresponding component of "u" will be truncated to zero. If all are zero, or are truncated to zero, vien will be zero. Flag nerr indicates any input error.

> With no truncation, (ux, uy, uz) = (ax, ay, az) / sqrt (ax**2 + ay**2 + az**2).

1990 March 14. Modified to always return a unit vector. 1990 March 21. Deleted change of 1990 March 14.

Input: ax, ay, az, np, tol.

Out put: ux, uy, uz, vlen, nerr.

Glossary:

ax, ay, az Input. The x, y, z components of a vector. Size np.

Output Indicates an input error, it not 0. 1 if np is not positive.

Size of arrays ax, ay, az, ux, uy, uz, vien. np Input

Output The x, y, z components of a unit vector. Size np. A component will be zero if the corresponding component of vector "a" is no greater than tol, or no greater than tol times the length of "a".

tol Input Numerical tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11.

Magnitude of vector "u", after any truncation of vlen(n) Output components has been done, but before division by vlen to form a unit vector.

SUBROUTINE APTVXUC

call aptvxuc (au, av, bu, bv, np, tol, cw, vlen, nerr)

Version: aptyxuc Updated 1990 January 18 14:20. aptvxuc Originated 1989 December 29 11:00.

Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. Author:

xport read .245100:aptslibe / 1 1 Source:

lib aptslibelx aptblibe aptvxuciend / 1 1.

aptslibe is a LIB library of FORTRAN source files. aptblibe is a BUILD library of Cray-compiled binaries.

To find, for each of the no sets of input data, the vector Purpose:

(cross) product "a" x "b" of the pair of 2-D vectors a = (au, av) and b = (bu, bv), and to divide by its magnitude vien, to produce the unit vector c = (0.0, 0.0, cw), parallel to "a" x "b". If cw is less than the estimated error in its calculation, based on tol, it will be truncated to zero, and vien will be zero. Directions u, v and w are orthogonal.

Flag nerr indicates any input error.

au, av, bu, bv, np, tol. Input:

Out put: cw, vlen, nerr.

Glossary:

au, av Input The u and v components of input vector "a". Size np.

The w components are zero.

The unit vectors in the directions u, v and w form

a positive unit triple.

The u and v components of input vector "b". Size $\ensuremath{\text{np}}_{\star}$ bu, by Input

The w components are zero.

The w components of output vector "c". Size np. CW Output

Will usually be +1.0 or -1.0.

The u and v components are zero.

Vector (cross) product of vectors "a" and "b", normalized to unit magnitude. The value of cw will be truncated to zero if less than the estimated error in its calculation, based on tol. This indicates that "a" and "b" are essentially parallel.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

Input. Size of arrays au, av, bu, bv, cw, vlen. np

Numerical tolerance limit. tol Input

On Cray computers, recommend 1.e-5 to 1.e-11.

Magnitude of the vector product "a" x "b", after any vlen(n) Output

truncation of components has been done. Will be zero if all comporants of vector "c" are zero.

Size np.

SUBROUTINE APTVXUN

dall aptvxun (ax, ay, az, bx, by, bz, np, tol, ux, uy, uz, vlen, nerr)

Version: aptvxun Updated 1990 March 14 16:00. aptvxun Originated 1989 November 10 11:20.

Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.

Source: xport read .245100:aptslibe / 1 1
lib aptslibe!x aptblibe aptvxun|end / 1 1.
aptslibe is a LIB library of FORTRAN source files.
aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find the veutor products "a" x "b" of the np vector pairs a = (ax, ay, az) and b = (bx, by, bz), and divide by their magnitudes vien, to produce the unit vectors u = (ux, uy, uz), parallel to "a" x "b". Any components of vector "u" less than the estimated error in their calculation, based on tol, will be truncated to zero. If all are zero, or are truncated to zero, the output vector "u" will be zero, and vien will be zero. Flag nerr indicates any input error.

History: 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes.

Input: ax, ay, az, bx, by, bz, np, tol.

Output: ux, uy, uz, vlen, nerr.

Calls: aptvuna (source in aptslibe, binary in aptblibe).

Glossary:

ax, ay, az Input The x, y, z components of input vector "a". Size np.

bx, by, bz Input The x, y, z components of input vector "b". Size np.

ux,uy,uz Output The x, y, z components of output vector "u". Size np.
Vector (cross) product of vectors "a" and "b",
normalized to unit magnitude. A component will be
truncated to zero if less than the estimated error
in its calculation, based on tol.

nerr Output Indicates an input error, if not 0.

1 if np is not positive.

np Input Size of arrays ам, ау, ах, bx, by, bz, ux, uy, uz, vlen.

tol Input Numerical tolerance limit.
On Cray computers, recommend 1.e-5 to 1.e-11.

vien(n) Output Magnitude of the vector product "a" x "b", after any truncation of components has been done. Will be zero if all components of vector "u" are zero.

Size np.

SUBROUTINE APTXNUP

call aptxnup (nopt, tplanck, np, Knu, nerr)

Version: aptxnup Updated 1990 February 12 10:50, aptxnup Originated 1990 January 31 17:00,

Authors: Eugene H. Canfield, LLNL, 1-298, Talephone (415) 422-4125. Arthur L. Edwards, LLNL, 1-298, Telephone (415) 422-4123.

Source: **xport read .245100:aptslibe / 1 1

lib aptailbelx aptblibe aptknuplend / 1 1, aptailbe is a LIB library of FORTRAN source files, aptblibe is a BUILD library of Cray-compiled binaries.

Purpose: To find, for each of np temperatures tplanck, a frequency xnu sampled fandomly from a Planck or a Wien spectrum.
Flag nerr indicates any input error (np not positive).

The Planck distribution function is: $p(x) = (15.0 \ / \ pi^**4) \ ^* \ x^**3 \ / \ (exp \ (x) \ - 1.0),$ where $x = xnu \ / \ tplanck, and <math>< x> = 3.83223...$ The Wien distribution function is: $p(x) = x^**3 \ ^* \ exp \ (-x) \ / \ 6.0.$

where $\langle x \rangle = 4.0$,

History: See Barnett and Canfield, UCIR-473, June 1970.

1990 February 6 11:20. Truncated plfn, to limit number of terms

required to converge,

Input: nopt, tplanck, np.

Output: xnu, nerr.

Glossary:

nerr Output Indicates an input error, if not 0.

1 If np is not positive.

nopt Input Indicates type of spectrum to sample from:

O for a Planck spectrum. 1 for a Wien spectrum.

np Input Size of arrays tplanck, xnu.

tplanck Input Black body temperature of frequency distribution.

Same units as xnu. Size np.

xnu Output Frequency sampled randomly from spectum. Size np.

Same units as tplanck.

APPENDIX

SUBROUTINES BY FUNCTION

FUNDAMENTAL CONSTANTS

Find the values of the fundamental constants of Physics and Chemistry, and energy conversion factors

in cm-g-sh-keV in m-kg-s (SI)		:		aptcon1
יייי ווו אין ט אין אין			,	

MATHEMATICS AND STATISTICS

Find any real root of a general quadratic equation

a single equation		1	aptqrts
any number of equations	(vectorized)		aptqrtv
	•		

Find the mean and standard deviation of a set of values aptmean

MONTE CARLO SAMPLING

Sample randomly from a probability distribution

values from a linear distribution on an interval one value from each linear distribution on an interval	aptslid aptsliv
points in a major plane (2-D)	
uniformly in a triangle	apttloc
uniformly in a triangle or quadrangle	aptgloc
direction vectors in any coordinate system (3-D)	
uniform distribution	aptscat
cosine-power distribution along a specified axis	aptscap
direction vectors in a specified plane (3-D)	•
uniform distribution	aptscad
frequencies from a Planck or a Wien spectrum	aptxnup
velocities from a relativistic Maxwellian distribution	aptmaxw

FUZZY GEOMETRY

Impose limits on the values of

a fractional distance (scalar) any number of fractional distances (vectorized)	aptfdad aptfdav
the components of a vector	
in a major plane (2-D), lower	aptvlic
in a major plane (2-D), several options	aptvtoc
in any coordinate system (3-D), lower	aprvlim
in any coordinate system (3-D), several options	aptvtol

Round off a floating point number

to a	specified	relative	or	absolute	precision	aptrnds
------	-----------	----------	----	----------	-----------	---------

GEOMETRY

Transform bet	ween Cartesian,	cylindrical	and	sphorical
coordinate	systems			

	coordinates (3-D) coordinates and bound vectors (3-D)	aptcaya aptcayv
Do	the basic vector operations	
	<pre>linear combination in a major plane (2-D) in a major plane (2-D) in any coordinate system (3-D) in any coordinate system (3-D) difference</pre>	aptvadc aptvsuc aptvadd aptvsum
	in a major plane (2-D) in any coordinate system (3-D) dot (scalar) product	aptvdic aptvdis
	in a major plane (2-D) in any coordinate system (3-D) cross (vector) product	apt vdoc apt vdot
	in a major plane (2-D) in a major plane (2-D), normalized to unit vector in any coordinate system (3-D) in any coordinate system (3-D), normalized normalize to a unit vector	aptvaxc aptvxuc aptvaxb aptvxun
	in a major plane (2-D) in a major plane (2-D), replace in any coordinate system (3-D) in any coordinate system (3-D), replace	aptvubc aptvuac aptvunb aptvuna
Do	the basic matrix operations	
	product of a 3-D vector and a 3 by 3 matrix product of two n by n matrices	aptmopv aptmprd
Fi	nd the angle relationships	
	area included between adjacent sides in a major plane (2-D) in any coordinate system (3-D) bisectors	aptvaxc aptvaxb
	in a major plane (2-D) in any coordinate system (3-D) cosine	aptbanc aptbang
	in any coordinate system (3-D) cosine (between unit vectors)	aptvang
	in a major plane (2-D) in any coordinate system (3-D) cosine and sine	apt vdoc apt vdot
	in a major plane (2-D) sine (between unit vectors) in a major plane (2-D)	aptvanc aptvaxc
	in any coordinate system (3-D)	aptvaxb

Test for the special geometric relationships

points 1	peing coincident	
on an	axis (1-D)	aptvdil
inar	major plane (2-D)	aptvdic
	z space (3-D)	aptvdls
	y coordinate system (3-D)	aptdist
	being on lines	•
	major plane (2-D)	aptptlc
	z space (3-D)	aptptln
	peing within a bounded region	
	major plane (2-D)	
	riangle, and distances to sides	aptting
	Ladrangle, and distances to sides	aptgine
	sing parallel or congruent	apequite
		aust Inla
	major plane (2-D)	aptinic
	z space (3-D)	aptlnln
	ing in a plane	
	z space (3-D)	aptlnpl
	being parallel	
	major plane (2-D)	aptvaxc
in an	y coordinate system (3-D)	aptvaxb
vectors	being perpendicular	
in a :	major plane (2-D)	aptvdoc
in an	y coordinate system (3-D)	aptvdot
planes	being parallel or congruent	
	z space (3-D)	aptplpl
	eing tangent to a sphere	
	z space (3-D)	aptplsp
	being congruent	
	z space (3-D)	aptspsp
	being tangent to a sphere	ирсорор
	z space (3-D)	aptspsp
1.1. AY	Lapace (5-b)	арсарар
Do the bas	ic geometric operations	
	as goometate specialists	
inversi	on of a point or vector through a specified	
point		
•	major plane (2-D)	aptinvo
	z space (3-D), and the operator	aptinvp
	z space (3-D), with scaling, and the operator	aptsclu
	scaling of a point or vector in the direction	арсьста
	specified axis (i.e., Lorentz transformation)	
		antaala
	major plane (2-D)	aptsclc
	z space (3-D), and the operator	aptscll
	z space (3-D), with reflection,	
	the operator	aptscll
	scaling of a point or vector	
	z space (3-D), and the operator	aptsclu
	z space (3-D), with inversion, and the operator	aptsclu
	ion of a point or vector	
from	a plane perpendicular to a major plane (3-D)	
	a point or vector in a major plane (2-D)	aptrefc
	a point or vector in xyz space (3-D)	aptrefl
	a plane in xyz space (3-D), and the operator	aptrefs
	The state of the s	• • • •

rotation of a point or vector	
by a specified angle around a specified axis	
in a major plane (2-D)	aptroto
in xyz space (3-D), operator only	aptrota
by specified angles around the 3 major axes (3-D),	
operator only	aptrots
to rotate a specified vector onto another vector	
(3-D), operator only	aptrotv
to rotate a specified plane onto another plane	
(3-D), operator only	aptrotp
to rotate a specified vector in a specified plane	
onto another vector in another plane (3-D),	
operator only	aptrott
apply the operator generated by aptrota, aptrotp,	
aptrots, aptrott, aptrotv or aptmopv to points or vectors	aptmopv
translation of a point	арстору
in a major plane (2-D)	anttran
in xyz space (3-D)	apttrac apttran
combined operations	apectan
multiply two matrix operators together	aptmprd
apply matrix operator to points or vectors	aptmopv
approximaters operator to pornes or voctors	прешору
Find the distance	
from a point to another point	
on an axis (1-D)	ant richt 1
in a major plane (2-D), and direction	aptvdil aptvdic
in xyz space (3-D), and direction	aptvdis
in any coordinate system (3-D), and direction	aptdist
from a point to a line	apturst
in a major plane (2-D)	aptptlc
in xyz space (3-D)	aptptln
from a point to the sides of a triangle	abchern
in a major plane (2-D), and in or out?	apttine
from a point to the sides of a quadrangle	apecane
in a major plane (2-D)	aptqdic
in a major plane (2-D), and in or out?	aptqinc
from a point to a plane in xyz space (3-D)	apadaiio
in any orientation, and the nearest point	aptptpl
bounded by a triangle, and the nearest point, more	apttrip
from a point to a second-order surface	apoczap
bounded by a quadrangle (3-D), and the nearest point	aptquad
from a line to another line	apaquaa
in a major plane (2-D)	aptinic
in xyz space (3-D)	aptlnln
from a line to a plane	
in xyz space (3-D)	aptlnpl
Find the initial vector direction between two points	
in a major plane (2-D), and find distance	antidic
in a major plane (2-D), and find distance in xyz space (3-D), and find distance	aptvdic
in any coordinate system (3-D), and find distance	aptvdis aptdist
in any coordinate system (3-D), and tind distance	aptuist

Find the alternate geometric representation of a

line in a major plane (2-D) given two points, find vector, distance given point and vector, find another point line in xyz space (3-D)	aptvdic aptvadc
given two points, find vector, distance given point and vector, find another point line in any coordinate system (3-D)	aptvdis aptvadd
given two points, find initial vector, distance plane in xyz space (3-D) given three points, find normal vector	aptdist aptvpln
Find the vector perpendicular (normal) to a	
line in a major plane (2-D) plane in xyz space (3-D)	aptvplc aptvpln
Find the vertex areas in a major plane (2-D) of a	
triangle quadrangle, and shape (convex, boomerang, bowtle)	aptvaxc aptqvac
Find the local coordinates of a point	
in a quadrangle in a major plane (2-D), with any number of points, one quadrangle in a quadrangle in a major plane (2-D), with	aptqfdc
any number of points, quadrangles	aptfdqc
Find the intersection(s) of a line with	
a line in a major plane (2-D) a circle in a major plane (2-D) (two points) a plane in xyz space (3-D)	aptinic aptinic aptinpi
Find the intersection(s) of a linear track with	
a line, both in a major plane (2-D) a major plane (3-D) a plane in xyz space (3-D) an axisymmetric cylindrical surface with	aptrkle aptrksl aptrkpl
constant radius (3-D) an axisymmetric cylindrical surface (3-D) a centrisymmetric spherical surface (3-D) a general implicit second-order surface (3-D)	aptrkcl aptrkcy aptrkrl aptrkis
Find the intersection(s) between	
two circles in a major plane (2-D) (2 points) two planes in xyz space (3-D) (a line) a plane and a sphere in xyz space (3-D) (a circle) two spheres in xyz space (3-D) (a circle)	aptcinc aptplpl aptplsp aptspsp

Move a point a specified distance in a specified direction, and find the final position, direction

in any coordinate system (3-D) aptmove in axisymmetric cylindrical coordinates (3-D) aptmove in spherical coordinates (3-D) aptmovs

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract #W-7405-Eng-48.

DATE FILMED 11/05/190

