## APTBLIBE: <br> Geometrical and Monte Carlo Sampling Routines for the Cray Computer

Arthur L. Edwards

## April 1990



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APTBLIBE:
Geometrical and Monte Carlo Sampling
Subroutines for the Cray Computers
Arthur L. Edwards. UCRL-ID--103432
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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
iib 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, 2D 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 statisuics ( 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 docurnent.

The latest self-consistent set of values of the fundamental constants of physics and chemistry are provided in two subroutines, aptconl ( 180 values in $\mathrm{cm}-\mathrm{g}$-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 componsats, 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 ?-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 dll 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 " 1 ". 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, accessiblity, readability, generality, flexibility, ease of maintenance, and ease of $\mu$ se.

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 helps 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 deciarations 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 $1 . \mathrm{E}-12^{* *}(1 / \mathrm{n})$, when the tested value x is to be used in the form $\mathrm{x} * * \mathrm{n}$. 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 $1 . \mathrm{E}-99 \mathrm{might}$ 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,
&
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.
Source: xport read .245100:aptslibe / 1 1
    lib aptslibelx aptblibe aptbanc!end / 1 1
    aptslibe is a LiB library of FORTRAN source files.
    aptblibe is a BUILD llbrary of Cray-complled binarles.
Purpose: To find, for each of np sets of Input data, the bisector
    bd " (bdu, bdv) of the angle "abc" formed bv the polnts
    a * {au, av), b = (bu, bv), and c = (cu, cv) in the uv plane,
    and polnt d'= (du, dv), the intercept of the bisector on
    the llne "ca". If points "a", "b" and "c" are collnear,
    vector "bd" will be,zero, and polnt. "d" will be polnt "b".
Input: au, av, bu, bv, cu, cv, np, tol.
Output: bdu, bdv, du, dv, nerr.
Calls: aptvalc, aptvuac (sources in aptslibe,
    binarles in aptblibe)
glossary:
au, av Input The u and v coordinates of point "a". Slze np.
bdu, bdv Output The }u\mathrm{ and v components of the vector "bd" which
    blsects angle "abc", and connects polnts "b" and""d".
bu, bv Input The }u\mathrm{ and v coordinates of point "b". Size np.
cu, cv Input The u and v coordinates of point "c". Size np.
du, dv Output The u and v coordinates of point "d" on line "ca".
        The intercept of bisector' "bd" on line "ca".
        Slze np.
nerr Output Indicates an input error, if not 0.
        1. If np is not positive.
np Input Slze of arrays au, av, bu, bv, cu, cv,
    bdu, bdv, du, dv.
t.01 Input Numerical tolerance limit
    On Cray computers, recommend 1.e-5 to 1.e-11.
```



## SUBROUTINE APTCINC



Refs: $\quad$. Whe 1986 Adjustment of the Fundamental Physlecal Constants", Codata BulletIn Number 63, November 1986, Pergamon Press.
2. Metric Practice Guide E 380-72en, 1973, American Society for Testing and Materlals, 1916 Race Street, Philadelph1a, Pa 19103.
3. File physcons in LIB library physilbe. Execute:

> xport read 245100 :physlibelend / $t v$
> lib physlibelx physconslend / $t v$
> allout hsp physcons $/ t v$
> trix aclolphyscons!tuNNNN!pl/tv

Source: xport read . 245100 aptslibe / 12.
1lb aptsilbelx aptblibe aptconllend / 11 .
aptsilbe $1 s$ a LIB library of FORTRAN source files.
aptblibe is a BUIID library of Cray-complled binaries.
Purpose: To provide the best avallable values of the fundamental physical constants and conversion factors of physics and chemfstry, in cmig-ghake-keV units. Sae aptconm for SI unfts. For each of $n$ p values of ind, the constant with local index ind is returned in array pgcon. The local indices ara tabulated below. For definitions of the constants, see the full listing of this subroutine, or reference 3 listed above. If any value of ind 1 s not in the range from 1 to 180 , the returned value of pgeon will be -1.e99.

| 1 | poa | 37 | pgittoam | 73 | $p \mathrm{pk}$ | 109 | pgmsubmu | 145 | pgratde |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | pgab185 | 38 | pgittog | 74 | pgketoam | 110 | pgmsubn | 146 | pgratdp |
| 3 | pgalpha | 39 | pgfrtojk | 75 | pgketofr | 111 | pgmsubp | 147 | pgratea |
| 4 | poalphal | 40 | pgfrtoke | 76 | pgketojk | 112 | pgmub | 148 | pgrated |
| 5 | pgantohz | 41 | pyfrtore | 77 | pgketorc | 113 | pgrmube | 149 | pgratemu |
| 6 | pgamtojk | 42 | pgg | 78 | pgkevtog | 114 | pgmubf | 1.50 | pgratep |
| 7 | pgamtoke | 43 | pggamma | 79 | pglamce | 115 | pgmubw | 151 | pgratmue |
| 8 | pqamtorc | 44 | pggamp | 80 | pglamceb | 116 | pgmud | 152 | pgratne |
| 9 | pgamu | 45 | pggampb | 81 | polamen | 117 | pgimudb | 153 | pgratnp |
| 10 | pgamud | 46 | pggampp | 82 | pglamonb | 118 | pgmudn | 154 | pgratpe |
| 11 | pgamue | 47 | pggamppo | 83 | pglamcp | 119 | pgrmue | 155 | pgratpmu |
| 12 | pgamumu | 48 | pgesolden | 84 | pglamcpb | 120 | pgmueb | 156 | pgrctoam |
| 13 | pgamun | 49 | pgosube | 85 | pglosch | 121 | pgmuen | 157 | parctofr |
| 14 | pgamup | 50 | pggsubmu | 86 | pgmagfa | 122 | pgmumu | 158 | porctog |
| 15 | pgamutog | 51 | pggsubn | 87 | pomdev | 123 | pgmumub | 159 | parctojk |
| 16 | pgastar | 52 | pggtoamu | 88 | pgmd $f$ | 124 | pgmumun | 160 | porctoke |
| 17 | pgasube | 53 | pgotofr | 89 | pymeev | 125 | pgmun | 161 | pgrmole |
| 18 | pgasubmu | 54 | pgatojk | 90 | pque 1 | 126 | pgmune | 162 | pgrydb |
| 19 | pgatm | 55 | pggtokev | 91 | pgrunrde | 127 | pgmunf | 163 | pgrydbc |
| 20 | pgatomx | 56 | pgotorc | 92 | pgmmrdp | 128 | pgmunt | 164 | pgrydbe |
| 21 | pgbohr | 57 | pgh | 93 | pgmmremu | 129 | pgmuntt | 165 | porydbev |
| 22 | pgc | 58 | pghart | 94 | pgmmrep | 130 | pgmuntn | 166 | posate |
| 23 | pgesubl | 59 | pghartev | 95 | prommmup | 131 | pgrmunw | 167 | pgsatez |
| 24 | pgcsub2 | 60 | pghbar | 96 | pgmmrne | 132 | pgmup | 168 | pgsb |
| 25 | pgcunit | 61 | pghbarc | 97 | pgmurnp | 133 | pgmupb | 169 | pasia |
| 26 | pgcuxun | 62 | Dghbarok | 98 | pgmmuev | 134 | pgmupn | 70 | pgsid220 |
| 27 | pgdrohm | 63 | pohlen | 99 | pgmay | 135 | pgmupp | 171 | pgsiow |
| 28 | pge | 64 | pghmass | 100 | pomnev | 136 | pgmuppo | 172 | pgsivolm |
| 29 | pgebase | 65 | pghok | 101 | pgmn $)$ | 137 | pgmuppn | 173 | pgtemp |
| 30 | pgec | 66 | pght ime | 102 | pgmoih | 138 | pgmuvac | 174 | pgt homx |
| 31 | pgeoh | 67 | pojfvr | 103 | proolhe | 139 | pgnsuba | 175 | Pgubb |
| 32 | pgeome | 68 | pgjktoam | 104 | pgmoxun | 140 | pgombl 85 | 176 | pgv76bl |
| 33 | pgeomp | 69 | pgjktofr | 105 | pgmpev | 141 | pgqcirc | 177 | pgumols |
| 34 | pgepsvac | 70 | pgjktog | 106 | pgmpl | 142 | pgqcirch | 178 | pgumolz |
| 35 | pgerad | 71. | ngjktoke | 107 | pgmsubd | 143 | pgohc | 179 | powien |
| 36 | Dofar | 72 | pgjktorc | 108 | pgensube | 144 | pgahr | 180 | $p 1$ |



Power. 1 ferk / in $=1.0$ o 17 W (watt.), $1 \mathrm{~W}=1 \mathrm{~J} / \mathrm{s}=1$.0e-17 jerk/sh.

Presaure or energy density. 1 ferk / cm** $3=1.0015 \mathrm{~Pa}$ (pascal). $1 \mathrm{~Pa}-1 \mathrm{~N} / \mathrm{m}^{*} \mathrm{~K}^{2}=1 \mathrm{~J} / \mathrm{m}^{* * 3}$.

Spaciflc hat. 1 jark / (g keV) $=8.617385 e+04 \mathrm{~J} /(\mathrm{kg} \mathrm{K})$,
Thermal conductivity, 1 jerk / (sh an keV) $=6.617385 e+11 \mathrm{~W} /(\mathrm{m} K)$.
Veloclty. $1 \mathrm{~cm} / \mathrm{sh}=1.0 \mathrm{e}+06 \mathrm{~m} / \mathrm{s}$.
Volume. $1 \mathrm{cm**}=1.0 \mathrm{e}-06 \mathrm{~m} * * 3$.
call apt conm (1nd, np, pgoon, nerr)

| Version: aptconm Updated 1990 March 2 15:30. |  |
| :--- | :--- |
|  | aptconm OrIginated 1989 March 2 15:30. |
| Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |  |

Refs: 1. "The 1986 Adfustment of the Fundamental physical Constants", Codata Bulletin Number 63, November 1986, Pergamon Press.
2. Metric Practice Guide E 380-72en, 1973, American Society for Testing and Materials, 1916 Race Street, Philadelphla, Pa 19103.
3. File physcons In LIB library physlibe. Execute:
xport read . 245100 ;physlibelend / t v
llb phyellbelx physconslend / t v
allout hsp physcons / t v
trix aclolphysconsltuNNNN!p1/tv
Source: xport read . 245100:aptslibe / 11
11b aptslibelx aptblibe aptcommend / 11.
aptsilbe is a LIB 1 ibrary of FORTRAN source flles. aptblibe is a BUILD library of Cray-complled binaries.

Purpose:
To provide the best avallable values of the fundamental physical constants and conversion factors of physics and chemlstry, In SI units. See aptconl for cm-g-shake-keV units. For each of np values of ind, the constant with local index ind $1 s$ returned in array pgcon. The local indices are tabulated below. For definitions of the constants, see the full listing of this subroutine, or reference 311 sted above. If any value of ind is not in the range from 1 to 217 , the returned value of pocon will be -1.e99.
1 pga
2 pgabi85 46 pgevtorm
46 pgevtor
47 pgiar
pgad
pgalpha pgalpha1
pgamtoev $\quad 49$ pggamma
Dgamtoht 51 pggampb
pgamtohz
pgamtof
pgamtok
pgamtokg
pgamtorm
pgamu
pgamud $\quad 58$ pgh
$\begin{array}{ll}\text { pgamue } & 59 \text { pghart. } \\ \text { pgamumu } & 60 \text { pghartev }\end{array}$
pogamun
poamun
pgamup
pgasube pgasubmu pgatm
3 pgatomx
4 pgbohr
5 pgc
26 pgcsubl
2 pgcsub2d
9 pgcunit
1 pgdrohm
2 pge
3 pgebase
pgec
pgeoh
pgeome
pgeomp
pgepsvac
pgerad
40 pgevtoam
11 pgevt oht.
42 pgevtohz
3 pgevtof
44 pgevt.ok

| 89 | pgjtokg | 133 | pompev | 177 | pgratea |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 90 | pgjtorm. | 134 | pgmip | 178 | pgrated |
| 91 | pgk | 135 | pgmsubd | 179 | pgratemu |
| 92 | pgkd | 136 | pgmsube | 180 | pgratep |
| 93 | pgkgtoam | 137 | pgmsubmu | 181 | pgratmue |
| 94 | pgkgtoev | 138 | pgmsubn | 182 | pgratne |
| 95 | pgkgtoht | 139 | pgmsubp | 183 | poratip |
| 96 | pukgtohz | 140 | pgmub | 184 | pgratpe |
| 97 | pgkgtof | 141 | pgmube | 185 | pgratpmu |
| 98 | pgkgrok | 142 | pgrmubf | 186 | pgrmold |
| 99 | pgkgtorm | 143 | pgmubk | 187 | pormole |
| 100 | pgktoam | 144 | pgmubw | 188 | pgrmtoam |
| 101 | pgittcev | 145 | pgmud | 189 | pgrmtoev |
| 102 | pgktoht | 146 | pgmudb | 190 | pgrmtoht |
| 103 | pgktohz | 147 | pgmudn | 191 | pgrmiohz |
| 104 | pgktof | 148 | pgmue | 192 | pgrmtos |
| 105 | Pgktokg | 149 | pgmueb | 193 | pgrmiok |
| 106 | pgktorm | 150 | pgmuen | 194 | pgrmtokg |
| 107 | pglamce | 151 | pgmumu | 195 | pgrydb |
| 108 | pglamceb | 152 | pgmumub | 196 | pqrydbc |
| 109 | pglamen | 153 | pgmumun | 1.97 | pgrydbe |
| 110 | pglamenb | 154 | pgmun | 198 | pgrydbev |
| 111 | pglamcp | 155 | pgmune | 199 | posate |
| 112 | pglamcpb | 156 | pgmunf | 200 | pgsatez |
| 113 | pglosch | 157 | pgmunk | 201 | pgsb |
| 114 | pgmagfa | 158 | pgmunt | 202 | pgsbd |
| 115 | pomdev | 159 | pgmuntb | 203 | pgsia |
| 116 | pand $f$ | 160 | pgmunten | 204 | posid220 |
| 117 | pomeav | 161 | pgmunw | 205 | pgsigw |
| 118 | prame $J$ | 162 | pgmup | 206 | pgsivolm |
| 119 | pgmmrde | 163 | pgmupb | 207 | pgt emp |
| 120 | pormordp | 164 | pgmupn | 208 | pgtempt |
| 121 | pgmmremu | 165 | pgimupp | 209 | pgt homx |
| 122 | pgmmrep | 166 | pgmuppb | 210 | pgubb |
| 123 | pgmmmup | 167 | pgmuppn | 211 | pgubbd |
| 124 | pgmmrne | 168 | pgmuvac | 212 | pgu76bl |
| 125 | pgrmernp | 169 | pgnsuba | 213 | pgumolt |
| 126 | pmmuev | 170 | pgombl85 | 214 | pgumoltz |
| 127 | pommuj | 171 | fgacirc | 215 | pgwlen |
| 128 | pgmnev | 172 | paqcirch | 216 | powlend |
| 129 | pgmn' | 173 | pgahe | 217 | pl |
| 130 | pmolh | 174 | pgqhir |  |  |
| 131 | pamolhe | 175 | pgratde |  |  |
| 132 | pgmoxun | 176 | pgratdp |  |  |


$1 \mathrm{~T}=1 \mathrm{~Wb} / \mathrm{m}^{* * 2}-\left(1,0 e+07 \mathrm{~J} / \mathrm{m}^{* * 3}\right) * * 0.5$.

## Power. 1 ferk / sh $-1.0 \mathrm{e}+17 \mathrm{~W}$ (watt) <br> $1 \mathrm{~W}=1 \mathrm{~J} / \mathrm{m}$ - $1, \mathrm{e}-17$ jerk / sh.

Pressure or energy dansity, 1 jerk $/ \mathrm{cm}^{* * 3} \sim 1,0 \mathrm{e} 15 \mathrm{pa}$ (pasoal). $1 \mathrm{~Pa}=1 \mathrm{~N} / \mathrm{m}^{*} 2=1 \mathrm{~J} / \mathrm{m**} 3$ 。

Speciflo heat. 1 Jork / ( keV ) $-8.6173850+04$ y / ( kg K ).
Thermal conductivity. 1 fark / (sh am keV) - a, 617385etil $\mathrm{W} /(\mathrm{m} \mathrm{K})$.
Valocity, $1 \mathrm{~cm} / \mathrm{sh}=1,0 \mathrm{e}+06 \mathrm{~m} / \mathrm{s}$,
Volume. 1 cm**3 $=1,00-06$ m**3.

## SUBROUTINE APTCSYS



## subroutine aptcsyy

| 6 | $v$ (n1, n2, lunlt, $u, v, w, a u, a v, a w, n p$, tol, nerr) |
| :---: | :---: |
| Version: | aptesyv Updated 1989 December 1 13:10. |
|  | aptesyv Orlginated 1989 November 2 14:10. |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100 aptsllbe / 1 i |
|  | lib aptsilbelx aptblibe aptosyviend / 11. aptslibe is a Lit llbrary of FORTRAN source files. |
| Purpose: | To transform the np points ( $u, v, w$ ) and |
|  | the assoclated bound vectors a - (au, av, aw) from coordinate system $n 1$ to coordinate system $n 2$. Allowed coordinate systems are cartesian, cylindrical, spherlcal. |
|  | Note: If $(u, v, w)$ is at the orlgin, then au and av are |
|  | Independent of the coordinate system, and aw changes sign |
|  | between the spherlcal coordlnate system and the other two. Angles may be in degrees (lunit $=0$ ) or rndlans (iunlt = 1) |
|  | Results will be truncated to zero if less than the estimated error In thelr calculation, based on tol. Disallowed input |
|  | values of $n 1, n 2$, lunlt, or $n p$ are indlcated by a nonzero value of nerr. |
| Input: | n1, n2, lunit, $u, v, w, a u, a v, a w, n p, t o l$. |
| out put: | $u, v, w, a u, a v, ~ a w, ~ n e r r . ~$ |
| Glossary: |  |
| $a u, a v, a w$ | In/Out The $u, v, w$ components of a bound vector at. $\langle u, v, w\rangle$. slze np. |
| Iunit. | Input Indicates undt to be used for angles: 0 If angles are in degrees. 1 If angles are in radians. |
| n1 | Input Indicates initial coordinate system type: |
|  | 0 for cartesian coordinates. $u=x, v=y, w=z$. <br> 1 for cyllndrical coordinates. $u$ madlus from ? |
|  | axis, $v=$ angle $\ln x y$ plane, counterclockwise from $x$ axis, w . $z$. |
|  | 2 for spherical coordinates. $u=$ radius from orlgin, $v$ wangle in $x y$ piane, counterclockwlse from $x$ axis, $w=a n g l e$ from $z$ axis. |
| n2 | Input Indlcates final coordinate system. Seen nl . |
| nerr | Output Indlcates an input error, if not 0 . |
|  | 1 If np is rit positive. |
|  | 2 1f elther $n 1$ or n 2 is not 0,1 , or 2 . |
|  | 4 if lunit is not 0 or 1 . |
| rp | Input Number of points ( $u, v, w$ ), and number of bound vectors (au, av, aw). |
| t.ol | Input Numerical tolerance ldmlt. Any angle with a sine or cosine (absolute value) less than tol wlll be adjusted to make its sine or cosine $=0$. Any spatial coordlnate or vector component with a final value less than the estimated error in its calculation, based on tol, wlll be truncated to zero. |
| $u, v, w$ | In/out The coordinates of a point. Slze np. See $n 1, \mathrm{n} 2$. Wlll be truncated to zero, lf less than the estimated error in thelr calculation, base on tol. |



## SUBROUTINE APTFDAD

| Version: | aptfdad Updated 1990 January 18 16:40. aptfdad Originated 1989 November 2 14:10. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read .245100:aptslibe / 11 <br> lib aptslibelx aptblibe aptfdadlend / 11. <br> aptslibe is a LIB library of FORTRAN source flles. aptblibe is a BUILD library of Cray-complled binarles. |
| Purpose: | To adjust the value of $f d$, relative to the limits 0 and 1 , based on the opition noptfd and the numerical tolerance limit tol. Values of fa initially in the range from tol to $1+$ tol may be adjusted to the range from tol to 1 - tol. Values of id outside the range from 0 to 1 may be adjusted to that range. The flag nl im indicates if and how fd was adjusted. <br> Flag nerr indicates any error'in nopt fd. |
| Input: | fd, noptfd, tol. |
| Output : | fd, nlim, nerr. |
| Clossary: |  |
| fd | Input Fractional distance. |
| fd | Outpot Fractional distance, with range limised if noptifd is 1 or 2. |
| nerr | Output Indicates an input exror, if not 0 . 1 if nopt fd is not between 0 and 2. |
| n11m | Output 0 if no limit imposed on fd, 1 if the limit of noptid = 1 is imposed, 2 if the 11 mit of noptfd - 2 is 1 mposed. |
| nopt fd | Input Option to 11 mit range of fd : 0 for no 11 mit ; 1 to increase fd to tol, if in the range from -tol to tol, and decrease fd to $1.0-t 01$, if in the range from 1.0 - tol to $1.0+$ tol; and 2 to impose the limits for noptfd $=1$, and then 11 mlt fd to the range from 0.0 to 1.0 . |
| tol | Input Numerical tolerance limit. Needed if noptfd-1 or 2. On Cray computers, recommend 1.e-5 to $1 . e-11$. |

## SUBROUTINE APTFDAV



| 4 | fdk, fdl, ngood, nerr) |
| :---: | :---: |
| Version: | aptifdqc 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 11b aptslibelx aptbl'be aptfdqc/end / 1 1. aptslibe 1s a LIB litrary of FORTRAN source flles. aptblibe 1s a BUILD 11 brary of Cray-complled binarles.``` |
| Purpose: | To find, for each of thi np sets of input data, the fractional distances $f d k$ and $f d l o$ : the point $p=(p u, p v)$, between the opposite edges "da" and "bc", and "ab" and "cd", respectively, of the 2-D quadrilatera: In the uv plane with vertices $a=(a u, a v), b=(b u, b v), c=(c u, c v\rangle$, and $d=(d u, d v)$. Flag nerr indicates any input error. |
| Input: | $a u, a v, b u, b v, c u, c v, d u, d v, p u, p v, n p, t o l$. |
| Output: | fdk, fdl, ngood, nerr. |
| Calls: | aptqrtv (source in aptslibe, binary in aptblibe) |
| Glossary: |  |
| $a u, a v$ | Input The $u$ and $v$ coordinates of point "an in the uv plane. slze np. |
| bu, bv | Input The $u$ and $v$ coordinates of point "b" in the uv plane. Slzenp. |
| cu, CV | Input The $u$ and $v$ coordinates of point " $c$ " in the uv plane. Slze np. |
| du, dv | Input The $u$ and $v$ coordinates of point " $d^{*}$ in the uv plane. size np. |
| $f d k$ | Output Fractional distance of point. "p" from the line segment "da" to the line segment "bc". Slze np. <br> Values between $-t o l$ 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. |
| fdl | Ourput Fractional distance of point "p" from the line segment "ab" to the line segment "cd". Size np. <br> Values between -tol and tol will be adjusted to tol. Values between 1.0 - tol and $1.0+$ tol wlll be adjusted to 1.0 - tol. See ngood. |
| ngood | Output Indicates range of fractional distances fak and fdl: <br> 0 if elther fdk or fdl is outside the range from -tol to $1.0+$ tol. Also if both are. <br> 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. <br> 2 if fdk and fdl are hoth 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 $\begin{gathered}\text { SIze of arrays } p u, ~ \\ f d k, ~ f d l .\end{gathered}$ |
| pu, pv | Input The $u$ and $v$ coordinates of point " $p$ " in the uv plane. Slze np. |
| tol |  |


| Version: | aptinve Updated 1990 March 13 11:30. aptinve Originated 1990 January 4 13:20. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | ```xport read . 245100:aptslibe/1 1 lib aptslibe!x aptblibe aptinvclend / 1 1. aptslibe ds a LIB library of FORTRAN source flles. aptblibe ls a BUILD library of Cray-aompiled binarles.``` |
| Purpose: | To invert the $n p$ points or vectors $p-(p u, p v)$ through the point a = (au, av), all in the uv plane. If "p" are unbound vectors, point $a=(a u, a v)$ should be at the origin. The new components of "P" willd be truncated to zero if less than the estimated error in their aalculation, based on tol. Flag nerr indicates any input error. |
| Input: | Itype, au, av, pu, pv, np, tol. |
| Out put: | pu, pv, nerr. |
| Glossary: |  |
| au, av | Input The $u$ and $v$ components of the inversion point "an. |
| herr | Output Indicates an input error, if not 0 . 1 if np is not positive. |
| $n p$ | Input Number of 2-D points or vectors (pu, pv). |
| pu, pv | In/Out The $u$ and $v$ coordinates of a 2-D point, or the $u$ and $v$ components of a 2-D vector. Slze np. Truncated to zero if less than the estimated error in their calculation. See tol. |
| tol | Input Numerical tolarance limit. On Cray computers, recomend $1 . e-5$ to $1 . e-11$. |

## subroutine aptinve



## SUBROUTINE APTINIC




## SUBROUTINE APTLLNLN

```
aall apt.lndn (ax, ay, az, bx, by, bz, bx, cy, az,
dx, dy, dz, np, tol, dpenjn, fracab, fracod,
ex, oy, &z, fx, fy, fz, Itrun, lpar, norr)
Varsion: aptInIn Updatad 1990 March 14 16:00.
    aptinln orlginated 1989 November 2 14:10.
Author: Arthur L. EdWards, LLNL, L.-298, Telophone (415) 422-4123.
Source{ xport read . 245100gaptisl1be/ 1/1
    1lb aptsllbalx aptbllbo aptInlnlend / 1 1.
    aptslibe Ls a LIB 1Ibrary of FORTRAN source flles.
    aptblibe ls a BUILD Llbrary of Gray-domplled binarlea.
```

Purposei To flnd, for atach of np sets of input data, the milnimum
distance dpmin between the 1 ine through the points
$a=(a x, a y, a z)$ and $b=(b x, b y, b z)$, and the IIne through
the polnts $c=(c x, c y, c z)$ and $d=(d x, d y, d z)$, and the
polnt $a=\mid \Theta x, e y, \quad b z)$ on llne "ab", and the point
$f=(f x$, $f y, f z$ on 11 ne "ad", at which the mindmum distance
dpmin occurs. If dpmin ls amaller than the estlmatad error $\ln$
its calculation, it wlll be truncatad to zero, and ltrun -1
wlll be returned.
Tho fractlonal distance fracab of polnt "e" along 11 ne "ab",
and the fract. Ional distance fraced of polnt "f" along line
"cd", are also returned.
If the llnes are paralld, lpar - 1 wlll be returned.
If a line seqment 1 s too short, Lpar $=2$, 3 or 4 wlll be
returned.
Hestory: 1990 March 14. Changed tol to 0.0 In call to unlt vertor
subrout.Ine. Allows small magnitudes.
Input: $\quad a x, a y, a z, b x, b y, b z, c x, c y, c z, d x, d y, d z, n p, t o l$.
Output: dpmin, fracab, fracod, ex, oy, ez, fx, fy, fz,
Itrun, Ipar, nerr.
Calls: aptivdls, aptvdot, aptvuna fources in aptsilbe,
binarles in aptbllbe).
Glossary:

$d x, d y, d z$ Input The second point on line segment "cd". Slze np.
ex, ay, ez Output. The $x, y, z$ coordinates of the point on line "ab"
nearest Ilne "cd". Size np.
$f x, f y, f z$ Output The $x, y, z$ coordinates of the polnt on line "cd"
nearest l.Ine "ab". Slze np.
fracab Output. Fractional distance of "e" along line "ab". Slze np.
Meaningless if lpar $\mathbf{m} 2$ or 4.
fraced Output Fractional distance of "f" along llne "ed", Slze np.
Meaningleus lf lpar $=3$ or 1.
Ipar Output 0 lfllnes are not parallel, 1 If they are, and
polnts "e" and "f", can be moved arbitiarily by
equal distances along the llnes, Size np.
2 if IIne segment "ab" is too short.
3 if ilne segment "ed" is t.oo shart.
4 If "ab" and "cd" are both too short.
Itrun Gutput 0 if dpmin not truncated to zero, based on tol.
1 If dpmin is truncated to zero, based on tol.
slze np.


| $\text { call apt } 1$ | pl (px, py, pz, sx, sy, sz, ax, ay, az, vnx, vny, vne, np, tol, dpmin, dint, fracps, qX, qu, qz, lpar, nerr) |
| :---: | :---: |
| Version: | aptlnpl Updated 1990 March 15 13:40. aptlnpl Orlginated 1989 November $214: 10$. |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100:aptalibe/11 <br> 1lb aptsilbelx aptbllbe aptinpllend / 11. <br> aptsilibe is a LIB library of FORTRAN source flles. <br> aptblibe is a BUILD library of Cray-complled blnarles. |
| Purpose: | To flnd, for each of np sets of input data, the point of Intersection of the 11 ne through points $p-(p x, p y, p z)$ and $s=(s x, s y, s z)$, with the plane through the point a. (ax, ay, az) with normal vector vn . (vnx, vny, vnz). The polnt of Intersection wlll be deflned hy ita distance dint from polnt "p", Its fractional distance fracps along the llne from "p" to "s", and Its coordinatess as (qx, qy, qz). <br> The perpendlcular distance dpmin from the plane to polnt "p" is also returned. <br> If point " $p$ " colnoldes with polnt "s", based on tol, the result wlll be the same as if line "ps" is parallel to the plane. If vector "un" is too short, based on tol, the result wlll be the same as if line "ps" lles in the plane. If 11 ne "ps" is parallel to the plane, lpar wlll be 1 . If, in addition, dpain is not zero, dint, fracps, and the coordinates of " q " wlll be very large. If the line is parallel to the plane and dpmin is zaro, then the line is in the plane, and dint and fracps w1ll be zero, and the coordinates of "q" Wlll be ( $\mathrm{px}, \mathrm{py}, \mathrm{pz}$ ). |
|  | Flag nerr indlcates any Input |
| History: | 1990 March 14. Changed tol to 0.0 in call to unit vector aubroutlne. Allows small magnitudes. <br> 1990 March 15. Changed results when vector "vn" is too short. Now gives name results as if line "ps" is In the plane. |
| Input : | $p x, p y, p z, s x, s y, s z, a x, ~ a y, ~ a z, ~ v n x, ~ v n y, ~ v n z, ~ n p, ~ t o l . ~$ |
| Out put: | dint, dpmin, fracps, cix, qy, qz, lpar, nerr. |
| Calls: | aptvadd, aptvdis, aptvdot, aptvuna, aptvunb (sources in aptsilbe, binarles in aptblibe). |
| Glossary: |  |
| $a x, a y, a z$ | Input. The $x, y, z$ coordinates of polnt "a" In the plane. slze inp. |
| dint | Output The distance of the polnt of Intersection "q" from point "p". Positive if in the same direction as that from "p" to "g", Size np. Meaningless if lpar is not zero. |
| dpmin | Output. The perpendlcular distance to polnt "p" from the plane. Positive if polnt "p" is in the same direction from the plane as the normal vector "vn". If less than the estimated error in its calculation, dpmin wlll be truncated to zero. size np, Meaningless if ipar $-2,3$, or 4. |
| fracps | Output. Fractional distance of polnt "q" along the llne segment from point "p" to polnt "g". Size np. May de negative or greater than 1. Maningless if lpar is not zero. |
| 1 par | Output 0 if the lifie lis not parallel to the plane, size np. <br> 1 If it ls. See dpmin, dint, fracps, $q x$, $q y, q z$. <br> 2 If line "pg" is too short, based on tol. <br> 3 If vector "vn" is too short, based on tol. <br> 4 If "ps" and "vn" are both too short, based on tol. |


| narr | Output | Indicates an input orror, if not 0 . 1 . 1 nip ls not positiva. |
| :---: | :---: | :---: |
| np | Input | Slze of arraya. |
| $p x, p y, p z$ | Input | The $x, y, a$ cooridinates of point " $p$ " on the $11 n e$. Must diffar irom "an, based on tol, slze np. |
| $q \times, q y, q z$ | Out put | The $x, y, z$ coordinatas of the polnt of intersection of the line thisough " $p$ " and "s" Wlth the plane through point "a" with normal vector "un". Meantngleas if lpar is not zero. |
|  | Input | The $x, y, z$ coordinates of point "s" on the line. Must differ frym "p", based on tol, size np. |
| tol | Input | ```Numerical tolaralice 11mbt. On Cray computhrs, recommend 1.e-5 to 1.e-11.``` |
| $v n x, y, z$ | Input | The $x, y, z$ compdnents of vector "vn" normal to the plane. Magnlthide must exceed tol. Slze np. |


| Varalona | $\begin{array}{lllll}\text { aptmaxw } & \text { Updated } & 1990 \text { January } 31 & 16: 30 . \\ \text { aptmaxw } & \text { Orlginated } \\ 1990 & \text { January } & 31 & 16: 30 .\end{array}$ |
| :---: | :---: |
| Authors: | Eugene H. Canfleld, LLNL, L-298, Talephone (415, 422-4125, Arthur L. Edwards, LLNL, 1,-298, Teleplione (413) 422-4123. |
| Source: | xport read . 245100 aptesilibe / 11 <br> Llb aptsllbelx aptblibe aptmaxwland / 11 , <br> aptalibe is a Lib llbrary of FORTRAN soufce flles. <br> apliblibe is a BUILD llbrary of cray-complied binarles. |
| Purpose: | To find, for aach of np spealfled temperaturas tgas, the relativistic veloolty functions beta and gamma, by sampling from a relativistio Maxwellian diatribution of partioles with a rest mass energy of erest (same unita as tgas). Flag nerr indicates any Input error. |
| Input: | t.gas, np, erest. |
| Out put: | beta, ganma, nerr. |
| Glossary: |  |
| beta | Output Ratio of particle veloolty to the speed of light, beta - v/a ( 0 - 2.997924580+08 $\mathrm{m} / \mathrm{s}$ ). Range is from 0.0 to $1 . \mathrm{Slze}=\mathrm{np}$. |
| erest | Input The rest mass of the particles (same units as toga). |
| ganma | Output Ratio of relativistic mass to particle rest mass garma $=$ sqrt (1.0 - beta**2). Range in from 0.0 to infinity. size np. |
| nerr | Output Indicates an Input error, if not zero. 1 if no ls not poaltive. |
| np | Input Slze of arrays tgas, beta, gamma, |
| tgas | Input Average particle tomperature (same unlts as arest). size np. |

## SUBROUTINE AETMEAN

| Varsion: | 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. |
| Sources | xport read . 245i00;aptsilibe / 11 <br> 11b aptallbelx aptblibe aptmeanlend / 11. <br> aptsilbe is a LIB library of FORTRAN source flles. <br> aptblibe la a BUILD llbrary of Cray-complled binarlas. |
| Purpose: | To find, for the no values of $x$, the mean value xmean and the standard deviation xdev of $x$ from xmean. <br> Flag nerr indicates any Input error. |
| Input: | $x$, np, tol. |
| out put: | xmean, xdev, nerr. |
| Glossary: |  |
| nerr | Output If not 0 , Indicates an Input error. 1 if np f not positive. |
| np | Input Slze of array $x$. |
| tol | Input Truncation error limit. On Cray computers, recommend 1.e-11. |
| $\times$ | Input A scalar value, Slze 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. |

## SUEROUTINE APTMOPV



## SUBRCUTINE APTMOVE



| 6 | usch, usth, usph, dpmove, np, tol, rho, cth, sth, aph, sph, urh, uth, uph, nerr) |
| :---: | :---: |
| Version: | aptmovs Úpdated 1990 March 14 16:00. aptmeys Originated 1989 December 417:00. |
| Aut hor: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100 aptslibe / 11 <br> llb aptslibelx aptblibe aptmovslend / 11. <br> aptsilbe is a LIB library of FORTRAN source flles. <br> aptblibe is a BUILD library of Cray-complled 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. <br> Any component of point " $p$ " or vector " $u$ " less than the estimatad error in its calculation, based on tol, will be truncated to zero. If tol $=0$, no truncation tests are done. Flag nery 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, ephs, sphs, usrh, usth, usph, dpmove, np, tol. |
| Out put: | rho, cth, sth, cph, sph, urh, uth, uph, nerr. |
| Calls: | aptvona (source in aptsilibe, binary in aptblibe). |
| Glossary: |  |
| cph | Output The cosine of the final value of phi fangle from the 2 axis). <br> May be truncated to zero, if less than the estimated numerical arror in their calculation based on tol. slze np. |
| cphs | Input The cosine of the initial value of phi. See uph. Slze np. |
| cth | Output The cosine of the final value of theta (angle in the xy plane counterclockwise from $x$ axis). <br> May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Slze np. |
| cths | Input The cosine of the initial value of theta. See cth. slze np. |
| dpmove | Input The distance from point "ps" to noint "p". sizenp. (Assuming vector "us" is a unit vector.) |
| nerr | Output Indicates an input error, if not 0 . Lif np is not positive. |
| np | Input Size of arrays. |
| rho | Output The spherical radial component of final poine "p". May be truncated to zero, if less than the estlmated numerical error in their calculation based on tol. Slze np. |
| rhos | Input . The spherical radial component of initial point "ps*. Slze np. |
| sphs | Input The sine of the inltial value of phi, See cph. size np. |
| sph | Output The sine of the final value of phi. See cph. <br> May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. slze np. |


| sths | Input | ```The sine of the inltial value of theta. See cth. Slze 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. Slze np. |
| t. 01 | 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 "un. May be truncated to zero, if less than the estlmated 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. Slzenp. |
| 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". Slze np. |
| usth | Input | The theta component of initial inlt 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 thelr calculation based on tol. See cth. slze no. |

## SUBROUTINE APTMPRD

call aptmprd (nrows, smati, smat 2, tol, smat, nerr)


|  | dpmove, np, tol, <br> pz, pr, eth, sth, uz, ur, ut, nerr) |
| :---: | :---: |
| Version: | aptmvey Updated 1990 March 14 16:00. aptrmvey Originated 1989 Decembar 4 11:00. |
| Author: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | ```xport read .245100;aptalibe / 1 1 lib aptslibe\|x aptblibe aptmvaylend/11. aptslibe is a LIB llbrary of FORTRAN source flles. aptblibe la a BuILD library of cray-complled binaries.``` |
| Purpose: | To find, for each of the np sets of input data, the new polnt $p=(p z, p r, c t h, ~ s t h)$ and unlt direstion vector $u=(u z, u r, u t)$, resulting from moving from the point $\mathrm{ps}=$ ( $\mathrm{psz}, \mathrm{psr}$, oths, sths) in the direction of the unit vector us - (usz, usi, ust) for a distance dpmove, in cylindrical coordinates. <br> If $\mathrm{kth}=0$, all cths -1.0 , all sths $=0.0$, and cth and sth will not be oalculated, and none need be dimensioned. Any component of polnt. "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 tents are done. Flag nerr indicates any input error. |
| History: | 1990 March 14. Changed tol to 0.0 in call to unlt vector subroutine. Allows small magnitudes. |
| Input: | kth, psz, psr, cths, sths, usz, usr, ust, dpmove, np, tol. |
| Output: | pz, pr, cth, sth, uz, us, ut, nerr. |
| Calls: | aptivina (source in aptsilbe, blnary in aptblibe). |
| Glossary: |  |
|  | Slzenp. |
| cth | Output The cosine of the final value of theta (angle in the xy plane counterclockwise from $x$ axis). <br> May be truncated to zero, if less than the estimated numerical error in their calculation based on tol. Size nd, if kth - 1. Otherwise, not calculated. |
| cths | Input The cosine of the initia! vilue of theta. See cth. Size np, if kth $=1$. Otierwise, scalar 1.0. |
| dpmove | Input The distance from point "ps" to point "p". size np. (Assuming vector "us" is a unit vector.) |
| kth | Input Indicates size of arrays cth, cths, sth, sths: <br> 0 If array size is 1 , with cths- 100 , sths $=0.0$, and cth and sth are not to be calculated. <br> 1 If array size is nh, input values of cths and sths will be used, and cth and sth will be calculated. |
| nerr | Output Indicates an input error, if not 0 . 1 if np is not positive. <br> 2 If kth is not 0 or 1. |
| np | Input Size of arrays. |
| pr, pz | Output The $r$ and $z$ components of final point "p". Size np. May be truncated to zero, if less than the estimated numerical error in thair calculation based on tol. |
| psr, psz | Input The $r$ and $z$ coordinates of initial point "ps", Slze np. |
| sths | Input The sine of the initlal value of theta. See cth. slze 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 thelr calculation based on tol. slze np, if kth - 1. Otherwise, not calculated. |


| tol | Input | Numerlcal tolerance limit. If zero, no tests done. On Cray computers, recommend $1 . e-5$ to 1.e日-11. |
| :---: | :---: | :---: |
| ur | Output | The $r$ component of final unit direation vector "u". May be truncated to zero, if less than the estimated numerical error in thelr calculation based on tol. slze np. |
| usir | Input | The r component of inftial unit direction vector "us". Slze np. |
| ust | Input. | The theta component of initial unit direction vector "us". See ath. Slze np. |
| usz | Input | The 2 component of inftial unit direction vector "us". |
| ut | Out put | The theta component of final unit direction vector "u". May be truncated te zero, $1 f$ less than the est Imated numerlcal error in their calculation based on tol. See cth. Slze np. |
| 4 z | Out put | The $z$ component of final unlt direction vector "u". Slze ny. |

## SUBROUTINE APTPLPL



| Ex, fy, zz | output | The $x, y, z$ coordinates of the polnt on the line of interseation of planes "a" and "aN nearest polnt "a" Maaninglass, but point "a", Li lpar la not 0. |
| :---: | :---: | :---: |
| dpmin | Out put |  Otherwise, zero. Slze np. |
| Ipar | Output | Indicatien relative orlentation of planes "an and " $\mathrm{CN}^{\prime \prime}$ : <br> 0 If the planas intersect. <br> 1 If the planes are parallel, based on tol. <br> 2 If veotor "b" is too short, based on tol. <br> 3 If veator "d" is too short, based on tol. <br> 4 if vectorn "b" ard "d" are both too ahort. <br> orlentation is indeterminate if lpar - 2, 3 or 4. sizenp. |
| Itrun | Out put | If 1, Indicates planes are parallel and colncidant. Slze np. |
| nerr | Output | Indicates an input error, if not 0 . 1 1f np is not positive. |
| tol | Input | ```Numerical tolerance 11mit. On Cray computers, recommend 1.e-5 to 1,0-11.``` |
| ux, uy, uz | Out put | The $x, y, z$ components of the unit vector parallel to the line of intersection of planes "a" and " c ", lf lpar = 0. Meaningless, but parallel to the IIne "ac" if lpar is not zero. Slze np. |



| raph | Input | The radlum of the sphere ounterod at polnt "p" Slze np. The abmolute value la uad. |
| :---: | :---: | :---: |
| tol | Input | Numerloal toleranae 11 mlt . <br> On Cray domputers, recommand $1, a-5$ to $1, a-1$ |

## SUGROUTINE APTTPLLC



Author: Arthut L. fidwards, LLNL, L-298, Telephone (419) 422-4123.
Source: xport raad . 245100 iapliallbe $/ 11$
11b aptilibelx aptblibe aptptiolund / 11.
aptalibe in a LIE libitary of FORTRAN source flles, aptblibe la a BUito library of Craymompllad blnarles.

Purposen to ilnd, for anoh of fib ata of input data, the minimum distance dpmin from the point po ( $p u, p v$ ) to the atralght line thrnugh
 the uv plane. Dlraotions $u, v$ and $w$ are orthogonal.
opt ion noptifd allowa the eraotional diatance fdmiln of the proximal polnt along i. Ine "ab" to be oalculated, and allows the range of tamin to be 11 mlted . Flag nl 1 Indicates when such 1 Imitation has beem 1 mposed. If $111 \mathrm{~m} m 2$, dpmin 1 s the distance from poldit "p" to the nearast and of line a $a$ gmant "ab".

The value of dpmin w1ll be truncated to zero if less than the antimated arror in Its calaulation, based on tol, and if so, itrun - 1 wlll be returned.

If the pointe "a" and "b" colnolde, based on tol, dpmin will be the distance from point "a" to point "p", and if dpmin is not zaro, ltrun wllise-1.

Flag nerr Indlcates any 1 nput error.
History: 1990 Fobruary 12 15120. Added Input argument noptifd, optlonal output arguments $\mathfrak{f d m} \mathrm{n}, \mathrm{nllm}$.

Input: $p u, p v, a u, a v, b u, b v, ~ n p, ~ t o l, ~ n o p t i f d . ~$
output: dpriln, famln, nllm, ltrun, nerr.
Calla: aptfdav, apteaxa, aptvalo, aptvdoo (sources in aptallbe, binarles in aptblibe).

## Glossary:

| $a u, a v$ | Input | The $u$ and $v$ coordinates of polnt "an on llne "ab". slze np. All polnta are in the uv plane. |
| :---: | :---: | :---: |
| bu, bv | Input | ```The u and v coordinates of polint "b" on 1lna "ab". slze np.``` |
| dpmin | Out put | Distance from polnt "p" to the lina "ab". Size np. Truncated to zero if less than the est imated error In its calculation, based on tol, and if so, Itrun - 1 wlll be returned. <br> If pointe "a" and "b" are colnoident, dpmin is the diatance from point " $p^{\prime \prime}$ to polnt. "a", and ltrun $=-1$ Is raturned, unlasa dpmin - o.0. If noptid la 2 , and famin la indtially not in the rango from 0.0 t.0 1.0 , dpmin is the diatance from point "D" to the nearest of pointes "am and "b", and nilm - 2 is returned. <br> The value of dpmin ds positive, if point "p" is to the left of the vector "ab" in the uv piane, |
| famin | Out.put, | Fractional distance between polnt "a" and polint "b" of the point nearest polnt "p". See noptid. Slze np, if noptifd is not -1 . |
| 1t.run | Out put | 0 1f dpmin is not truncaced to zero. Slze np. <br> 1 If dpmin la truncatad to zero, when less than its est Imated error, based on tol. <br> -1 If dpmin la not zero, and polntes "a" and "b" colnclde, based on tol. |


| nerr | output | Indloates an Input error, if not 0 . <br> 1 If np la not poaltiva. <br> 2 If nopt fd la not $-1,0,1$, or 2 . |
| :---: | :---: | :---: |
| n11m | output | 0 If no limit imposed on tomin, 1 if the limit of noptifd - 1 In 1 mposed, $21 f$ the 1 Imlt of noptifd $=2$ Ls imposed, siza np, if noptifd is not -1. If 2 , dpmin la the distanoe from point "p" to the nearest and of llne gegment "ab". |
| nopt fd | Input | Option to limlt range of idmin: o for no 1 Imlt <br> -1 to not caldulate $t$ dmin or nilm. <br> 0 to $I I n d$ Idmin, but impose no limlts. <br> 1 to Incrase fdmin to tol, if In the range from -tol to tol, and decrease edmin to $1.0-\mathrm{tal}$, If In the range from $1.0-$ tol to $1.0+$ tol. <br> 2 to impose the $1 / \mathrm{mlta}$ for nopt $\mathrm{fd}-1$, and then $11 \mathrm{mlt} \mathrm{fdm} / \mathrm{n}$ to the range from 0.0 to 1.0 , and adjust the magnitude, but not the sign of dpmin If the later limit 1 is imposed. |
| np | Input | Slze of arrays pu, pv, au, av, bu, bv, itrun. <br> If noptid is not -1 , the aize of arrays fdmin, nilm. |
| pu, pv | Input | The $u$ and $v$ coordinates of point "p". Slzen np. |
| tol | Input | Numarlcal tolerance limit. <br> On Cray computers, recommend $1,0-5$ to 1.e-11. |

## SUBROUTINE APTPTLN

```
oald aptptin (px, py, pz, ax, ay, az, bx, by, bz, np, tol,
6
noptfd, dpmin, fdmin, ax, ay, dx, n11m, itrun, nerr)
Version: aptptin Updatad 1990 February 14 10:00.
    aptptin Orlginated 1989 Novamber 2 14:10.
Author: Arthu% L, Edwards, LLNL, L-298, Telephone (415) 422-4123.
Source: xport read . 245100:aptislibe / 1 1
    llb aptsllbelk aptblibe aptptinlend / 1 1.
    aptsllbe is a LIE Llbrary of FORTRAN source flles.
    apthlibe 1s a BUILD llbrary of Craymompllad binarles.
```

Purpose: To flnd, for ach of np sets of input data, the minimum distance dpmin from the point $p=$ (pu, py, pzi to the stralght line through the polnts $a=\langle a x, a y, a z)$ and $b=(b x, b y, b z\rangle$, to IInd the coordinates $a-(c x, o y, c z)$ of the proximate polnt on Ifne "ab", and to find the fractional diatance fdmin of that point along the 1lne segment "ab". The value of dpmin will be truncated to zero if legs than the estimated error In its caldulation, based on tol, and if so $1 t r u n-1$ will be returned. Flag nerr indloates any input error.

Option nopt fd allows the line "ab" to be treated as a finfte segment, by 1 imiting the range of fimin. Flag nlim indicates when such IImitation has beem imposed.

If the points "a" and "b" colncide, based on tol, dpmin will be the distance from point "a" to point " $p^{*}$, and if dpmin is not zero, ftrun will be -1.

History: 1990 February 12 16:00. Fixad bug affeoting fdmin when np 18 greater than 64.

Input: $\rho x, p y, p z, a x, a y, a z, b x, b y, b z, n p, t o l$, nopt fd.

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

Glossary:

| $a x, a y, A z$ | Input | The $x, y, z$ coordinates of point "a" on line "ab". Slze np. |
| :---: | :---: | :---: |
| $b x, b y, b z$ | Input | The $x, Y, z$ coordinates of point "b" on line "ab". Slze np. |
| cx, cy, cz | Out put | The $x, y, z$ coordinates of the polnt on the llne "ab" neareat point "p". Polnt "p" if' dpmin = 0. Slze np. |
| dpmin | Out put | Distance from point "p* to the line "ab". Size np. Truncated to zero if lesa than the estimated error In its calculation, based on tol, and if so, torun - 1 wlll be returned, Perpendicular distance, unless itrun $=-1$, or $n l l m=2$. |
| famin | Out put | Fractlonal distance between point "a" and point "b" of the point ${ }^{N} c^{M}$, Size np. |
| Itrun | Output | 0 If dpmin is not truncated to zero. 1 If dpmin is truncated co zero, when less than its est Imated error, baged on tol. Size np. -1 $1 f$ dpmin is not zero, and points "a" and "b" colnclde, based on tol. |
| nerr | Out.put | ```Indlcates an Input error, if not 0. l If np ls not positive. 2 If noptfd is not 0, 1, or 2.``` |
| n.11m | Out put | 0 if no limit imposed on fanin, 1 if the 11 mlt of noptifd - 1 is imposed, 2 if the 11 mlt of noptid $=2$ Is imposed. Slze np. <br> If the latter 1 lmit. $1 s$ Imposed, dumin will be the distance from point "p" to the nearest end of the IIne segment. |


| nopt fd | Input | Option to 1 imit range of $\operatorname{fdmint} 0$ for no 1 lm 1 t ; <br> 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 famin to the range from 0.0 to 1.0 . |
| :---: | :---: | :---: |
| $n p$ | 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. <br> On Cray computers, recommend $1 . e-5$ to $1 . e-11$. |


| Version: | aptptpl Updated 1990 March 15 11:50. <br> aptptpl Originated 1989 November 2 14:10. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100:aptslibe / 11 <br> lib aptslibe!x aptblibe aptptpllend/11. <br> aptsilibe is a LIB library of FORTRAN scurce fles. <br> aptblibe is a surid library of Cray-complied binaries. |
| Purpose: | To find, for each of np sets of input data, the minimum distance dpmin to the point $p=(p x, p y, p z)$, from the plane through the point a - (ax, ay, az) with nomal vector $b-(b x$, by, bz), and the coordinates $c=(c x, c y, c z)$ of the point in the plane nearest point "p". <br> Flag itrun indicates truncation of dpmin to zero (1) or t.oo small a magnitude of vector "b" (2): <br> 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: | px, py, pz, ax, ay, az, bx, by, bz, np, tol. |
| Out put : | dpmin, cx, cy, cz, itrun, nerr. |
| Calls: | aptvadd, aptvdis, aptvdot, aptvunb (sources in aptsilibe, binaries in aptblibe). |
| Glossary: |  |
| ax, ay, az | Input The $x, y, z$ coordinates of point "a" in the plane. slze np. |
| bx,by,bz | Input The $x, y, z$ components of vector "b" normal to the plane. Magnitude must exceed tol. S.lze np. |
| cx, cy, cz | Output The $x, y, z$ coordinates of the point in the plane nearest point "p". Sizenp. <br> Returned as point "p" if normal vector "b" is too short, based on tol (1trun - 2). |
| dpmin | Output The perpendicular distance co point "p" from the planc 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 (1trun-1). Returned as zero if normal vector "b" is too short, based on tol (1trun-2). |
| Itrun | Output Indicates a special result for one data set: <br> 1 If the valiue of dpmin is truncated to zero, when less than the estimated error in its calculation, based on tol. <br> 2 If normal vector "b" is too short, based on tol. The orlentation 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. |
| np | Input size of arrays. |
| 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 APTCDIC

| 4 | pu, pv, np, tol, <br> pab, pbc, pod, pda, dpmin, nerr) |
| :---: | :---: |
| Version: | aptqdic Updated 1990 February 21 11:00. aptqdic Originated 1990 February 21 11:00. |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100:aptslibe/11 <br> lib aptslibe!x aptblibe aptqdiclend / 11. <br> aptslibe is a LIB library of FORTRAN source flles. <br> aptblibe is a BUILD library of Cray-complled binarles. |
| Purpose: | To find, for each of the np sets of input data, the distances pab, pbc, pcd and pda from the point $p=(p u, p v)$ to the sides of the quadrangle with vertices a - $(a u, a v), b-(b u, b v)$, $c=(c u, c v)$, and $d-(d u, d v)$, in counterclockwise order in the uv plans, and the minimum dpmin of pab, pbc, ped and pda. The values of pab, pbc, pcd and pda will be truncated to zero, if less than the estimated error in thelr calculation, based on tol. Flag nerr indicates any input error. |
| Input: | au, av, bu, bv, cu, cv, du, dv, pu, pv, np, tol. |
| Out put : | pab, pbc, ped, pda, dpmin, nerr. |
| Calls: | aptptlc (source in aptslibe, binary in aptblibe). |
| Glossary: |  |
| au, av | Input The $u, v$ coordinates of vertex "an of the quadrangle. slze np. |
| bu, bv | Input The $u, v$ coordinates of vertex "b" of the quadrangle. Slze np. |
| $\mathrm{cu}, \mathrm{cv}$ | Input The $u, v$ coordinates of vertex " $c^{n}$ of the quadrangle. size np. |
| dpmin | Output Minimum of absolute values of distances pab, pbc, pcd and pda. slze np. |
| du, dv | Input The $u, v$ coordinates of vertex " $d^{*}$ of the quadrangle. Slze np. |
| nerr | Output Indicates an Input error, if not 0 . 1 if np is not positive. |
| np | Input $S$ ize of arrays $p u, p v, a u, a v, b u, b v, c u, c v, d u, d v$, pab, pbc, pcd, pda. |
| pab | Output Distance from point "p" to quadrangle side "ab". Truncated to zero, if less than the estimatederror in its calculation, based on tol. Absolute value. |
| 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. Absolute value. |
| ped | Output Distance from polnt "p" to quadrangle side "cd". Truncated to zero, if less than the estimated error in fts calculation, based on tol. Absolute value. |
| 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. Absolute value. |
| $p u, p v$ | Input The $u$ and $v$ coordinates of point " $p$ " in the uv plane. Slze np. |
| tol | Input Numerical tolerance limit. On Cray computers, recommend l.e-5 to 1.e-11. |

## SUGROUTINE APTOFDC



## SUBROUTINE APTQINC



| 'nloc | output | Indicates the location of point "p" relative to the quadrangle "abcd": <br> -1 If all quadrangle vertices colncide. <br> 0 if point. "p" is outside the quadrangle mabcd", or is inside, but the quadrarigle vertices were specifled in clockwise order, or $1 f$ ktype $=-1$, is inside a bowtie or in certaln areas inside a boomerang. <br> 1 if point "p" is inside the quadrangle mabod", and elther all four distances pab, phe, ped and pda are non-negative, or if ktype $=0,1$ or 2 , the quadrangle is a poomerang or bowtle and the distances pass specific tests. |
| :---: | :---: | :---: |
| np | Input | Size of arrays $p u, p v, a u, a v, b u, b v, c u, c v, d u, d v$, pab, pbc, pcd, pda. |
| ntype | I/O? | Shape type of quadrangle. Input if ktype -2 . Output if ktype $\mathbf{m} 1$. Size np $1 f$ ktype $=1$ or 2. 0 if quadrangle is convex. <br> 11-14 1f quadrangle has just one concave vertex at point "an, "b", "c", of "d", resp. (a boomerang). 21-24 If quadrangle has just two तdjacent concave vertices at ends of sides "cd", "da", "ab", or "bc", respectively (a bowtle). |
| pab | Out put | Distance from point "p" to quadrangle side "ab". Truncated to zero, if less than the estimated errar in its calculation, based on tol. |
| pbc | Out put | Distance from point " $D$ " to quadrangle side "bc". Truncated to zero, if less than the estimated error in its calculation, based on tol. |
| ped | Out put | 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 polnt "p" to quadrangle side "da". Truncated to zero, if less than the estimated error in its calculation, based on tol. |
| pu, py | Input | The $u$ and $v$ coordinates of point " $p$ " In the uv plane. \$1zenp. |
| tol | Input | Numerical tolerance limit. <br> On Cray conputers, recommend 1.0 .5 to $1 . e-11$. |

## SUBROUTINE APTQLOC



root 1 Output The first or only real root, $1 f$ (nroota. ge. 1).
root 2 Output The second real root, if (nroots .eq. 2).
tol Input Numerlaal toleranad 11 m 1 t .
Must not be zero if nopta $=1$ On Cray oomputers, recommend $1 . e-5$ to $1 . \theta-11$.

## SUBROUTINA APTRQRTV


for np set's of coofflelonts aa, bb, ac.
The solution is vactorlzed over the sots of coefficlents, which are calculated in sections of 64 for less, for the flnal section).
The method minlmizes truncation error, and Indlcates when truncation error may still be signiflcant, based on tol. Option noptg allows the user to speclify the value of $\mathrm{qq} \times \mathrm{bbac}^{2}-4.0$ * aa coc, fnatead of using the value calculated here.

Note: aptqrts is a scalar version of aptqriv.
History: 1990 January 19 15:00. Flxad bug for a $=0.0$ or $b=0.0$ 1990 March 21 14:00. Changed to allow truncation of small positive qa to zero.

1 nput: noptq, aa, bb, cc, qq, np, tol.
Output: $q$ q, nroots, root1, root2, itrun.
Glossary:

| a a | Input. | Coefficlonts of $x * * 2$ In a quadratic equation, Sizen mp. |
| :---: | :---: | :---: |
| bb | Input. | Coefflclenta of $x$ In a quadratic aquation. size np. |
| cc | Input. | Coefficlents of 1 In a quadratic equation. slze np. |
| 1trun | Out put | Truncition error Indicator. 0 if lnsigndilcant. |
|  |  | 1 If the magnitude of $q 9$ is less than the estimatod truncation error, based on tol. This fidicates that the roots are near a minlmum or maximum, or that the quadrat.lc is almost the square of a llnaar function. The value of $q q 1 s$ truncated to zero. <br> 2 If the input value of $q q$ (noptq-1) differs from the calculated value by more than the estimated truncation error, based on tol, Slze np. |
| nerr | Output | Indicates an input error, if not 0 . i if np ls not positive. |
| noptq | Input | Option for getting value of $4 q=b b * 2-4.0 * a a * c c:$ 0 to not use input qq, but calculate from aa, bb, co. 1 to use the input value of qq (more accurate). A nonzero value of tol must be used with thls opt lon, for comparision of the input with the calculated value. |

-1 If ( $\{a$, eq, 0,0 ) , and, (bb, eq, 0,0)).
Equation is null (oc , eq. 0.1 or bad (ce, ne. 0.).
0 If (bb**2.1t. 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 1f (bb**2 .gt. 4,0* aa* cc).
SIzenp.

| 49 | Input | If noptq-1. Equal to qq - bto**2-4.0 * aa * oa, but. calculatiad more accurately, due to cancollation of terma reaulting from the compoalte nature of da, bb, and/or do. slaenp, |
| :---: | :---: | :---: |
| $q 9$ | Output | If noptq $=0$, Equal to $4 q \times b b * 2-4.0 * a * 0 a$, calculated locally. $81 z \mathrm{ng}$. |
| root 1 | Output | The flest or only real root, if (nroots, ge. 1). Sluenp, root 2 Output The gecond real root, lf (nroota, eq, 2), slzenp. |
| tol | Input | Numerlual tolerance 11 mlt . <br> Must not be zero if napta $m 1$. <br> On Cray computera, recommend 1,e-5 to 1,a-11. |

## SUGROUTINE ASTCNAD

| aall aptc | ad $\left(p x_{1} d y, p x_{1} a x_{1} a y_{1} a x_{1} b x_{1} b y_{1} b y_{1}\right.$ $a x_{1} \sigma y_{1} a z, d x_{1} d y_{1} d z_{1}$ noptef, tol, dpmin, edka, fdla, $q x_{1}$ gy, qu, nllmk, ndiml, Itrun, nalda, noon, nerry |
| :---: | :---: |
| Varalon: | aptquad Updated 1989 Novamber 2916110. aptquad Crlglnated 1909 Novamber 2 141:10. |
| Authars | Arthur L. Edwarda, LLNL, L-298, Telephone (415) 422-4123. |
| Souras | xport ratad .2491001apta11be / 11 <br> Ilb aptellbelx apthllbe aptquadlend / 11. <br> aptallbe is LIE libraty of FORTANN source flles. <br> aptblibe 1 a a $\quad$ 日UlD 1 lbrary of Cuyy-compllad binarlas. |
| purpose: | To Ind the minimum diatance dpmin from the exterinal point $p=$ ( $p x$, $p y, p z$ ), to the aurfaco bounded by a 3-D quadrarigle with verticas $(a x, a y, a z),(b x, b y, b z),(a x, a y, a z),(d x, d y, d z) y$ to flnd the point $q=(q x, q y, q z)$ on the surface nearest the external polnt: and to I nd the fractlonal distances fdkq and fala of that polnt between opposite sides of the quadrangle. Opt lon nopt id allowa the ranger of fdkg and fdla tio ba 11 mlted . neault and ercor flags are returnad. |
|  | The equation of the surface ( $b, a, b, a, d$ are vectora) 1 a ; $\begin{aligned} & r=a+(b-a) \\ &(a-b+a-d k+(d-a) *\{d\}+ \\ &(d) \end{aligned}$ |
|  | $\begin{aligned} r \times a *(1-f d k) *(1 \cdots(d)) & +b *\{d k *(1-f d d)+ \\ & +d *(1-f d k) *(d) \end{aligned}$ |
|  | Where $r$ 1a vector $(x, y, z)$, and $f d k$, $f d$ are fractional diatances betwaen opposite edges. |
| Mathods | Uses functional fteration, tangent plane approximation, and acoeleration. The rate of convergenae depends on the problem. For 2 Initilal values of fdk, lteratively find fdt nearast the external polnt, the best fdk for that $\mathbb{i d l}$, eto. If two minima are feund, use the least value of dpmin. |
| Input: 1 | $p x, p y, p z, a x, a y, a z, b x, b y, b z, c x, \quad c y, \quad z z, d x, d y, d z$, tol. |
| Out put: | dpmin, fdkq, fdiq, qx, qy, qz, nlimk, nllmi, itrun, nside, ncon, narr. |
| Callsi | aptrciad, aptptin, aptptpl, aptudis, aptupln (sources in aptsilbe, blnarles in aptb!! (ha). |
| Glossary: |  |
| $a x, a y, a z$ | Input The $x, Y, z$ coordinatea of quadrangle vertex ${ }^{\text {Kan }}$. |
| bx, by, bz | Input The $x, y, z$ coordinates of quadrangle vertex "b". |
| cx, cy, cz |  |
| $d x, d y, d z$ | Input The $x, y, z$ coordinates of quadrangle vertex "d". |
| dpmin | Gutput. Minimum distance from point $p m$ ( $p x$, $p y, p z$ ) to the surface bolinded by the edges of the 3-D quadrangle whth vertlces (ax, ay, az), (bx, by, bz), (cx, cy, cz) and (dx, dy, dz). |
| fdka | Output fractional distance of the point $q$ - (qX, qy, qz) batween opposite edges of the quadrangle, from the edge bounded hy (ax, ay, az) and (dx, dy, dz). A value of exactly 0.0 or 1.0 may Indicate actual minimum polnt outside quadrangle, Values withln inal of 0.0 or 1.0 may be shifted slightiy inside quadrangle, See nllmk. |


| fala | Out put | Fractional diatance of the point $q$ - (qx, $q y, q z)$ batween oppoalte adges of the quadrangle, from the edge bounded by (ax, ay, az) and (bx, by, bx). A value of exactly 0,0 or 1.0 may Indloate actual minimum polnt outalde quadrangla. Values withln tol of 0.0 or 1.0 may be shlfted allghtly fralde quadrangle. See nilml. |
| :---: | :---: | :---: |
| 1 Itrun | Out put | 0 If no ohange is made in the calaulatiod value of domin, 1 If dperin is changed to zero, when less than the estimated error in fte calculation. |
| neon | Output | Error flag. <br> 1 or 2 if flrst two guasses fall to converge. <br> 3 for total fallure to find solution. |
| narr | output | Indicates an Input error, if not 0 . 1 is added if noptifd is not between 0 and 2. |
| n11mk | Output | 0 If faka not adjusted. <br> 1 It near 0.0 or 1.0 , shifted inalde quadrangle. <br> 2 If outside range 0.0 to 1.0 , shlfted to 0.0 or 1.0 . |
| n11ml | Output. | 0 If ediq not adjusted. <br> 1 Lf near 0.0 or 1.0 , shlfted inside quadrangle. <br> 2 Lf outalde range 0.0 to 1.0 , shifted to 0.0 or 1.0 . |
| nopt fid | Input | Option to limit the ranges of fdkq, fdlas <br> 0 for no limlt, <br> 1 to Increase to tol, if in the range from -tol to tol, and dearase to 1.0 - tol, If In the range from 1.0 - tol to $1.0+$ tol (move a polint near ant adge slightly finside the quadrangle), and <br> 2 to 11 mlt to the range from 0.0 to 1.0 (move a polnt outalde the trlangle to an edge). |
| nalde | Out put. | 1 If the polit. neareat $p=(p x, p y, p z)$ in the extended surface through the quadrangle in actually $q-(q x, q y, q z)$, within tolerance tol. 0 If $q$ - ( $q x$, qy, qz) le only the polnt on the edges of the quadrangle nearest ( $p x$, py, pzi, but the vector connecting " $p$ " to " $q$ " is not: normal to the surface. |
| $p x, p y, p z$ | Input | The $x, y, z$ coordinates of the external polnt "p", |
| $q x, q y, q z$ | Out put. | The $x, y, z$ coordinates of the polnt ${ }^{N} q^{n}$ nearest to $p=(p x, p y, p z)$ on the blquadrat!c surface. |
| t.01 | Input | Numerlcal tolerance limlt. Convergence oriterion for dpmin. On Cray computera, recommend 1.e-5 to 1.e-11. |

## gUGROUTINE APTGVAC

call aptqVad (au, av, bu, bv, ou, ov, du, dv, np, tol, nopt,

4
arpa, arpb, arpa, arpd, ntype, qu, qV, nerri

| Varston: | aptquad | Updatad | 1990 |  | bruary |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | aptquac | Orloinated | 1990 |  | bbruary |  |  |

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Sourca: xport read . 245100 iaptalite / 11
IIb aptallbelx aptbilba aptquacland / 11.
aptalibe ls a LIB library of FORTPAN source files.
aptbliba 1 a BUIDD llbrary of Cray-complled blnarles.
Purpose: To flnd the shape and slze of np quadrangles In the uv plane, with vertlaes $a=\left(a u_{1} a v\right), b=(b u, b v), a=(a w, a v)$ and $d=$ (du, dv) counterclorkwlse around the quadrangle, Opt lonally (nopt 0 or 2), the vertex parallelogram areas arpa, arpb, arpo and arpd will bu returned, and (nopt -2 or 2) the number and location of any concave (negative area) vertices wlll ba returned, encoded in ntypa, and if the quadrangle is a bowtle, the Intersection of the sides $q$ - (qu, qu), will be returned. The nat area of the quadrangle is
0.25 (arpa + arpb + arpo + arpd).

Flag nerr lidicates any lnput error.
Input $\quad a u, a v, b u, b v, d u, c v, d u, d v$, np, tol, nopt.
Out put: ntype, arpa, arpb, axpo, arpd, nerr.
Cal1s: aptivdic, aptvaxc
$\quad$ (sources in aptsilbe, binarles In aptbllbe).

## Glossary:

| arpa | Output | Parallelogram area at vertex Ma" (nopt $=0$ or 2). Size np. |
| :---: | :---: | :---: |
| arpb | Output | parallelogram araa at vertex "b" (nopt - 0 or 2 ). Slzenp. |
| arpe | Out put | ```Parallelogram area at vertex "CN (nopt m O or 2). Slze np.``` |
| a rpd | Out put | Parallelogram area at vertex "d" (nopt -0 or 2). Size np. |
| $a u, a v$ | Input | The $u$ and $v$ coordinates of vertex " $a^{\prime \prime}$ of quadrangle. Slze np. |
| bu, bv | I nput | The $u$ and $v$ coordinatas of vertex "b" of quadrangle. Slze np. |
| cu, CV | Input | The $u$ and $v$ coordinates of vertex ${ }^{m "}$ of quadrangle. Size np. |
| du, dv | Input | The $u$ and $v$ coordinates of vartex ${ }^{n} d^{\mu}$ of quadrangle. Slze np. |
| narr | Out put. | Indleates an 1 nput error, if not 0 . <br> 1 If np is not positive. <br> 2 If nopt 1 s not 0,1 or 2. |
| nopt | I nput: | ```Output optIon: O or 2 to return vertax parallelogram areas. 1 or 2 to return shape type gode ntype. 2 to return areas, ntype, and bowtle intergectloris``` |
| $n \mathrm{p}$ | Input | Slze of arrays $a u, a v, b u, b v, c u, c v, d u, d v$, and if nopt - O or 2, arpa, arpb, arps and arpd, and If nopt $=1$ or 2, ntype. |


| ntype | Out put | Shape type of quadrangle (nopt $=1$ or 2). <br> 0 if all vertices are convex. Regular. <br> 11 If only vertex "a" is concave. Boomeratig. <br> 12 If only vertex "b" is concave. Boomerang. <br> 13 If only vertex "c" is concave. Boomerang. <br> 14 If only verter "u" is concave. Boomerang. <br> 21 If only vertices " $\mathrm{c}^{\prime}$ and "d" are concave. <br> Bowtie. <br> 22 if only vertices "d" and "a" are concave. Bowtie. <br> 23 if only vertices "a" and "b" are concave. Bowtie. <br> 21 if only vertices " $b$ " and " $c$ " are concave. Bowtie. <br> 31 If only vertex "a" is convex. Inverted boomerang. <br> 32 if only vertex "b" is convex. Inverted boomerang. <br> 33 If only vertex." $c^{\prime \prime}$ is convex. Inverted boomerang. <br> 34 If only vertex "d" is convex. Inverted boomerang. <br> 40 if all yertices are concave. Inverted regular. |
| :---: | :---: | :---: |
| qu, qv | Output | 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. <br> On Cray computers, recommend 1.e-5 to 1.e-11. |

## SUBROUTINE APTREFC



SUBROUTINE APTREFL


## SUBROUTINE APTREFS



## SUBROUTINE APTRKCL



SUGROUTINE APTRKCY


| $n \mathrm{p}$ | Input | Slze of arrays pz, pr, uz, ur, ut, az, ar, bz, br, dintmn, dintmx, nint, pinz, plinr. |
| :---: | :---: | :---: |
| pinr | Output | Cylindrical radial $r$ coordinate of intersection point. Slzenp. |
| pinz | Out put. | ```CyIIndrical axial z coordinate of intersection point. Slze 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 cyilndrical 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 counterclockwlse from $x$ axis. Slze np. |
| uz | Input | Initial axial $z$ component of unit direction vector along track. Size np. |
| tolf | Input | Truncation error limit to imposed on the fractional distance of the intersection (pinz, pinr) along the line segmant 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. |
| t.01s | Input | Truncation error limit to be imposed on uz, ut and pinr. Magnitudes of ut and uz less than tols whll be increased to tols. Values of pinr less than tols * pr will be increased to tols * pr. On Cray computers, recommend $1 . e-5$. <br> A value of zero may produce unpredictable results. |



Author: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
Source: kport read .245100:aptslibe / 11
Ilb aptillbelx aptblibe aptrklslend/id.
aptsllbe is a LIE library of FORTRAN source files. aptbllbe is a BUILD llbrary of Cray-complled blnaries.

Purpose: To find, for each of np sets of Input data, the distance dint to the intersection $q .(q x$, $q y, q z)$ of the linear tiack through polnt $p=(p x, p y, p z)$ with direction vector $v=(v x, v y, v z)$, and the general second order surface for whlch the equation is


```
    axx "x**2 + ayy* y**2 + azz* z**2 = = 0
```

and for which dint is between dintinn and dintmx. If two such Intersections occur, the one with the smaller magndtude of dint wlll be returned, if no such intersection is found, nint will be 0 , and dint and the coordinatee of point "q" wlll be very large. Flag nerr indlcates any input error.

The vector normal to the surface is $s=(d f / d x, d f / d y, d f / d z$. The sign of the direction of the Intersection is determined by the dot product $v * s$.

History: 1990 March 14. Changed tol to 0.0 in call to unlt vector subroutine. Allows small magnitudes.
Input: $\quad \mathrm{x}, \mathrm{py}, \mathrm{pz}, v \mathrm{x}, \mathrm{vy}, v z$, $a c, a x$, $a y, a z$ axy, ayz, azx, axx, ayy, azz, dlntmn, dintmx, np, tol.

Output: nint, $q x, q y, q z, d i n t$, nerr.
Calls: aptqrtv, aptvadd, aptvunb (sources in aptslibe, blnarles in aptblibe).

Glossary:

| a. | Input | ```Coefflclents 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. <br> Positive lf in the same direction as vector "v". Acceptable only if between dintmn and dintmx. |
| dintmn | Input | The minimum allowable value of dint. |
| dint.mx | Input | The maxlmum allowable value of dint. |
| nerr | Out.put. | Indicates an input error, if not 0 . 1 If np is not positive. |
|  |  | 1 If the track through polnt "p" in direction " $v$ " Intersects the surface at a distance dint between dintme and dintmx. <br> 0 If no such intersection was found. <br> -1 If vector "v" is too short, based on tol. |
| $n \mathrm{p}$ | Input | Stze of arrays. |
| $\mathrm{px}, \mathrm{py}, \mathrm{pz}$ | Input | The $x, y, z$ coordinates of polnt " $\mathrm{P}^{\prime}$ ". |
| $q x, q y, q z$ | Output | The $x, y, z$ coordinates of the point of intersection of the line through point "p" with unit direction vector ${ }^{*} V{ }^{\prime \prime}$, and the surface, if nint $=1$. |

## vx, vy,vz Input The $x, y, z$ components of direation vector "v".

 If the magnitude is too small, nint will be -1 .tol Input Numerical tolerance 11 mlt .
On Cray computers, recommend $1 . e-5$ to 1.e-1.1.

## SUBROUTINE APTRKLC

| $4$ | dintmn, dintmx, np, tol, <br> nint, eu, ev, dint, nerr) |
| :---: | :---: |
| Verston: | aptrklo Updated 1990 Maroh $1416: 00$. <br> aptrkio orlginated 1990 January 11 15:10. |
| Author: | Arthur L, Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100;aptslibe / 11 <br> 11b aptalibelx aptiblibe aptrklolend / 11. <br> aptsilibe if a LIB library of fORTRAN source flles. <br> aptblibe is a BUILD llbrary of Cray-oomplled binaries. |
| Purpose: | To find, for each of the np sets of Input data, any Iritersection polnt e- (eu, ev) of the linear track through polnt a - (au, av) with the direction vector ab-(abu, abv), and the 11 ne scgment from point $\mathrm{a}=(\mathrm{au}, \mathrm{av})$ to point $d$ - (du, dv), all in the uv plane of uvw space, for which (1) the distance from point "a" to point. "s" is beeween the IImits dintmen and dintmx, (2) point. "e" is between point "c" and "d", and (3) the track crosses line "cd" from left to right in the uv plane. This is a zone exit if the points " $\mathrm{cm}^{\prime \prime}$ and "d" are the vertioes of a zone edge, counteraloakwise around the zone in the uy plane. Flag nint indicates the type of Intersection found. The distance dint of the interseation from point "a" is also returned. <br> Flag nerr indicates any input error. |
| Hilstory: | 1990 March 14, Changed tol to 0.0 In call to unit vector subroutine. Allows small magnitudes. |
| Input: | au, av, abu, abv, cu, ov, du, dv, dintmn, dintimx, nn, tol. |
| Out put : | nint, eu, ev, dint, nerr. |
| Calls: | aptfdav, aptvadc, aptvaxc, aptydio, aptrubc (sources in aptsilibe, binaries in aptblibe). |
| Glossary: |  |
| au, av | Input The $u$ and $v$ coordinates of point "a". Slze np. In the uv plana. |
| abu, abv | Input The $u$ and $v$ components of 2-D ditection vector "ab". Must not both be zero. Slze np. |
| $\mathrm{cu}, \mathrm{ev}$ | Input The $u$ and $v$ coordinates of point "c" in the uv plane. Must differ from "d", based on tol. Slze np. |
| $d u, d v$ | Input The $u$ and $v$ coordinates of point ${ }^{\prime \prime} d^{H}$ in the $u v$ plane, Must differ from "c", based on tol. Size np. |
| dint. | Output The distance of the point of intersection "e" from polnt "a". Positive if in the same direction as vector "ab". Sizenp. |
| dintimn | Input Minimum allowed value of distance to intersection. size np. |
| dintmx | Input. Maximum allowed value of distance to intersection. slze np. |
| eu, ev | Output The $u$ and $v$ coordinates of the polnt of Intersection of the 1ine through point "a" With direction vector "ab", and line "od", all in the uv plane. |
| nerr | Output Indicates an input error, if not 0 . 1 if np ls not positive. |
| nint. | Output Number of acceptable intersections found. 0 if none. <br> 1 If an acceptable intersection was found. <br> 2 If the track colncides with part of line "cd". |
| np | Input Slze of arrays. |
| tol | Input Numerlcal tolerance limit. On Cray computers, recommend 1.e-5 to 1.e-11. |

## SUBROUTINE APTRKPL



| $\mathrm{px}, \mathrm{py}, \mathrm{pz}$ | Input | The $x, y, z$ coordinatee of politi "p". |
| :---: | :---: | :---: |
| $q x, q y, q z$ | output | The $, x, y, z$ coordinates of the point of interseation of the line through polnt "p" with unlt direotion vactor "v", and the plane through polnta "a", How. and "a", if tpar *O. Slze np. <br> Meaningluss, but large if Ipar w 1. <br> Maanlnglass, but zaro $1 f$ lpar $-2,3$ or 4. |
| vx,vy,vz | Input | The $x, y, z$ componanta of direotion vector "v". |
| tol | Input | Numerlcal tolarince 11 mlt . On Cray aomputera, recommend $1,0.5$ to $1, a-11$. |

## SUBROUTINE APTRKRL




## SUBROUTINE APTRNDS



## SUBROUTINE APTROTA



SUBROUTINE APTROTC
call aperoto (au, av, bu, bv, cu, cv, np, tol, nerr)


| - |  |
| :---: | :---: |
| Version: | aptrotp Updated 1989 March 14 16:00. <br> aptrotp Originated 1989 November 2 14:10. |
| Aut hor: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100:aptslibe/ 11 <br> 1lb aptslibe!x aptblibe aptrotplend/21. <br> aptsilibe is a LIB library of FORTRAN source files. <br> aptblibe is a BUILD library of Cray-compled binaries. |
| Purpose: | To find the rotation matrix operator rotm, for rotating the plane containing the vectors a m (ax, ay, az) and $b-(b x$, by, bz) to be parallel to the plane contalning the vectors $c=(c x, c y, c z)$ and $d=(d x, d y, d z)$, around an axis parallel to both planes. Any components of rotm within tol of $-1.0,0.0$, or 1.0 , w111 be truncated to those values. Flag nerr indicates any input error. |
| Higtory: | 1990 March 14. Changed tol to 0.0 in call to unit vector subroutine. Allows small magnitudes. |
| Input: | $a x, ~ a y, ~ a z, ~ b x, ~ b y, ~ b z, ~ c x, ~ c y, ~ c z, ~ d x, ~ d y, ~ d z . ~$ |
| Output : | rotm, nerr. |
| Cal1s: | aptvaxb, aptvuna, aptvxun (sources in aptsilibe, binaries in aptblibe). |
| Clossary: |  |
| ax,ay;az | Input The $x, y, z$ components of a vector. |
| $b x, b y, b z$ | Input The $x, y, z$ components of a vector. |
| $\mathrm{cix}_{\mathrm{x}} \mathrm{cy}, \mathrm{cz}$ | Input The $x, y, z$ components of a vector. |
| $d x, d y, d z$ | Input The $x, y, z$ components of a vactor. |
| nerr | Output Indicates an input error, if not 0. <br> 1 If the magnitude of any input vector is too small, or the twa vectors in a plane are almost parallel. |
| rotm | Output Rotation operator (a unitary $3 \times 3$ matrix). Must be sized rotim(3,3). |
| tol | Input Numerical tolerance ilmit. Used to test and adjust unit vector components and point coordinates. On Cray computers, recommend $1 . e-5$ to $1 . e-11$. |

## SUBROUTINE APTROT'S



## 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'ly. Ectwardy, LINL, I-298, Telephone (415) 422-4123.
Source: xport react , 45)00;apt,0libe / 1 1
    I1b aptirim!x luptbilbe aptrottlend / 2 1.
    aptslibe'{s a tris ld%rary of FORTFAN source flles.
    aptblibe ls a Bulld liprary of Craymcompiled binarles.
Purpose: To find the rotation matrlx operator rotm, for rotating the
    vector a = (ax, ay, az) and the plane containlng vectors "a" and
    b - (bx, by, bz), to be parallel to vector c - (cx, cy, cz) and
    the plane containing vectors "c" and d m (dx, dy, dz).
    Any component.s of rotm within tal of -1.0, 0.0, or 1.0,
    wlll be truncated to those values.
    Flag nerr indlcates any I nput error
    If vectors "a" and "b" are the llrat two vectors of the positive
    vector triple (a,b, a x b), and c and d are the flrst two
    vectors of the positive vector triple (c, d, c x d), then rotm
    rot.ates (a, b, a x b) onto (c, d, c x d), or equlvalently,
    redefinas the coordinate axes to be (a, b, cx d) instead of
    (c, a, c x d). (a x b indlcates the vector product of a and b.)
H1story: 1990 March.24. 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: rotm, nerr.
Calls: aptvxun, aptvunb (sources in aptslibe
    binaries in aptblibel
Glossary:
```



```
rotm Output Rotation operator (a unitary 3 x 3 matrix)
    Must be sized rotm(3,3).
tol Input Numerical colerance 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: aptrotv Updated 1990 March 14 16:00.
        aptrotv Origlnated 1989 November 2 14:10.
Author: Arthur L, Edwarás, LLNL,, L-298, Telephene (415) 422-4123.
Source: xport read . 245100:aptslibe / 1 1
    llb aptsilbelx antblibe aptrotvlend / 1 1.
    aptslibe is a lim library of FORTRAN source flles.
    aptblibe is a BUILD library of Cray-complled binarles.
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,
    wlll be truncated to those values.
    flag nerr Indlcates any input error.
HIstory: 1990 March 14. Changed tol to 0.0 In call to unlt 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\mathrm{ components of vector "a".
bx,by,bz Input The }x,y,z\mathrm{ components of vector "b".
nerr' Output Indicates an input error, if not 0.
    1 If the magnilude 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
    unft vector components and polnt coordinates.
    On Cray computers, recommend 1.e-5 to 1.e-11.
```


## SUBROUTINE APTSCAD



## SUBROU'SINE APTSCAP

| Version: | aptscap Updated 1990 January 10 10:30. <br> aptscap Originated 1990 January 10 10:30. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 42'-4123. |
| Source: | xport read .245100:aptsllbe / 11 <br> lib aptsilbelx aptblibe aptscaplend/'11. <br> aptslibe is a LIB library of FORTRAN source flles. <br> aptblibe is a BUILD llbrary of cray-complled binarles. |
| Purpose: | To flnd np unit vectors b = (bu, bv, bw), representing random directions in a cosine""pm distitibution in 3-D space, centered on an axis in the direction of vector a = (au, av, aw), with the restirlctions that the magnitudes of the components be no smaller than the speclfled limits tolu, tolv, tolw, respectively. Flag nerr indlcates any input error. <br> If "ba" Is the expected value of the component of vector "b" In the direction of vector "a", then: $\begin{aligned} & \mathrm{ba}=(\mathrm{pm}+1.0) /(\mathrm{pm}+2.0) \text {. (ba .ge. } 0.5) . \\ & \mathrm{pm}=(2.0 \text { ba }-1.0) /(1.0-\mathrm{ba}) \text { (pm.ge. } 0.0) . \\ & \mathrm{pm}=0.0 \text {. 1sotropic in half-space. } \\ & \mathrm{pm}=1.0 \text { cosine distribution in halt-space. } \end{aligned}$ |
| Calls | aptmopv, aptrotv, apt.vilm. <br> (sources In aptsilibe, binarles in aptblibe). |
| Input: | np, tolu, tolv, tolw, au, av, aw, pm. |
| Out put : | bu, bv, bw, nert. |
| Glossary: |  |
| $a u, a v, a w$ | Input The $u, v$ and $w$ components of a vector in the direction of the center of a cosine**po distribution. |
| bu | Output The u component of a undt vector reprosenting 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 foordinates. Slze np. Magnitude may be no smaller than tolu: |
| bv | Output. The $v$ component of a unlt vector representing a direction chosen randomly from a cosine* "pm distribution in 3-D space, centered in the direction of vectior "a". Coordinates $u, v$ and $w$ may be any 3 orthogonal coordinates. Size np. Magnitude may be no smaller than tolv. |
| DW | Output The w component of a unlt 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, slze np. Magnitude fay be no smallar than tolw. |
| nerr | Output Indleates an inpit error, if not 0. 1 If np is not positive. |
| np | Input Slze of irrays. |
| pm | Input Power used for the cosinen"pm spatial distribution from which undt vector "b" is to be chosen. |
| tolu | Input Minimum magnitude of all bu components. On Cray computers, recommend 1.e-5. |
| tolv | Input Minimum magnit.ude of all bv components. On Cray computers, recommend 1.e-5. |
| colw | Input Minimum magnitude of all bw components. On Cray computers, recommend $1, e-5$. |

call aptscat (np, au, av, aw, nerr)


## SUYROUTINE APTSCLC

| Versions | aptscia Updated 1990 March 14 16:00. aptscic orlolnated 1990 January $\$ 15: 00$. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | ```xport read . 245100;aptsilbe;111 llb aptallbelx aptblibe aptsalalend / 1 1. aptslibe is a LIB library of FORTRAN source Illes. aptiblibe is a BuILD library of Cray-complled binarles.``` |
| Purpose: | To Ilnearly scale the np polnts or vactors <br> $p-(p u, p v)$ by the factor "geale", In the direction of the vector a " (au, av), with the polnt $b=(b u, b v)$ invarlant. <br> All are in the uv plane. If $p=$ ( $p u, p y$ ) are unbound vectors, Invarlant point "b" must be at the origin. <br> This is the spatial part of a Lorentz transformation. <br> Flag nerr indicates any input error. |
| History: | 1990 March 14. Changed tol to 0.0 In call to unlt vector subroutine. Allows small magnltudes. |
| Input: | scale, au, av, bu, bv, pu, pv, np, tol. |
| Output : | pu, pv, nerr. |
| Calls: | aptrube (source in aptslibe, blnary in aptblibe) , |
| Glossary: |  |
| au, av | Input The $u$ and $v$ components of the uv plane vector defining the direction of linear scalling. |
| bu, bv | Input The $u, v$ coordinates of the uv plane invariant point. |
| nerr | ```Output- Indicates an input error, if not 0. l if np is not positive. 2 If the magnitude of vector "a" la too mmall, relative to tol.``` |
| np | Input. Slze of arrays pu, pv. |
| pu, pv | In/Out. The $u$ and $v$ coordinates of a point, or components of a vector I the uv plane. Slze np. |
| tol | Input. Numerical tolerance limit. Used to test and adjust unlt vector, matrix element, and polnt components. <br> On Cray computers, recominend $1 . e-5$ to $1 . e-11$. |

## sueroutine aprscll



## SUGROUTINE APTSCLI



Gall aptsild (xa, pa, xb, pb, np, xran, nerr)
Vorsion: aptsild Upthted 1990 Fabruary 111000. aptalld Orlglnatod 1990 fabruary 2 14:10

Authors Arthur L. Edwards, LLNL, L-298, Telaphone (415) 422-4123.
Source: xport raad . 2451001aptalibe / 11
1lb aptslibelx apthlibo aptslidland / 11
aptslibe li a LIB HLIrary of FORTRAN source flles.
aptblibe is a BUItD Library of Cray-comilled binarles.
Purpose: To flnd np values of $x$, by sampling from a linear dlatrlbut lon function having probabllity pa at $x a$, and probabllity pb at $x b$ Flag narr indleatos any Input error.

If both pa and pb aro rion-nogative, tho expocted value of $x$ is $\langle x\rangle=f a$ xa $f(f b \quad x b$; Where $f a=(2.0 * p a+p b) /(3.0 *(p a+p b))$ and $\mathrm{fb}=(\mathrm{pa}+2.0$ * pb$) /(3.0 *(\mathrm{pa}+\mathrm{ph}))$.

If pa is negative, and pb is positlve, thon nerr 3 no values of $x$ W1ll be ampled between $x a$ and $x a{ }^{\prime}=(x a-p b-x b$. $\mathrm{pa} /(\mathrm{pb}-\mathrm{pa})$, and $\langle x\rangle=f a^{\prime}$ * $x a+f b^{\prime}$ * $x b$ Where $f a^{\prime}=p b /(3.0 *(p b-p a))$ and $\mathrm{fb}=(2.0 * \mathrm{pb}-3.0 \cdot \mathrm{pa}) /(3.0 \cdot(\mathrm{pb}-\mathrm{pa}))$

If pa 1 s positive, and pb ls negat: lve, then nerr $=3$, no values of $x$ will be sampled betwoen $x b$ and $x b^{\prime}=(x b$ a $p a-x a$ - $p b) /(p a-p b)$, and $\langle x\rangle=f a^{\prime}$ * $x a+f^{\prime}$ * $x b$, Where fa' = (2.0 * pa-3.0 * pb) / (3.0 * (pa - pb) and $f b^{\prime}=p a /(3.0 *(p a-p b))$.

If both pa and pb aro non-positlve, chen nerr $=2$, and no valuas of $x$ will be amplad.

History: 1990 February 5 13:20. Modlflad to ellminate sampling from any range of $x$ with negat ive probabllity.

Input: $\quad x a, p a, x b, p b, n p$,
Output: xran, nerr

| Glossary: nerr | Out put | Indlates an lnput error, if not 0 . <br> 1 li np is not positive. <br> 2 If both pa and ph are non-positive. <br> No $x$ values are sampled. <br> 3 If elther pa or po is negative, and the othor is positive. Values of $x$ are sampled only from the positive part of the probabllity distilbution. |
| :---: | :---: | :---: |
| $n \mathrm{n}$ | Input. | Slze of array xran. |
| pa, po | Input | Relat lve probabllitles of random varlables $x a$ and $x b$, respectively, Probablilty $p(x)$ is linear in $x$. The values of pa and pb nead not be normalized. If nelther pa nor pb $1 s$ positive (nurr - 2), no values of $x$ will be sampled. If elther pa or pb is negat.Ive, and the other is positive, (nerr m 3), $x$ values will only be sampled from the posit.ive part of the probabllity distribution. To $f 1 n d$ pa and $p b$, when $\langle x\rangle$ ls glven: $x \text { xna }=(2.0 \cdot x a+x b) / 3.0$ <br> $x m b=\langle x a+2.0 * x b\rangle ; 3.0$. <br> For $\langle x\rangle$ between $x a$ and xma, $p b 1 s$ negative, and: $\mathrm{pb}=-((x \mathrm{ma}-\langle x\rangle) /(\langle x\rangle-x a))$ * pa. <br> For $\langle x\rangle$ betweon tina and $x m b$ : <br> $(\langle x\rangle-x m a)^{n} p a=(x m b-\langle x\rangle)$ "pb. <br> For <x> betwean xmb and $x b$, pa is negat $\mid v o$, and: $p a=-(\langle\langle x\rangle-x m b) /(x b-\langle x\rangle))$, pb. |
| $x a, x b$ | Input: | Values of random varlable $x$ with relat lve probllitiles pa and pb , respectively. |
| *raņ | Out put | Randomly sampled value of $x$ In range from xa to xh , Slzo np. |

## SUBROUTINE APTSLIV

call aptsilv (xa, pa, $x b, p b, n p, x r a n$, nerr)


## SUBROUTINE APTSPSP




| call apttloc lau, av, bu, bv, cu, cv, np, tol, 6 fdk, fdl, pu, pv, nerr) |  |
| :---: | :---: |
| Version: | apttloc Updated 1970 February 8 14:30. |
|  | apttioc Originated 3 990 February 8 14:30. |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . $245100:$ aptsllbe / 11 |
|  | lib aptslibe!x aptblibe apttloclend / 11. |
|  | aptslibe is a LIB library of FORTRAN source files. |
|  | aptblibe is a BUILD library of Cray-complled binaries. |
| Purpose: | To find np points $p=(p u, p v)$, by sampling from a undform distribution over the triangle in the uv plane with vertices $a=(a u, a v), b=(b u, b v), c=(c u, c v)$, in any order around the triangle. |
|  | Varlables fdk and fdl are the local coordinates in the triangle. For any polnt $p=$ ( $p u, p v$ ) in the triangle: |
|  | pu m $a u+f d k$ * (bu - au) + fdk * fdl * (cu - bu) |
|  | $p v=a v+f d k$ * (bv-av) + fdk * fdl * (cv-bv) |
|  | $f \mathrm{dk}=(\mathrm{l}-\mathrm{a}) \mathrm{x}(\mathrm{c}-\mathrm{b})) /(\mathrm{b}-\mathrm{a}) \mathrm{x}(\mathrm{c}-\mathrm{b})$ ) |
|  | $f d l=-((p-a) \times(b-a)) /((p-a) \times(c-b))$, |
|  | 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 distribulion for fok and fdl is: |
|  | $\operatorname{prob}(\mathrm{fdk}, \mathrm{fd} 1)=\mathrm{fdk}$ |
|  | which is linear for fak, unlform for fdl. |
|  | Flag nerr indicates any input error. |
| Input: | au, av, bu, bv, cu, cv, np, tol. |
| Out put: | fdk, fdi, 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. |
| bu, bv | Input. The $u$ and $v$ coordinates of vertex "b" of triangle. |
| $\mathrm{cu}, \mathrm{cv}$ | Input The $u$ and $v$ coordinates of vertex " $c$ " of triangle. |
| nerr | Output Indicates an input error, if not 0 . 1 if np is not positive. |
| np | 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 i .0 to 1.0 . Size np. |
| fdl | Output Fractional distance of point "p" between the triangle sldes "ab" and "ca". Range 0.0 to 1.0 . slze np. |
| pu, pv | Output Sampled point p. Size np. |
| tol | Input Numerical tolerance limlt. |
|  | On Cray computers, recommend 1.e-5 to 1.e-11. |

## SUBROUTINE APTTRAC

| Version: | apttrac Updated 1990 March 13 11:30. apttrac Orlginated 1990 January 4 12:00. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | ```xport read .245100:aptslibe / 1 1 lib aptslibe!x aptblibe apttrac!end / 1 1. aptslibe is a LIB library of FORTRAN source flles.s. aptblibe is a BUILD library of cray-complled binmries.``` |
| Purpose: | To translate the origin to the 2-D point $a=(a u, a v)$, by subtracting the vectior "a" from the np 2-D points $\mathrm{p}=(\mathrm{pu}, \mathrm{pv})$. 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. |
| Out put: | pu, pv, nerr. |
| glossary: |  |
| nerr | ```Output. Indi :ates 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). |
| t. 01 | Input Numerlcal tolerance limit. On Cray computers, recommend $1 . e-5$ to $1 . e-11$. |
| pu, pv | In/Out The $u$ and $v$ coordinates of 2-D polnt " $p$ ". Size np. <br> Truncated to zero if smaller than the est.dmated error in thelr calculation, based on tol. |

## SUBROUTINE APTTRAN

```
call apttran (ax, ay, az, px, py, pz, np, tol, nerr)
Version: apttran Updated 1990 March 13 11:30.
    apttran Origlnated 1989 November 2 14:10.
Althor: Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123.
Source: xport read .245100:aptslibe / 1 1
    lib aptsllbe!x aptblibe apttran!end / 11.
    aptslibe 1s a LIB llbrary of FORTRAN source flles.
    aptbllbe is a BUILD library of Cray-complled binaries.
Purpose: To translate the origin to the polnt a = {ax, ay, az)
        by subtracting the vector "a" from the np polnt.s
        p m (px, py, pz). New coordinates less than the estlmated error
        In their calculation, based on tol, wlll be truncated to zero.
        Flag nerr indicates ary Input error.
Input: ax, ay, az, px, py, pz, np, tol.
out put: px, py, pz, nerr.
```

```
glossary:
nerr Output Indlcates an Input error, if not o.
    1 if np is not positive.
                            2 If the magnitude of (ax, ay, az) is no greater than
                tol.
np Input Number of points (px, py, pz).
tol Input Numerlcal tolerance limit.
    On Cray computers, recommend 1.e-5 to 1.e-11.
px,py,pz In/Out The }x,y,z\mathrm{ coordinates of point "p". Size np.
    Truncated to zero If smaller than the estimated
    error in their calculation, based on tol.
```

| call aptt $\&$ $\&$ | 1p ( $p x, p y, p z, a x, a y, a z, b x, b y, b z$, <br> cx, cy, cz, noptfd, tol, <br> dpmin, fda, fdb, fdc, $x m i n, y m i n, z m i n$, nlima, nlimb, nlitnc, itrun, nside, nerr) |
| :---: | :---: |
| Version: | apttrip Updated 1990 January 18 14:20. <br> apttrlp Originated 1989 November 2 14:10. |
| Aut hor: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read .245100:aptslibe / 11 <br> lib aptsllbelx aptblibe apttriplend / 11. aptslibe is a LIB library of FORTRAN source flles. aptblibe is a BUILD library of Cray-compiled binarles. |
| Purpose: | To find the distance dpmin from a point $p=(p x, p y, p z)$. to a plane defined by the three points $a=(a x, a y, a z)$, $b=\langle b x, b y, b z\rangle$, and $c=(c x, c y, c z\rangle$, and the point rmin $=(x m \ln , y m\\|n, z m\\| n$ nearest to point $p$, and in the plane, subject to constraints that may be imposed by option nopt fd and the value of tol. |
|  | Opt Ionally, to find the fractional distances (fda, fdb, fdc) of point rmin along the trlangle's altitudes. <br> Flags nlima, nlimb, nlime indlcate when fda, fdb, fdc have been restrained. Flag itrun indicates when dpmin has been truncated to zero. Flag nside indicates when the minlmum point is inside the trlangle. Flag nerr indicates any input error. |
| Input: | $a x, a y, a z, b x, b y, b z, c x, c y, c z, p x, p y, p z, ~ t o l$. |
| Out.put: | $d p m i n, f d a, f d b, f d c, x m i n, y m i n, z m i n$, nlima, nlimb, nllmc, itrun, nside, nerr. |
| Cal1s: | aptfdad, aptpt $1 n$, aptvdis, aptvpin (sources in aptslibe, binarles in aptblibe). |
| Glossary: |  |
| $a x, a y, a z$ | Input The $x, y, z$ coordlnates of point "a". |
| bx, by, bz | Input The $x, y, z$ coordinates of point "b". |
| cx, cy, cz | Input The $x, y, z$ coordinatas of point "c". |
| dprin | Output Distance from point "p" to the nearest (constralned) point in the platle defined by points "a", "b", "c". a value less than the estlmated error in its calculation is truncated to zero (itrun = 1). dpmin is positive when the external point is on the slde 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". |
| $f d b$ | Output Fractional distance of point (xmin, ymin, zmin) from side "ca" to vertex "b". |
| fdc | Output Fractional distance of point ( $x \mathrm{~m} / \mathrm{n}, \mathrm{ym} / \mathrm{n}, \mathrm{zm} \mathrm{m} \mathrm{n}$ ) from slde "ab" to vertex "c". |
| 1trun | Output 0 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 . <br> 1 is added if nopt fd is not between 0 and 2 . <br> 2 is added if 3 polnts representing triangle are colinear or congruent. |
| nl1ma | Output 0 if no limit imposed on fda, 1 if the limit of nopt fd $=1$ is imposed, 2 if the 1 lml t of nopt $\mathrm{fd}=2$ is imposed. |
| nlimb, c | Output Like rilma, but for fdb, fdc, respectively. |


| nopt fd | Input | Option to 11 mit range of fda, $f d b$ fdc: <br> -1. for no limit, no calculation of fda, fedb, fdc, <br> 0 for no limlt, <br> 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 polnt near an edge slightly inslde the trlangle), and <br> 2 to 11 mit to the range from 0.0 to 1.0 (move a polnt outside the triangle to an edge). |
| :---: | :---: | :---: |
| nside | Out put | 0 If minimum point outside the triangle, 1 if inside. 0 if moved to edge, when nopt fd $=2$. |
| $\mathrm{px}, \mathrm{py}, \mathrm{pz}$ | Input: | The $x, y, z$ coordinates of point "p". |
| tol | Input | Numerlcal tolerance limit for dpmin, fda, fdb, fdc. On Cray computers, recommend $1 . e-5$ to $1 . e-11$. |
| $x m 1 n$ | Out put | The $x$ coordinate of $p t$ in plane nearest point "p". May be constralned by option noptfd. |
| $y \mathrm{~min}$ | Out.put | The $y$ coordinate of pt in plane nearest point "p". May be constralned by option noptif. |
| zmin | Out put | The $z$ coordinate of $p t$ in plane nearest point. "p". May be constrained by option noptif. |

## SUBROUTINE APTVADC




## SUBROUTINE APTVANC



## SUBROU"'INE AP'TVANG

| Version: | aptvang Updated 1990 March 14 16:00. aptvarig Orlginated 1990 January 5 12:10. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LiNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read .245100:apts.libe / 11 <br> lib aptslibelx aptblibe aptvanglend / 11. <br> aptslibe is a LIB library of FORTRAN source flles. <br> aptblibe is a BUILD llbrary of Cray-complled binaties. |
| Purpose: | To flnd t : - cosine costh of the angle between the pair of vectors $a=(a x, a y, a z)$ and $b=(b x$, by, bz), for ach of $n p$ sots of input data. The value of costh wlll 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. |
| Out put. | costh, nerr. |
| Calls: | aptvdoc, aptvunb (sources 1 l aptslibe, binaries in aptblibe). |
| 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. Slze np. |
| costh | Output Cosine of the angle between the vectors "a" and " L ". Will be truncated to zero, if less than the estlmated error in its calculation, based on tol. |
| nerr | Output. Indicates an input error, if not 0. $l$ lf np is not positive. |
| $n \mathrm{n}$ | Input size of arrays ax, ay, $a z, b x, b y, b z$, costh. |
| t. 01 | Input Numerical tolerance 11 mlt . On cray computers, rerommend $1 . e-5$ to $1 . e-11$. |



## SUBROUTINE AFTVAXC

| Version: | $\begin{array}{lllll}\text { aptvaxc } & \text { Updated } 1990 \text { January } 18 & 16: 40 . \\ \text { aptvaxc } & \text { Originated } & 1989 \text { November } 2 & 14: 10 .\end{array}$ |
| :---: | :---: |
| Aut hor: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422.4123. |
| Source: | ```xport read .245100:aptslibe / 1 1 lib aptslibe!x aptblibe aptvaxc!end / 1 1. aptslibe is a LIB library of FORTRAN source flles. aptblibe is a BUILD library of Cray-complled -binaries.``` |
| Purpose: | To find the vector products cw of the $\mathrm{np} 2-\mathrm{D}$ vector pairs $a=(a u, a v)$ and $b=(b u, b v)$. 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, $c w=a u$ * $b v-a v * b u$. |
| Input: | $a u, ~ a v, ~ b u, ~ b v, ~ u p, ~ t o l . ~$ |
| Output: | cw, nerr. |
| Glossary: |  |
| $a u, a v$ | Input The $u$ and $v$ component.s of input vector "a". Size np. The $w$ components are zero. Directions $u, v$ and $w$ are orthogonal. |
| bu, bv | Input The $u$ and $v$ components of input vector "b". stze $n p$. The $w$ components are zero. |
| cW | 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. <br> Equal to the area of the parallelogram with sides "a" and "b". <br> 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 $a u, a v, b u, b v, c w$. |
| tol | Input Numerical tolerance limit. <br> On Cray computers, recommend l.e-5 to 1.e-11. |


| Version: | $\begin{array}{lll}\text { aptvdic } & \text { Updated } 1990 \text { March } 7 \text { 17:00. } \\ \text { aptvalc } & \text { Orlginated } 1989 \text { December } 29 \quad 15: 50 .\end{array}$ |
| :---: | :---: |
| Author: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | ```xport read . 245100:aptslibe / 1 1 1lb aptslibe!x aptbllbe aptvdic!end / 1 1. aptslibe is a LIB llbrary of FORTRAN source flles. aptbllbe 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 $a=(a u, a v)$ to point $b=(b u, b v)$, and its magnitude dab, the distance from "a" to "b", all In the uv plane. Directions $u, v$ and $w$ are, orthogonal. <br> Any component of vector "d" less than the estimated error in Its calculation, based on tol, wlll be truncated to zero. <br> Flag nerr indicates any input error. <br> With no truncation, (du, $d v)=(b u, b v)-(a u, a v)$, and distance dab $=\operatorname{sqrt}\left(d u * * 2+d v^{* * 2}\right)$. |
| Input : | $a u, a v, b u, b v$, np, tol. |
| Output: | du, dv, dab, nerr. |
| Glossary: |  |
| $a u, a v$ | Input The $u$ and $v$ coordinates of point "a". Slze np. The $w$ coordinates are zero. Directions $u, v$ and $w$ are orthogonal. |
| bu, bv | Input The $u$ and $v$ coordinates of point. "b". Slze np. The $w$ coordinates are zero. |
| $d a b$ | Output Distance between points "a" and "b", equal to the lengt.h of $2-D$ vector $d m$ (du, dv). May be truncated to zero, if less than the estimated error In its calculation. See tol. Size np. |
| $d u, d v$ | Output The $u$ and $v$ components of 2-D vector "d". Size np. <br> The $w$ coordinates are zero. <br> 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. |
| $n p$ | Input The size of arrays $a u, a v, b u, b v, d a b, d i s, d v$. |
| tol | Input Numerical tolerance 11 mlt . Used to truncate the components of $2-D$ vector $d=(d u, d v)$. On Cray computers, recomuend 1.e-5 to 1.e-11. |




## SUBROUTINE APTVDOC



## SUBROUTINE APTVDO'T



## SUBROUTINE APTVLIC

| Version: | apt.vilc Updated 1990 January 18 14:20. aptvilc orlginated 1990 January 3 13:40. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (115) 422-1123. |
| Source: | ```xport read .245100:aptsllbe / 1 1 1lb aptslibelx aptblloe aptvllolend / 1 1. aptsllibe is a LIB llbrary of FORTRAN source flles. aptblibe is a folld library of Cray-compllod blnarios.``` |
| Purpose: | To adjust the np 2-D vectors a $=$ (au, av), by 1 mposing the lower llmats tolu and tolv on the magnltudes of the components au and av, respectively, while retalning the indtal magnitude of the vector "a". If all are inltlally zoro, tho output vector "a" wlll be zero, and vien wlll bd zero. Flag nerr indicates any 1 nput error. |
| Input: | au, av, np, tolv, tolv. |
| out.put: | au, av, vlen, nerr. |
| Glossary: |  |
| $a u, a v$ | Input. Tho $u$ and $v$ components of Input vector "a". slan np. Dlrections $u, v$ and $w$ are orthogonal. |
| au, av | Output The $u$ and $v$ components of output vector "a". Slze np. Magnitudes wlll be at least tolu, Lolv, respectively, subject to the requilrement that the flnal magnitude of vector "a" be the same as tho Inltial magnitude. |
| nerr | Output Indicates an Input error, it not 0. 1 lf np is not positive. |
| np | Input Size of arrays au, av, vien. |
| tolu | Input Numerical tolerance 11 mlt for component au. On Cray computers, recommend $1,0-5$ to 1.e-11. |
| tolv | Input Numerical tolerance 11 mlt for component av. On Cray computers, recommend $1 . e-5$ to $1 . e-11$. |
| vien ( $n$ ) | Output Magnitude of vector "a". |


| version: | aptvilm Updated 1990 January 18 16:40. aptulim orlgifated 1989 December 1913:40. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | xport read .245100:apts11be / 11 <br> lib aptslibelx aptblibe aptvilmlend / 11. <br> aptsilibe is a Lifs llbrary of FORTRAN source filles, <br> aptblibe is a BUID library of Cray-complled blnaries. |
| Purpose: | To adjust the np vectors a - (au, av, aw), by imposing tho lower limits tolu, colv, and tolw on the magnitudes of the components au, av, and aw, respectively, whlle retalning the inltial magnltude of the vector "a", If all are inltially zoro, the output vector "a" wlll be zero, and vlen wlll be zaro. flag nerr indicates any input error. |
| Input: | $a u, a v, a w, ~ n p, ~ t o l u, ~ t o l v, ~ t o l w . ~$ |
| Out put : | au, av, aw, vlen, nerr. |
| Gilossary: |  |
| au, av, aw | Input The $u, v, w$ components of input vector "a". slze np. |
| au, av, aw | Output. The $u, v, w$ components of output vector "a". Size np. Magnitudes wlll be at least tolu, tolv, tolw, respectively, subject to the requiroment 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. |
| nip | Input size of arrays au, av, aw, vien. |
| tolu | Input Numerical tolerance 1 Imlt for component au. On Cray computers, recommend l.e-5 to 1.e-11. |
| tolv | Input Numerical tolerance 11 mlt for component av. On Cray computers, recommend 1.e-5 to 1.e-11. |
| colw | Input Numerical tolerance limit for component aw. On Cray computers, recommend l.e-s to $1 . e-11$. |
| vien (n) | Output Magnltude of vector "a". |

## SUBROUTINE APTVPLC

```
call aptvplc (au, av, bu, bv, np, tol, cu, cv, vlon, nerr)
Varsion: aptvplc Updated 1990 March 13 11:30.
    aptvplc Orlglnated 1989 December 28 13:20.
Authur: Arthur L. Edwards, LLNL, L,298, Telephone (415) 422-4123.
Source: xport read .245100:aptsllbe / 1 1
    11b aptslibelx aptbllbe aptvplclend / 1 1.
    aptslibe ls a LIB llbrary of FORTRAN source flles
    apt.blibe is a BUILD library of Cray-complled blnarles.
Purpose: To flnd the vector c=(cu, cV) normal to the dlno doflned by
    the two polnts a = (au, av), b = (bu, bv), and In the uv plane,
    for each of the np sets of points "a" and "b". The dlrections
    u, v,w are orthogonal. The magnltudo vlen of the normal vector
    "c" is equal to the length of the line sagment. "ab". If vlen is
    zero, lihe points "a" and "b" are congruent. By convontlon,
    the direction of the normal vector is from rlght to left,
    relative to the direction from "a" to "b" In the uv plane.
    The components of "c" wlll be truncated to zero, if less than
    the estlmated numerlcal error In thelr calculation, based on
    tol.
Input: au, av, bu, bv, np, tol.
Output: cu, cv, vleri; nerr.
Glossary:
\begin{tabular}{|c|c|c|}
\hline \(a u, a v\) & Input: & The \(u\) and \(v\) coordlnates of polnt "a". Slze np. \\
\hline bu, bv & Input. & The \(u\) and \(v\) coordinates of point. "b". size np. \\
\hline \(\mathrm{Cu}, \mathrm{cv}\) & Out put & The \(u\) and \(v\) components of normal vector " \(c\) ". May be truncated to zero, if less than the estlmated numerical error in thelr calculation. See tol. \\
\hline nerr & output & Indleates an Input error, if not: 0. 1 If np ls not posltive. \\
\hline \(n \mathrm{n}\) & Input. & The number of sets of points "a" and "b" for which the normal vector "c" is to be calculatod. Must be positive. \\
\hline tol & Input & Numerlcal tolerance 11 mlt for cu , cv . On Cray computers, recommend \(1 . e-5\) to \(1 . e-11\). \\
\hline vlen ( \(n\) ) & Out put. & The magnitude of the normal vector "e". Slie np. zero if polnts "a" and "b" aro congruent. \\
\hline
\end{tabular}
```



## subroutine aptvguc

```
call aptvsuc (nopt.f, fa, au, av, fb, bu, bv, np, tol,
6
cu, ev, clan, norr
Verslon: aptvauc Updated 1990 Aprl1 3 16:00.
aptvsuc orlginated 1989 Apr11 3 16:00.
Author: Arthur L, Edwards, LINL, L,-298, Telephone (115) 422-1123.
Source: xport read . 245100:aptslibe / 1 1
    1lb aptsllbolx apt.blibe aptvsuclend / 1 1.
    aptslibe is a LIB library of FORTRAN source flles.
    aptbllbe is a BUILN llbrary of Cray-complled blnarlos.
```

Purpose: To flnd, for each of the np sets of Input data, the welghted

$o(n)=f a * a(n)+f b * b(n), n=1, n p$ (nopt $f=01$, or
$c(n)=f a(n) \neq a(n)+f b(n) * b(n), n=1, n p$ (noptif $=11$
and to flad clen, the magnitude of vector "c".
Any component of vector "c" less than the estimated orror in
Its calculation, based on tol, wlll be truncated to zero
Flag nerr Indlates any Input error.
Spectal cases:
sum: $\quad c \pi a+b \quad$ (nopt $f=0, f a=1,0, f b=1,0)$
difference: $\quad c=a-b \quad$ (nopt $f-0, t a-1.0, f b=-1.0)$.
blsector: $\quad c=0.5 *(a+b) \quad$ (nopt $f=0, f a=f b=0.5)$.
Interpolation: $c=f a * a+(1.0-f a) * b(n o p t f=0)$,
$c=(1.0-f b) * a+f b * b \quad(n o p t i=0)$.
Input: noptf, fa, $a u_{1} a v, f b, b u, b v$, np, tol.
Output: cu, ev, cien, norr.
Glossary:

| $a u, a v$ | Input | The $u$ and $v$ components of vector "a". Sizo np |
| :---: | :---: | :---: |
| bu, bu | Input | The $u$ and $v$ componants of vector "b". Stze np. |
| clen | Out put | Magnitude of vector "c". May be truncated to zero, If less than tho est Imated error in its calculation. See tol. Slze np. |
| $\mathrm{cu}, \mathrm{cv}$ | Output | The $u$ and $v$ components of vector "c". Slzenp. Whll be truncated to zero if less than the estimated numertcal arror in thate calculation basod on tol. |
| fa | 1 nfut | Coefflclent of vector "a". Size 1 (nopt. $f=0$ or np (nopt f = 1). |
| fo | Input | ```Coefflclent of vector "b", Slze 1 (nopt.f=0) or np (noptf = 1).``` |
| nerr | Output | Indicates an input error, if not 0. 1 if np $1 s$ not positive. 2 If nopt ifs not 0 or 1. |
| nopt f | Input | size option for fa, fb: <br> 0 If fa and fb are scalars. <br> 1 If ta and fb are arrays with size np. |
| np | Input | stze of arrays. |
| tol | Input | Numerlcal tolerance 11 mlt . Used to truncate the components of vector " c ". <br> On Cray computers, recommend $1 . e-5$ to 1.e-11. |

## SUBROUTINE APTVSUM



## SUBROUTINE APTVTOC

| Version: | aptivtoc Updated 1990 January 18 19:20. apt.vtoc OrIglnated 1989 November 15 16:40. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LINL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100 ;aptslibe / 11 . <br> 11b aptslibelx aptblibe aptvtoclend / 11. <br> apt:slibe is a LIB llbrary of FORTRAN sourco flles. <br> aptbllbe is a BUILD library of Cray-compllad binarles. |
| Purpose: | To adjust the values of the components of the np 2-D vactors a (ad, av), according to the optton kadj, and the numerlcal tolerance limits tolu and tolv, and to renormallze to a unit vector if option $k$ norm $=1$. Flag nerr indicates any input error. |
| Input: | au, av, np, kadj, knorm, tolu, tolv. |
| Out put: | au, av, vlen, nerr. |
| Glossary: |  |
| $a u, ~ a v$ | Input The $u$ and $v$ components of Input vector "a". size np, Directions $u, v$ and $w$ are orthogonal. |
| au, av | Output The $u$ and $v$ components of output voctor "a". size np. May be adjusted, according to the option kadj, and the numerlcal tolerance llmits tolu and tolv. |
| nerr | Output Indicates an lnput error, it not 0 . <br> $l$ if np is not positive. <br> 2 If kady is not from 0 to $\%$. <br> 3 if knorm is not 0 or 1. |
| karij | Input ' Option for adjusting the components (au, av\}. <br> Values from 0 to 7 are allowad: <br> 0 to use a limiting value equal to the tolerance limit times the vector magniltude. <br> Add 1 to use a limitifing value equal to the tolerance 11mit. |
|  | Add 0 to use the same tolerance limit., tolu, for au and av. <br> Add 2 to use tolu for au, tolv for av. <br> Add 0 to t.runcat.e the component to zero if less than the 11 mlting value. <br> Add 4 to Increase components less than the 11 mlting value, to the liniting value, with the same slgn. |
| knorm | Input Option for normallzing the adjusted vector "a" to a unlt vector. 0 - no, $1=$ yes. |
| $n \mathrm{n}$ | Input Slze of arrays au, av, vlen. |
| colu | Input Numerical tolerance limit for component au, and for au and av, for kady $=0,1,4$, and 5 . On cray computers, recommend $1 . e-5$ to $1, e-11$. |
| tolv | Input. <br> Numerical tolerance 11 mit for component av, for kady $=2,3,6$, and 7. <br> On Cray computers, recommend $1 . e-5$ to $1.0-11$. |
| vlen ( $n$ ) | Output Magnitude of the Input vector "a", after an! adjustment of components has been done, butt before any remormallzatlon (knorm $=1$ ). <br> Wlll be zero if all components of "a" aro zero, or are truncated to zero. |



## SUBROUTINE APTVUAC

```
call aptvuac (au, av, np, tol, vlen, nerr)
Version: aptvuac Updated 1990 March 14 17:30.
    aptvu'ac originated 1989 November 2 14:10.
Author:' Arthur L. Edwards, LINL, L-298, Telephone (4.15) 422-4123.
Source: xport read . 245100:aptslibe / 1 1
    lib aptslibe!x aptblibe apt.vuac!end / 1. 1.
    aptslibe is a LIB library of FORTRAN source flles.
    aptblibe ls a BUILD library of Cray-compiled binarles.
Purpose: To find the np unit vectors a = (au, av) parallel to the np
    Inltlal vectors a = (au, av), all in the uv plane (2-D). Any
    components of the indtial vector "a" no,greater than tol, or no
    greater than tol times the initlal length of "a", wlll be
    truncated to zero. If all are zero, or are truncated to zero,
    vlen wlll be zero.
    Flag nerr indlcates any input error.
    With no truncation,
    (au, av)=(au,av) / sqrt (au**2 + av**2)
H1story: 1990 March 14. Modifled to always return a unlt vector.
Input: au, av, np, tol.
Output: au, av, vlen, nerr.
Glossary:
au, av Input The u and v components of inltial vector "a" In the
    uv plane. Slze np.
    Wlll be truncated to zero if inltially no greater
    than tol, or no groater than tol times the initial
    length of "a".
au, av Output. The u and v components of unlt vector "a" in the
    uv plane. Size np.
nerr: Sutput Indicates an input error, it not 0.
    l if np is not positive.
np Input size of arrays au, av, vlen.
tol Input Numerlcal toverance limlt.
    On Cray computers, recommend l.e-5 to 1.e-11.
vlen(n) Output Magnitude of the input vectior "a", after any
    truncation of components t.as been done, but before
    division by vlen to form a unit vector.
```

| Version: | aptvubc Updated 195う March 14 17:30. <br> aptvubc Orlginated 1989 November 29 10:00. |
| :---: | :---: |
| Author: | Arthur L. Edwards, LLNL, L-298, Telephone (415) 422-4123. |
| Source: | xport read . 245100:aptslibe/11 <br> lib aptsilibe!x aptblibe aptvubc!end/11. <br> aptsilbe is a 21 B library of FORTRAN source. flles. <br> aptblibe is a BUILD Library of Cray-complled binaries. |
| Purpose: | To find the $n p$ unlt vectors $h=(b u, b v)$ parallel to the $n p$ 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 initlal length of "a", then the corresponding compouent of "b" wlll be tfuncated to zero. If all are zero, or are truncated to zero, vien wlll be zero. Flag nerr Indicates any input error. <br> With no truncation, <br> (bu, bv) = (au, av) / sqrt (au**2 + av**2) |
| History: | 1990 March 14. Modifled to always return a unit vector. |
| Input: | au, av, np, tol. |
| Out put : | bu, bv, vlen, nerr. |
| Glossary: |  |
| $a u, a v$ | Input The $u$ and $v$ components of vector "a" In the uv plane. slze np: |
| bu, bv | Output. The $u$ and $v$ components of vector "b" In the uv plane. Slize np. <br> 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 . lif np is not positive. |
| $n \mathrm{n}$ | Input Size of arrays au, av, bu, bv, vlen. |
| tol | Input Numerical tolerance 11 mit. 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 vlen to form a unlt vector. |

## SUBROUTINE APTVUNA



## SUAROUTINE APTVUNB



## SUBROUTINE: APTVXUC



## SUBROUTINE APTVXUN



## SUBROUTINE APTXNUP

```
call apt.xnup (nopt, r.plansk, np, xnu, nort)
Vorslon: aptxnup Updatod 1990 Fobruary 12 10150
    aptxnup Orfginated 1990 January 31 1%100.
Authors: Eugone H. Canfluld, liNL, l-298, Talophone (115) 422-4123.
    Arthur l., Edwards, LLNL, L,-298, Tolephonu (415) 12?-1123,
Sourea: xport road . 245100:aptallbe/11
    llb aptallbalx aptbl/be apt.xnuplend / 1 1.
    aptalibe is a lib library of fORTRAN gourca lllos.
    aptblibu is a BUILD library of cray-complled bimatlon,
Purpose: To flnd, for each of np temperatures tplanck, a frequency xnu
    sampled tandomly from a Planck or a Wlon spoctrum,
    flaq norr indlcates any Input. arror (np not positiva).
The Planck distrlbutlon funct.Ion 1a,
    p(x) = (15.0/p(**4)* x**3 / (exp (x) - 1.0),
    whare }x=x\mathrm{ mu/ tplanck, and }\langlex>=3,83223..
The Wlen digtrlbution function 1s:
    p(x)=x**3 * exp (-x) / 6.0.
where <x: = 1.0,
H1story: See Harnott and Canfleld, UCIR-473, June 19%0.
    1990 february 6 11:20. Truncatod pltn, to Hmlt number of torm!
    requirad to converge.
Input: nopt, tplanck, np.
Out.put: xnu, nerr.
Glossary:
nerr Output Indlcates an Input error, lf not 0.
    lf np la not positive.
nopt Input Indicates type of spectrum to sample from:
    O for a Planck spectrum,
    1 for a Wien spectrum.
np Input Sizo of arrays tplanck, xnu.
tplanck Infut Black body temperature of frequency distribution.
    Same unlts as xnu. Slzo np.
xnu Output Frequency sampled randomly from spoctum. Slze np.
    Same unlts as t.planck.
```


## APPENDIX

## SUBROUTINES BY FUNCTION

## FUNDAMENTAL CONSTANTS

Find the values of the fundamental constants of physics and Chemistry, arld energy conversion factors

```
in cm-g-sh-keV units
aptconl
in m-kg-s (SI) units
aptconm
```


## MATHEMATICS AND STATISTICS

```
Find any real root of a qeneral quadratic equation
    a single oquation 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
```



## FUZZY GEOMETRY

```
Impose limits on the values of
a fractional distance (scalar) aptfdad
any number of fractional distances (vectorized) aptfdav
the components of a vector
    in a major plane (2-D), lower
    in a major plane (2-D), several options
    in any coordinate system (3-D), lower
    in any coordinate systom (3-D), several optiong
Round off a floating point number
to a specified relative or absolute precision
aptrnds
```


## GEOMETRY

```
Transform between Cartesian, cylindrioal and sphorioal
    coordinate systems
    coordinates (3-D) aptcosys
    coordinates and bound vectors (3-D)
Do the basic vector operations
    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
        in a major plane (2-D)
        in any coordinate system (3-D)
    clot (scalar) product
        in a major plane (2-D)
        in any coordinate system (3-D)
    cross (vector) product
        in a mafor 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
        in a mafor plane (2-D)
        in a major plane (2-D), replace
        in any coordinate system (3-D)
        in any coordinate system (3-D), replace
Do the basic matrix operations
    product of a 3-D vector and a 3 by 3 matrix aptmopv
    product of two n by n matrices
Find the angle relationships
    area included between adjacent sides
    in a major plane (2-D)
    in any coordinate system (3-D)
bisectors
    in a major plane (2-D) aptbanc
    in any coordinate system (3-D) aptbang
cosine
    in any coordinate system (3-D)
cosine (between unit vectors)
    in a major plane (2-D)
    in any coordinate system (3-D)
cosine and sine
    in a major plane (2-D)
sine (between unit vectors)
    in a major plane (2-D) aptvaxc
    in any coordinate system (3-D) aptvaxb
```

Test for the spealal geometric relationships

| points being coincident on an axis (1-D) | apt vad. 1 |
| :---: | :---: |
| In a major plane (2-D) | aptvalc |
| In xyz space (3-D) | aptvals |
| in any coordinate system (3-D) | aptdist |
| points being on lines |  |
| In a major plane (2-D) | aptptic |
| in xyz space (3-D) | aptiptin |
| points beling within a bounded region |  |
| In a major plane (2-D) |  |
| a triangle, and distances to sides | apttinc |
| a quadrangle, and distances to sides | aptginc |
| linies being parallel or congruent |  |
| in a mafor plane (2-D) | aptinlc |
| in xyz space (3-D) | aptlnln |
| line being in a plane |  |
| in xyz space (3-D) | apt lnpl. |
| vectors being parallel |  |
| in a major plane (2-D) | aptrvaxc |
| in any coordinate system (3-D) | aptvaxb |
| vectors bedng perpendicular. |  |
| In a major plane (2-D) | apt vdoc |
| In any coordinate system (3-D) | aptvdot |
| planes being parallel or congruent |  |
| In xyz space (3-D) | aptplpl |
| plane being tangent to a sphere |  |
| in xyz space (3-D) | aptplsp |
| spheres being congruent |  |
| in xyz space (3-D) | aptspsp |
| sphere being tangent to a sphere in xyz space (3-D) | aptispsp |

Do the basic geometric operations
inversion of a point or vector through a specified point
in a mafor plane (2-D)
in xyz space (3-D), and the operator
in xyz space (3-D), with scaling, and the operator
linear scaling of a point or vector in the direction
of a specified axis (i.e., Lorentz transformation)
In a major plane (2-D)
aptinve aptinvp aptsclu

In xyz space $(3-D)$, and the operator
in xyz space (3-D), with reflection, and the operator
aptsolc
aptscll
aptscil
uniform scaling of a point or vector
in $x y z$ space ( $3-D$ ), and the operator
aptsclu
in xyz space (3-D), with inversion, and the operator aptsclu
reflection of a point or vector
from a plane perpendicular to a mafor plane (3-D)
of a point or vector in a mafor plane (2-D)
of a point or vector in xyz space (3-D)
from a plane in xyz space (3-D), and the operator
aptrefc
aptreed
aptrefs

```
    rotation of a point or vector
    by a specified angle around a specifiud axis
            In a mafor plane (2-D)
            In xyz space (3-D), operator only
    by specified angles around the 3 mafor axes (3-D),
            operator only
    to rotate a specified vector onto another vector
                (3-D), operator only
    to rotate a specified plane onto another plane
                (3-D), operator only
    to rotate a specified vector in a specified plane
        onto another vector in another plane (3-D),
        operator orily
    apply the operator generated by aptrota, aptrotp,
    aptrots, aptrott, aptrotv or aptmopv to points
        or vectors
    translation of a polnt
    In a major plane (2-D)
    In xyz space (3-D)
combined operations
    multiply two matrix operators together aptmprd
    apply matrix operator to points or vectors
Find the distance
    from a point to another point
    on an axis (1-D)
    In a major: plane (2-D), and direction
    In xyz space (3-D), and direction
    in any coordinate system (3-D), and direction
from a polnt to a line
    in a major plane (2-D)
    in xyz space (3-D)
from a point to the sides of a triangle
    in a major plane (2-1), and in or out?
from a point to the sides of a quadrangle
    in a major plarie (2-D)
    In a major plane (2-D), and in or out?
from a point to a plane in xyz space (3-D)
    in any orientation, and the nearest point
    bourided by a triangle, and the nearest point, more
from a point. to a second-order surface
    bounded by a quadrangle (3-D), and the nearest point
from a line to another line
    in a major plane (2-D)
    In xyz space (3-D)
from a line to a plane
    in xyz space (3-D)
apt rote aptrota
aptrots aptrotv
aptrotp
aptrote
aptimopv
apttrac
apttran
aptmprd aptmopv
aptvdil aptvdic aptvals aptdist
aptptlc aptiptln
apttinc
aptqdic
aptqinc
aptptpl.
apttrip
aptquad
apt.lnlc
aptinln
apt \(\ln p 1\)
```

Find the initial vector direction between two points
in a mafor plane (2-D), and find distance
In xyz space ( $3-D$ ), and find distance
in any coordinate system (3-D), and find distance
aptvdic aptvdis aptdist

```
Find the alternate geometrio represen: wion of a
    Inrie in a major plane (2-D)
    given two polnts, find vector, distance
    given polnt and vector, find another point
    line in xyz spade (3-D)
    given two points, find vector, distance
    given point and vector, find another point
    line in any coordinate system (3-D)
        given two points, find initial vector, distance
    plane In xyz space (3-D)
        given three polnts, find normal vector
Find the vector perpendicular (rormal) to a
    line in a major plane (2-D) aptuplc
    plane in xyz space (3-D)
Find the vertex areas in a major plane (2-D) of a
    triangle
    quadrangle, and shape (convex, boomerang, bowtie)
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
    any number of points, quadrangles
Find the intersection(s) of a line with
    a line in a mafor plane (2-D)
    a circle in a major plane (2-D) (two points)
    a plane in xyz space (3-D)
Find the intersection(s) of a linear track with
    a line, both in a major plane (2-D) aptrklc
    a major plane (3-D)
    a plane in xyz space (3-D)
    an axisymmetric cylindrical surface with
        constant radius (3-D)
    an axisymmetric cylindrical surface (3-D)
    a centrisymmetric spherical surface (3-D)
    a general implicit second-order surface (3-D)
Find the intersection(s) between
two circles in a major plane (2-D) (2 points) aptcinc
two planeg 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)
```

aptvdic aptvadc
aptvdis apt:vadd aptdist aptupln
aptvplc aptvpln
aptvaxc aptquac
aptqfdc aptfdqic
aptlnle aptlnic apt1npl
aptrklc aptrksl aptrkpl
aptrkcl aptrkcy aptrkrl aptrkis
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) aptmvcy
    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.


