crange-1.6.2

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Chapter 1

crange - The Berkeley Range-Energy Calculator

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Version

1.6.2

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1.1 Introduction

Thank you for choosing the Berkeley Range-Energy Calculator.

1.2 Pre-Installation

1.2.1 System Requirements

crange should run on any POSIX-based system that has the appropriate libraries installed (see Prerequisites).

1.2.2 Library Prerequisites

1.2.2.1 GNU Scientific Library

The GNU Scientific Library (http://www.gnu.org/s/gsl/) is required. This code was most recently tested with version 1.15, though any version with full complex variable support should work.

1.2.2.2 iniParser

The iniParser Library (http://ndevilla.free.fr/iniparser/), version 3.0 or later is strongly recommended. The code will still compile if it is not installed, but the resulting binary will not be able to read optional target or switch information, so only compiled-in defaults will be available.

1.3 Installation

See the INSTALL file.

1.4 Running

1.4.1 On the Command Line

Type crange -h to get the list of command-line options.

1.4.2 Task List

The crange program executes a list of tasks from a file. Here's an example:

```
r 1200 0 92 238 Al
e 0 9.2 79 197 CR-39
e 10600 9.2 79 197 CR-39
d 10600 0 79 197 Air
d 10600 300 79 197 Air
j 10600 0 79 197 Air
```

The first line tells the calculator to compute the range (in g cm^{-2}) of uranium (Z=92,A=238) at a kinetic energy of 1200 MeV per nucleon, in an aluminum target. The second line tells the calculator to compute the initial kinetic energy (in A MeV) of gold (Z=79,A=197) whose range in the plastic track-etch detector CR-39 was 9.2 g cm^{-2} . The third line asks for the final kinetic energy after passing through 9.2 g cm^{-2} of CR-39, given an initial energy of 10.6 A GeV. The fourth line tells the calculator to compute dE/dx (in A MeV g^{-1} cm^{2}) for gold with kinetic energy 10.6 A GeV in air. The fifth line computes REL instead of dE/dx with the REL cutoff set to 300 eV. The sixth line computes primary ionization. Arguments which are zero (0) are dummies which are necessary for place-holding.

The list of tasks may be of any length in any combination of ranges, energies or dE/dx. The order of the output will be the same as the order of the input.

1.4.3 Switching Optional Effects

The switch.ini file included with the source distribution shows the effects that may be turned on or off by the user. The values in the switch.ini file are the default values that are compiled into the program. The user may supply a modified switch.ini file on the command line. There are additional details in the file itself.

1.4.4 Adding or Modifying Targets

The target.ini file included with the source distribution lists the targets that are compiled in to the program by default. Most of the target data is taken from Sternheimer, Berger & Seltzer, [21]. The definitions of the material properties are in the target.ini file. The user may add additional targets or override existing target values by supplying a different target.ini file (with the same format!) on the command line.

1.5 Updates

Visit http://sdss.physics.nyu.edu/~bw55/dedx/ .

1.6 History

- 1.6.2: Fixed bug which was forbidding access to INI files. Minor changes relating to GitHub migration.

- 1.6.1: Fix version strings.
- 1.6.0: Make crange compatible with GNU autotools and GNU Scientific Library.
- 1.5.3: Simplified calculation switching and added a crange.h file
- 1.5.2: Increased value of MAXAB to acommodate a larger target data file
- 1.5.1: Fixed typo in one of the parameters of the electron capture corection

Chapter 2

Bug List

Global bma (double z1, double b)

Currently, this function is not called by anything.

Global djdx (double e1, double z0, double I0, double f0, double K, short sswitch, tdata *target)

The parameters needed are not contained in the target table.

Global effective_charge (double z0, double e1, double z2, short sswitch)

The Pierce & Blann formula is not actually available; it is simply commented out.

Global Fbrems (double x)

Currently, this function is unused.

Global qrange (double e, double z1, double a1, short sswitch, tdata *target)

Currently, this function isn't called by anything.

Global run_range (FILE *finput, FILE *foutput, short sswitch, tdata *extratargets)

The primary ionization parameters are currently hard-coded.

Chapter 3

Data Structure Index

3.1 Data Structures

Here are the data structures with brief descriptions:

RANGE_TABLE
Structure to store range tables 11
TDATA
Structure containing target data 12

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

config.h 15
crange.c
Source code for crange 18
crange.h
Header file for crange 28

Chapter 5

Data Structure Documentation

5.1 RANGE_TABLE Struct Reference

Structure to store range tables.

`#include <crange.h>`

Data Fields

- double z1
- double a1
- short sswitch
- tdata * target
- time_t timestamp
- double range [MAXE]

5.1.1 Detailed Description

Structure to store range tables.

This structure contains a range table and its associated metadata.

Definition at line 147 of file crange.h.

5.1.2 Field Documentation

5.1.2.1 double RANGE_TABLE::a1

The projectile mass.

Definition at line 149 of file crange.h.

5.1.2.2 double RANGE_TABLE::range[MAXE]

The actual table of range values.

Definition at line 153 of file crange.h.

5.1.2.3 short RANGE_TABLE::sswitch

The switch bit field.

Definition at line 150 of file crange.h.

5.1.2.4 tdata* RANGE_TABLE::target

A pointer to the TDATA structure used in constructing the table.

Definition at line 151 of file crange.h.

5.1.2.5 time_t RANGE_TABLE::timestamp

The time at which the table was created.

Definition at line 152 of file crange.h.

5.1.2.6 double RANGE_TABLE::z1

The projectile charge.

Definition at line 148 of file crange.h.

The documentation for this struct was generated from the following file:

- crange.h

5.2 TDATA Struct Reference

Structure containing target data.

`#include <crange.h>`

Data Fields

Material name

- char name [NAMEWIDTH+1]

General parameters

- double z2
- double a2
- double iadj
- double rho
- double pla
- double etad
- double bind

Density effect parameters

- double X0
- double X1
- double a
- double m
- double d0

5.2.1 Detailed Description

Structure containing target data.

This structure contains all the data related to target materials.

Definition at line 105 of file crange.h.

5.2.2 Field Documentation

5.2.2.1 double TDATA::a

Parameter used to interpolate the density effect between the values of X0 and X1.

Definition at line 130 of file crange.h.

5.2.2.2 double TDATA::a2

The mean atomic mass number.

Definition at line 117 of file crange.h.

5.2.2.3 double TDATA::bind

The total electronic binding energy [eV].

Definition at line 122 of file crange.h.

5.2.2.4 double TDATA::d0

Low-energy density effect parameter, only non-zero for conducting materials.

Definition at line 132 of file crange.h.

5.2.2.5 double TDATA::etad

The ratio of density to density at STP for gaseous targets. Should be set to zero for non-gaseous materials.

Definition at line 121 of file crange.h.

5.2.2.6 double TDATA::iadj

The logarithmic mean ionization potential [eV].

Definition at line 118 of file crange.h.

5.2.2.7 double TDATA::m

Parameter used to interpolate the density effect between the values of X0 and X1.

Definition at line 131 of file crange.h.

5.2.2.8 char TDATA::name[NAMEWIDTH+1]

The name of the material.

Definition at line 110 of file crange.h.

5.2.2.9 double TDATA::pla

The plasma frequency [eV].

Definition at line 120 of file crange.h.

5.2.2.10 double TDATA::rho

The density [g cm^{-3}].

Definition at line 119 of file crange.h.

5.2.2.11 double TDATA::X0

Value of $\log_{10}\beta\gamma$ at which the density effect turns on.

Definition at line 128 of file crange.h.

5.2.2.12 double TDATA::X1

Value of $\log_{10}\beta\gamma$ above which the high-energy form of the density effect may be used.

Definition at line 129 of file crange.h.

5.2.2.13 double TDATA::z2

The mean nuclear charge.

Definition at line 116 of file crange.h.

The documentation for this struct was generated from the following file:

- crange.h

Chapter 6

File Documentation

6.1 config.h File Reference

Macros

- #define HAVE_ERRNO_H 1
- #define HAVE_GSL_GSL_COMPLEX_H 1
- #define HAVE_GSL_GSL_COMPLEX_MATH_H 1
- #define HAVE_INIPARSER_H 1
- #define HAVE_INTTYPES_H 1
- #define HAVE_LIBGSL 1
- #define HAVE_LIBGSLCBLAS 1
- #define HAVE_LIBINIPARSER 1
- #define HAVE_LIBM 1
- #define HAVE_MEMORY_H 1
- #define HAVE_SQRT 1
- #define HAVE_STDINT_H 1
- #define HAVE_STDLIB_H 1
- #define HAVE_STRINGS_H 1
- #define HAVE_STRING_H 1
- #define HAVE_SYS_STAT_H 1
- #define HAVE_SYS_TYPES_H 1
- #define HAVE_TIME_H 1
- #define HAVE_UNISTD_H 1
- #define PACKAGE "crange"
- #define PACKAGE_BUGREPORT "benjamin.weaver@nyu.edu"
- #define PACKAGE_NAME "Berkeley Range-Energy Calculator"
- #define PACKAGE_STRING "Berkeley Range-Energy Calculator 1.6.2"
- #define PACKAGE_TARNAME "crange"
- #define PACKAGE_URL "http://cosmo.nyu.edu/~bw55/dedx/"
- #define PACKAGE_VERSION "1.6.2"
- #define STDC_HEADERS 1
- #define VERSION "1.6.2"

6.1.1 Macro Definition Documentation

6.1.1.1 #define HAVE_ERRNO_H 1

Definition at line 5 of file config.h.

6.1.1.2 #define HAVE_GSL_GSL_COMPLEX_H 1

Definition at line 8 of file config.h.

6.1.1.3 #define HAVE_GSL_GSL_COMPLEX_MATH_H 1

Definition at line 11 of file config.h.

6.1.1.4 #define HAVE_INIPARSER_H 1

Definition at line 14 of file config.h.

6.1.1.5 #define HAVE_INTTYPES_H 1

Definition at line 17 of file config.h.

6.1.1.6 #define HAVE_LIBGSL 1

Definition at line 20 of file config.h.

6.1.1.7 #define HAVE_LIBGSLCBLAS 1

Definition at line 23 of file config.h.

6.1.1.8 #define HAVE_LIBINIPARSER 1

Definition at line 26 of file config.h.

6.1.1.9 #define HAVE_LIBM 1

Definition at line 29 of file config.h.

6.1.1.10 #define HAVE_MEMORY_H 1

Definition at line 32 of file config.h.

6.1.1.11 #define HAVE_SQRT 1

Definition at line 35 of file config.h.

6.1.1.12 #define HAVE_STDINT_H 1

Definition at line 38 of file config.h.

6.1.1.13 #define HAVE_STDLIB_H 1

Definition at line 41 of file config.h.

6.1.1.14 #define HAVE_STRING_H 1

Definition at line 47 of file config.h.

6.1.1.15 #define HAVE_STRINGS_H 1

Definition at line 44 of file config.h.

6.1.1.16 #define HAVE_SYS_STAT_H 1

Definition at line 50 of file config.h.

6.1.1.17 #define HAVE_SYS_TYPES_H 1

Definition at line 53 of file config.h.

6.1.1.18 #define HAVE_TIME_H 1

Definition at line 56 of file config.h.

6.1.1.19 #define HAVE_UNISTD_H 1

Definition at line 59 of file config.h.

6.1.1.20 #define PACKAGE "crange"

Definition at line 62 of file config.h.

6.1.1.21 #define PACKAGE_BUGREPORT "benjamin.weaver@nyu.edu"

Definition at line 65 of file config.h.

6.1.1.22 #define PACKAGE_NAME "Berkeley Range-Energy Calculator"

Definition at line 68 of file config.h.

6.1.1.23 #define PACKAGE_STRING "Berkeley Range-Energy Calculator 1.6.2"

Definition at line 71 of file config.h.

6.1.1.24 #define PACKAGE_TARNAME "crange"

Definition at line 74 of file config.h.

6.1.1.25 #define PACKAGE_URL "http://cosmo.nyu.edu/~bw55/dedx/"

Definition at line 77 of file config.h.

6.1.1.26 #define PACKAGE_VERSION "1.6.2"

Definition at line 80 of file config.h.

6.1.1.27 #define STDC_HEADERS 1

Definition at line 83 of file config.h.

6.1.1.28 #define VERSION "1.6.2"

Definition at line 86 of file config.h.

6.2 crange.c File Reference

Source code for crange.

```
#include <crange.h>
```

Functions

- int main (int argc, char **argv)

  Main crange program.
- gsl_complex complex_hyperg (gsl_complex a, gsl_complex b, gsl_complex z)

  Confluent hypergeometric function.
- gsl_complex complex_lngamma (gsl_complex z)

  Complex logarithm of the Gamma function.
- double effective_charge (double z0, double e1, double z2, short sswitch)

  Computes effective projectile charge.
- double djdx (double e1, double z0, double I0, double f0, double K, short sswitch, tdata *target)

  Computes primary ionization.
- double dedx (double e1, double rel0, double z0, double a1, short sswitch, tdata *target)

  Computes dE/dx.
- double delta (double g, tdata *target)

  Computes the density effect.
- double olddelta (double g, tdata *target)

  Computes an obsolete version of the density effect.
- double bma (double z1, double b)

  Computes the Bloch, Mott and Ahlen corrections.
- double relbloch (double z12, double b1, double lambda, double theta0)

  Compute the relativistic Bloch correction.
- double lindhard (double zz, double aa, double bb, short sswitch)

  Compute the Lindhard-Sørensen correction.
- double Fbrems (double x)

  Compute a mathematical function related to bremsstrahlung.
- double range (double e, double z1, double a1, short sswitch, tdata *target, int *tno)

  Computes total range given initial energy.
- double qrange (double e, double z1, double a1, short sswitch, tdata *target)

  Computes total range by direct integration of dE/dx.
- double benton (double e, double z1, double a1, tdata *target)

Computes ranges at low energies.

- double renergy (double e, double r0, double z1, double a1, short sswitch, tdata ∗target)

  Extract energies from range tables.
- void run_range (FILE ∗finput, FILE ∗foutput, short sswitch, tdata ∗extratargets)

  Parses and executes the task list.
- short init_switch (char ∗switchfile)

  Initializes the value of of the switch bit field.
- tdata ∗ init_target (char ∗targetfile)

  Read optional target data file.
- void init_table (void)

  Initialize range-energy tables.
- double energy_table (int i)

  Returns the energy corresponding to a value in a range table.
- tdata ∗ find_target (char ∗target, tdata ∗extratargets)

  Finds target data corresponding to a target name.
- void print_target (tdata ∗target)

  Prints a target table entry in INI format.

6.2.1 Detailed Description

Source code for crange. This file contains all source code for the crange executable.

Definition in file crange.c.

6.2.2 Function Documentation

6.2.2.1 double benton (double *e*, double *z1*, double *a1*, tdata ∗ *target*)

Computes ranges at low energies.

This function is the result of empirical fits to very low energy 1 A MeV $<$ E $<$ 8 A MeV ion ranges. It follows the methods of Barkas & Berger, [5]. A simplified discussion, with a more complicated formula is given in Benton & Henke, [6]. As yet I know of no nicer way to deal with these low energies.

Parameters

e	Projectile kinetic energy in A MeV.
z1	Projectile charge.
a1	Projectile atomic mass.
target	A pointer to a TDATA structure.

Returns

Projectile range in g cm^{-2} .

Note

The array join[4] demarcates three energy regions represented by the three sets of coefficients in amn[3][4][4]. The demarcation is variable in order to minimize discontinuities at the boundary. The coefficients in cjoin[2][7], which is used to initialize join[4], are inherited from legacy code; I have not found them in the non-obscure literature. Approximately, the three regions are $E < 1$ A MeV, $1 < E < 7$ A MeV and $E > 7$ A MeV. I can find no reason why join[4] has four elements and not two.

Definition at line 1247 of file crange.c.

6.2.2.2 double bma (double *z1*, double *b*)

Computes the Bloch, Mott and Ahlen corrections.

This function computes the Mott correction of Ahlen, [1], the Bloch correction of F. Bloch, [8], and the Ahlen correction of Ahlen, [3]. All three of these corrections are rendered obsolete by the Lindhard-Sørensen correction, and are included here for historical interest and comparison with older calculations.

Parameters

z1	The projectile charge.
b	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).

Returns

The sum of the Bloch, Mott and Ahlen corrections.

Note

The variables lambda and theta0 are free parameters in the Ahlen correction. Theta0 also appears in the Mott correction. Here I have used Ahlen's recommended values, lambda = 1, theta0 = 0.1. An alternative formula, $\theta_0 = \sqrt{\alpha/(\beta\gamma\lambda)}$, is suggested by Waddington, Freier & Fixsen, [26].

Warning

The Mott correction has a severely limited range of validity, especially for high charges. It's so bad it can render the calculation not just inaccurate, but unphysical (dE/dx < 0) below about 10 A MeV for uranium. Ahlen recommends turning the Mott correction off for $Z/\beta > 100$. Here for $Z/\beta > 100$ the Mott correction is given the value at $Z/\beta = 100$. This prescription is given by Waddington, Freier & Fixsen, [26].

Bug Currently, this function is not called by anything.

Definition at line 768 of file crange.c.

6.2.2.3 gsl_complex complex_hyperg (gsl_complex *a*, gsl_complex *b*, gsl_complex *z*)

Confluent hypergeometric function.

Computes the confluent hypergeometric function. All input parameters are complex numbers. Uses the formula:

$$M(a,b,z) = 1 + \sum_{n=1} \frac{(a)_n}{(b)_n} \frac{z^n}{n!},$$

where

$$(x)_n \equiv \frac{\Gamma(x+n)}{\Gamma(x)}$$

is the Pochhammer Symbol.

Parameters

a	First parameter of the hypergeometric function.
b	Second parameter of the hypergeometric function.
z	A complex number.

Returns

The value $M(a,b,z)$, a complex number.

Warning

May not be stable for large values of $|z|$.

Definition at line 267 of file crange.c.

6.2.2.4 gsl_complex complex_lngamma (gsl_complex *z*)

Complex logarithm of the Gamma function.

Computes the fully complex logarithm of the fully complex Gamma function. Works in all portions of the complex plane, including the negative real axis.

Parameters

z	A complex number.

Returns

$\ln\Gamma(z)$, a complex number.

Warning

The Gamma function has poles at all integers <= 0.

Definition at line 299 of file crange.c.

6.2.2.5 double dedx (double *e1*, double *rel0*, double *z0*, double *a1*, short *sswitch*, tdata * *target*)

Computes dE/dx.

This is the core of the whole package, the dE/dx calculator. I have based this largely on the work of Salamon, [20]. Values of certain physical constants have been updated, as well as some of the corrections to the basic stopping power formula.

If the restricted energy loss parameter *rel0* is non-zero, dedx() computes restricted energy loss instead.

The dE/dx calculator includes a number of effects that are controlled by switches encoded in a bit field. Below we describe each bit field and the effect it controls.

- SSWITCH_ND : Density effect version. If this bit is set (which it is by default), a newer version of the density effect is used. See delta() and olddelta() for details.
- SSWITCH_SH : Inner shell correction. The inner shell correction is somewhat problematic. It arises when the projectile velocity is comparable to the velocity of inner shell electrons in the target medium. This is discussed by Fano, [9]. The shell correction can be included explicitly using this formula from Barkas & Berger, [5]. Alternatively, the shell correction can be "hidden" in the logarithmic mean ionization potential. Much more work is required before this topic can be fully understood.
- SSWITCH_LE : Relativistic shell correction. The Leung, or relativistic shell correction is a small effect which is due to relativistic inner shell electrons in very heavy targets. See Leung, [15], and Leung, [16]. SSWITCH_LE has no effect unless SSWITCH_SH is also turned on.
- The Lindhard-Sørensen effect (see lindhard()) is turned on by default. The Bloch, Mott & Ahlen effects are included for historical interestest. Right now these can be turned on by uncommenting a particular section of the code.
- SSWITCH_KI : Ultrarelativistic kinematic correction. This an estimate of the ultrarelativistic kinematic correction from Ahlen, [2]. It corrects to the finite mass (as opposed to size) of the nucleus in relativistic electron-nucleus collisions.
- SSWITCH_RA : Radiative correction. This is the radiative correction discussed in Ahlen, [2]. It arises from bremsstrahlung of scattered electrons in ultrarelativistic collisions. The form here is that of Jankus, [14]. The parameter Q from that paper is here set equal to the geometric mean between the the electron rest energy and $2m_e c^2\gamma$.
- SSWITCH_PA : Slowing due to pair production. This value and the value for the bremsstrahlung correction below are based on the work of Sørensen, [24].

- SSWITCH_BR : Slowing due to projectile bremsstrahlung. This version is that of Sørensen, [24], who has shown that this effect is much smaller than the version suggested by Weaver & Westphal, [27].. This is due to their treatment of the projectile and target nuclei as a point particles. That version appeared in some much older versions of this code, but has been replaced with Sørensen's version. We have not yet updated this code to reflect Sørensen's more recent paper [25].
- SSWITCH_BA : Barkas effect. This is the Barkas correction as calculated in Jackson & McCarthy, [13]. It is multiplied by a factor of two to bring it into agreement with Lindhard, [17]. It is not, however, equal to the results of Lindhard, and more work is needed to decide which, if any, form is correct. The recommended value seems to be the Jackson & McCarthy result multiplied by two. Jackson & McCarthy do not have reliable values of $F(V)$ for $V < 0.8$. For the purposes of the computation, the cut-off is placed at $V = 1.0$. I have followed the convention of Salamon in having the Barkas correction multiply just the "Bethe" portion of the stopping logarithm rather than the whole stopping logarithm. As there is considerable disagreement in the literature about the application of correction, and as changing the convention makes makes a difference of less than 1 A MeV even in calculating the energy of stopping uranium, I have chosen to leave it where it is. Furthermore, I have found that a simple power law V^{-2} is adequate to model Jackson & McCarthy's function for $V > 1.0$, so I have used this instead of the numbers found by reading off one of Jackson & McCarthy's figures (these values are stored in the array fva[10], but only the last value is used).

Parameters

e1	The projectile kinetic energy in A MeV.
rel0	Restricted energy loss parameter in eV.
z0	The projectile charge.
a1	The projectile atomic number.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

dE/dx in units of A MeV g^{-1} cm^2

Definition at line 545 of file crange.c.

6.2.2.6 double delta (double *g*, tdata * *target*)

Computes the density effect.

This function implements the density effect correction as formulated in Sternheimer & Peierls, [22] and as extended in Sternheimer, Berger & Seltzer, [21]. This version can distinguish between solids and gasses, and between metals and insulators. For conducting materials, there is a low-energy density effect.

Parameters

g	Projectile Lorentz factor.
target	A pointer to a TDATA structure.

Returns

The value of the density effect.

Definition at line 657 of file crange.c.

6.2.2.7 double djdx (double *e1*, double *z0*, double *l0*, double *f0*, double *K*, short *sswitch*, tdata * *target*)

Computes primary ionization.

This computes the primary ionization, the number of delta-rays produced per unit length. The formula is based on Bethe [7], as well as Fleischer *et al.*, [10].

Parameters

e1	The projectile kinetic energy in A MeV.
z0	The projectile charge.
I0	The binding energy of outermost electron in eV.
f0	The fraction of electrons in the outermost state.
K	A constant that depends on the target.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

Number of delta-rays per unit length in units of g^{-1} cm^2 .

Bug The parameters needed are not contained in the target table.

Definition at line 437 of file crange.c.

6.2.2.8 double effective_charge (double *z0*, double *e1*, double *z2*, short *sswitch*)

Computes effective projectile charge.

This is the modification of projectile charge due to electron capture. Hubert, Bimbot & Gauvin, [12], give an empirically determined function which depends on the target material. This version is used if SSWITCH_EC is set. Two older versions, from Anthony & Landford, [4], and Pierce & Blann, [19] are also available.

Parameters

z0	The bare projectile charge.
e1	The projectile kinetic energy in A MeV.
z2	The target mean nuclear charge.
sswitch	The switch bit field.

Returns

The effective projectile charge.

Bug The Pierce & Blann formula is not actually available; it is simply commented out.

Definition at line 366 of file crange.c.

6.2.2.9 double energy_table (int *i*)

Returns the energy corresponding to a value in a range table.

This utility returns an energy value from a (virtual) vector containing A logarithmically uniform distribution of energies between a minimum and maximum energy (defined by LOGTENEMIN and LOGTENEMAX), with a number of entries given by MAXE.

Parameters

i	The index of the vector.

Returns

The *i* th energy in A MeV.

Definition at line 1569 of file crange.c.

6.2.2.10 double Fbrems (double *x*)

Compute a mathematical function related to bremsstrahlung.

This function is used in an obsolete version of projectile slowing due to nuclear-nuclear bremsstrahlung. It appears in Heitler's treatment of bremsstrahlung, [11], which was adapted by Weaver & Westphal, [27].

Parameters

x	The input parameter.

Returns

The value of the function.

Bug Currently, this function is unused.

Definition at line 1039 of file crange.c.

6.2.2.11 tdata* find_target (char * *target*, tdata * *extratargets*)

Finds target data corresponding to a target name.

This function returns a pointer to a structure containing the target data corresponding to the input name. There is a built-in list. The built-in list may be added to or overridden by supplying an INI-type file on the command line, which will then be parsed & passed to this function. If the special target name "List" is passed to this function, the built-in list will be printed as an INI-type file.

Parameters

target	The name of a target.
extratargets	A pointer to an array of TDATA structures.

Returns

A pointer to a structure containing the target data. If the name of the target was not found, it will point to a dummy structure.

Definition at line 1596 of file crange.c.

6.2.2.12 short init_switch (char * *switchfile*)

Initializes the value of of the switch bit field.

This utility reads an INI-type file and sets the switch bit field accordingly.

Parameters

switchfile	The name of an INI-type file containing switch configuration.

Returns

The switch bit field.

Warning

If the iniparser library is not found, this function will only return the default value SSWITCH_DEFAULT.

Definition at line 1441 of file crange.c.

6.2.2.13 void init_table (void)

Initialize range-energy tables.

Sets all data in the array of RANGE_TABLE structures trange to zero.

Definition at line 1543 of file crange.c.

6.2.2.14 tdata* init_target (char * *targetfile*)

Read optional target data file.

This utility reads an INI-type file and returns an array of pointers to TDATA structures.

Parameters

targetfile	the name of an INI-type file containing target data.

Returns

A pointer to an array of TDATA structures. This pointer must be free()d!

Warning

If the iniparser library is not found, this function will only return a NULL pointer.

Definition at line 1481 of file crange.c.

6.2.2.15 double lindhard (double *zz*, double *aa*, double *bb*, short *sswitch*)

Compute the Lindhard-Sørensen correction.

This is the Lindhard-Sørensen correction including finite nuclear size effects as described in Lindhard & Sørensen, [18]. The defined variable SSWITCH_NS will turn off the nuclear size effect if it is set to zero. For values of the Lorentz factor above 10/R, where R is the nuclear size divided by the electron Compton wavelength, the correction is set to its asymptotic value which is described by Sørensen, [23]. This also avoids some difficulties with the evaluation of the confluent hypergeometric function (A. H. Sørensen, private communication).

Parameters

zz	The projectile charge.
aa	The projectile atomic mass.
bb	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).
sswitch	The switch bit field.

Returns

The value of the Lindhard-Sørensen correction.

Definition at line 897 of file crange.c.

6.2.2.16 int main (int *argc*, char ** *argv*)

Main crange program.

Standard C main() program.

Parameters

argc	Number of command line options.
argv	The command line options.

Returns

The exit status.

Definition at line 120 of file crange.c.

6.2.2.17 double olddelta (double *g*, tdata * *target*)

Computes an obsolete version of the density effect.

This function implements the density effect correction as originally formulated in Sternheimer & Peierls, [22]. Although it is now obsolete, I have included it here for compatibility with earlier codes.

Parameters

g	Projectile Lorentz factor.
target	A pointer to a TDATA structure.

Returns

The value of the density effect.

Definition at line 692 of file crange.c.

6.2.2.18 void print_target (tdata * *target*)

Prints a target table entry in INI format.

This utility prints a TDATA structure in INI format.

Parameters

target	A pointer to a TDATA structure.

Definition at line 1677 of file crange.c.

6.2.2.19 double qrange (double *e*, double *z1*, double *a1*, short *sswitch*, tdata * *target*)

Computes total range by direct integration of dE/dx.

This function computes total range by direct integration of the dedx() function. It does not create a range table or do table interpolation.

Parameters

e	Initial energy in A MeV.
z1	Projectile charge.
a1	Projectile mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

Total range in g cm^{-2} .

Bug Currently, this function isn't called by anything.

Definition at line 1183 of file crange.c.

6.2.2.20 double range (double *e*, double *z1*, double *a1*, short *sswitch*, tdata * *target*, int * *tno*)

Computes total range given initial energy.

This function computes total range given initial energy. The technique is quite clever, in that if from one call to the next, the projectile and target material parameters do not change, the calculation of range is performed by table interpolation rather than direct integration. The savings in calculation time can be enormous. However, the range of valid energies is limited by the size of the table. The function dE/dx is evaluated at most of the energies defined by the function energy_table(). Results are stored in the RANGE_TABLE array trange. The size of trange (set by MAXAB) is arbitrary and should be set to whatever is most useful. Certainly it should be no smaller than the number of target materials being used.

Parameters

e	Initial projectile kinetic energy in A MeV.
z1	Projectile charge.
a1	Projectile atomic mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.
tno	A pointer to the index of the most recently generated or used table.

Returns

Projectile range in g cm^{-2} .

Definition at line 1086 of file crange.c.

6.2.2.21 double relbloch (double *z12*, double *b1*, double *lambda*, double *theta0*)

Compute the relativistic Bloch correction.

This is the relativistic Bloch (or Ahlen) correction of Ahlen, [3]. The evaluation of this correction has been enormously simplified by the use of fully complex arithmetic.

Parameters

z12	The projectile charge.
b1	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).
lambda	A free parameter, described in bma().
theta0	A free parameter, described in bma().

Returns

The value of the relativistic Bloch correction.

Definition at line 838 of file crange.c.

6.2.2.22 double renergy (double *e*, double *r0*, double *z1*, double *a1*, short *sswitch*, tdata * *target*)

Extract energies from range tables.

This function extracts energies from a range table by table interpolation. It calls range() to initialze the range table or to find the correct table if it has already been computed.

Parameters

e	Projectile kinetic energy [A MeV].
r0	Range [g cm^{-2}].
z1	Projectile charge.
a1	Projectile atomic mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

The final energy of the projectile.

Definition at line 1348 of file crange.c.

6.2.2.23 void run_range (FILE * *finput*, FILE * *foutput*, short *sswitch*, tdata * *extratargets*)

Parses and executes the task list.

This utility function steps through the range, energy and dE/dx tasks specified in the input data file. The tasks are denoted by a single letter:

- *r* compute ranges
- *e* compute energies
- *d* compute dE/dx
- *j* compute dJ/dx (primary ionization)

The task letter should be followed by the energy (or range) at which to compute range (or energy), the charge and mass of the particle, and the name of the target material. Names of target materials can be found in the target.ini file. Target material names may be up to NAMEWIDTH characters in length and should contain no whitespace.

Parameters

finput	An open file pointer containing the task list.
foutput	An open file pointer to write results to.
sswitch	The switch bit field.
extratargets	A pointer to an array of TDATA structures.

Bug The primary ionization parameters are currently hard-coded.

Definition at line 1396 of file crange.c.

6.3 crange.h File Reference

Header file for crange.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <string.h>
#include <unistd.h>
#include <errno.h>
#include <time.h>
#include <gsl/gsl_complex.h>
#include <gsl/gsl_complex_math.h>
#include <config.h>
#include <iniparser.h>
```

Data Structures

- struct TDATA

  Structure containing target data.
- struct RANGE_TABLE

  Structure to store range tables.

Macros

- #define LOGTENEMIN 0.0
- #define LOGTENEMAX 6.0
- #define MAXE 200
- #define MAXAB 50
- #define M_PI 3.14159265358979323846264338327950288
- #define M_PI_2 1.57079632679489661923132169163975144
- #define M_LN10 2.30258509299404568402
- #define ALPHA 7.29735301383e-3
- #define ATOMICMASSUNIT 931.4943
- #define PROTONMASS 938.2723
- #define ELECTRONMASS 0.511003e+6
- #define SSWITCH_BA 0x001
- #define SSWITCH_SH 0x002
- #define SSWITCH_LE 0x004
- #define SSWITCH_ND 0x008
- #define SSWITCH_EC 0x010
- #define SSWITCH_NS 0x020
- #define SSWITCH_KI 0x040
- #define SSWITCH_RA 0x080
- #define SSWITCH_PA 0x100
- #define SSWITCH_BR 0x200
- #define SSWITCH_DEFAULT (SSWITCH_ND | SSWITCH_NS)
- #define NAMEWIDTH 8

Typedefs

- typedef struct TDATA tdata

  Define tdata.
- typedef struct RANGE_TABLE range_table

  Define range_table.

Functions

- gsl_complex complex_hyperg (gsl_complex a, gsl_complex b, gsl_complex z)

  Confluent hypergeometric function.
- gsl_complex complex_lngamma (gsl_complex z)

  Complex logarithm of the Gamma function.
- double effective_charge (double z0, double e1, double z2, short sswitch)

  Computes effective projectile charge.
- double djdx (double e1, double z0, double I0, double f0, double K, short sswitch, tdata *target)

Computes primary ionization.

- double dedx (double e1, double rel0, double z0, double a1, short sswitch, tdata *target)

  Computes dE/dx.
- double delta (double g, tdata *target)

  Computes the density effect.
- double olddelta (double g, tdata *target)

  Computes an obsolete version of the density effect.
- double bma (double z1, double b)

  Computes the Bloch, Mott and Ahlen corrections.
- double relbloch (double z12, double b1, double lambda, double theta0)

  Compute the relativistic Bloch correction.
- double lindhard (double zz, double aa, double bb, short sswitch)

  Compute the Lindhard-Sørensen correction.
- double Fbrems (double x)

  Compute a mathematical function related to bremsstrahlung.
- double range (double e, double z1, double a1, short sswitch, tdata *target, int *tno)

  Computes total range given initial energy.
- double qrange (double e, double z1, double a1, short sswitch, tdata *target)

  Computes total range by direct integration of dE/dx.
- double benton (double e, double z1, double a1, tdata *target)

  Computes ranges at low energies.
- double renergy (double e, double r0, double z1, double a1, short sswitch, tdata *target)

  Extract energies from range tables.
- void run_range (FILE *finput, FILE *foutput, short sswitch, tdata *extratargets)

  Parses and executes the task list.
- short init_switch (char *switchfile)

  Initializes the value of of the switch bit field.
- tdata * init_target (char *targetfile)

  Read optional target data file.
- void init_table (void)

  Initialize range-energy tables.
- double energy_table (int i)

  Returns the energy corresponding to a value in a range table.
- tdata * find_target (char *target, tdata *extratargets)

  Finds target data corresponding to a target name.
- void print_target (tdata *target)

  Prints a target table entry in INI format.

Variables

- range_table trange [MAXAB]

  The range-energy table.

6.3.1 Detailed Description

Header file for crange. This header file collects all the other header files needed to compile crange, as well as all defines, function declarations, etc.

Definition in file crange.h.

6.3.2 Macro Definition Documentation

6.3.2.1 #define ALPHA 7.29735301383e-3

The fine structure constant.

Definition at line 59 of file crange.h.

6.3.2.2 #define ATOMICMASSUNIT 931.4943

1 amu in units of MeV/c^2 .

Definition at line 65 of file crange.h.

6.3.2.3 #define ELECTRONMASS 0.511003e+6

Electron mass in units of eV/c^2 .

Definition at line 77 of file crange.h.

6.3.2.4 #define LOGTENEMAX 6.0

$\log_{10} E_{\max}$ Maximum energy in units of A MeV.

Definition at line 37 of file crange.h.

6.3.2.5 #define LOGTENEMIN 0.0

$\log_{10} E_{\min}$ Minimum energy in units of A MeV.

Definition at line 36 of file crange.h.

6.3.2.6 #define M_LN10 2.30258509299404568402

The value of $\ln 10$ in case it is not defined in math.h

Definition at line 50 of file crange.h.

6.3.2.7 #define M_PI 3.14159265358979323846264338327950288

The value of pi, in case it is not defined in math.h.

Definition at line 44 of file crange.h.

6.3.2.8 #define M_PI_2 1.57079632679489661923132169163975144

The value of pi/2, in case it is not defined in math.h.

Definition at line 47 of file crange.h.

6.3.2.9 #define MAXAB 50

The number of range tables. Arbitrary, but should be larger than the number of targets.

Definition at line 39 of file crange.h.

6.3.2.10 #define MAXE 200

The number of energies in the range-energy tables.

Definition at line 38 of file crange.h.

6.3.2.11 #define NAMEWIDTH 8

The maximum number of characters in a target name.

Definition at line 96 of file crange.h.

6.3.2.12 #define PROTONMASS 938.2723

Proton mass in units of MeV/c^2 .

Definition at line 71 of file crange.h.

6.3.2.13 #define SSWITCH_BA 0x001

Barkas effect bit.

Definition at line 82 of file crange.h.

6.3.2.14 #define SSWITCH_BR 0x200

Projectile Bremsstrahlung bit.

Definition at line 91 of file crange.h.

6.3.2.15 #define SSWITCH_DEFAULT (SSWITCH_ND | SSWITCH_NS)

Default bits set density effect and finite nuclear size.

Definition at line 92 of file crange.h.

6.3.2.16 #define SSWITCH_EC 0x010

Electron capture switcher bit.

Definition at line 86 of file crange.h.

6.3.2.17 #define SSWITCH_KI 0x040

Kinetic effect bit.

Definition at line 88 of file crange.h.

6.3.2.18 #define SSWITCH_LE 0x004

Leung effect bit.

Definition at line 84 of file crange.h.

6.3.2.19 #define SSWITCH_ND 0x008

Density effect switcher bit.

Definition at line 85 of file crange.h.

6.3.2.20 #define SSWITCH_NS 0x020

Finite Nuclear Size effect bit.

Definition at line 87 of file crange.h.

6.3.2.21 #define SSWITCH_PA 0x100

Pair Production energy loss bit.

Definition at line 90 of file crange.h.

6.3.2.22 #define SSWITCH_RA 0x080

Radiative correction effect bit.

Definition at line 89 of file crange.h.

6.3.2.23 #define SSWITCH_SH 0x002

Shell effect bit.

Definition at line 83 of file crange.h.

6.3.3 Typedef Documentation

6.3.3.1 typedef struct RANGE_TABLE range_table

Define range_table.

Define a range_table variable for convenience.

Definition at line 160 of file crange.h.

6.3.3.2 typedef struct TDATA tdata

Define tdata.

Define a tdata variable for convenience.

Definition at line 141 of file crange.h.

6.3.4 Function Documentation

6.3.4.1 double benton (double *e*, double *z1*, double *a1*, tdata * *target*)

Computes ranges at low energies.

This function is the result of empirical fits to very low energy 1 A MeV $<$ E $<$ 8 A MeV ion ranges. It follows the methods of Barkas & Berger, [5]. A simplified discussion, with a more complicated formula is given in Benton & Henke, [6]. As yet I know of no nicer way to deal with these low energies.

Parameters

e	Projectile kinetic energy in A MeV.
z1	Projectile charge.
a1	Projectile atomic mass.
target	A pointer to a TDATA structure.

Returns

Projectile range in g cm^{-2} .

Note

The array join[4] demarcates three energy regions represented by the three sets of coefficients in amn[3][4][4]. The demarcation is variable in order to minimize discontinuities at the boundary. The coefficients in cjoin[2][7], which is used to initialize join[4], are inherited from legacy code; I have not found them in the non-obscure literature. Approximately, the three regions are $E < 1$ A MeV, $1 < E < 7$ A MeV and $E > 7$ A MeV. I can find no reason why join[4] has four elements and not two.

Definition at line 1247 of file crange.c.

6.3.4.2 double bma (double *z1*, double *b*)

Computes the Bloch, Mott and Ahlen corrections.

This function computes the Mott correction of Ahlen, [1], the Bloch correction of F. Bloch, [8], and the Ahlen correction of Ahlen, [3]. All three of these corrections are rendered obsolete by the Lindhard-Sørensen correction, and are included here for historical interest and comparison with older calculations.

Parameters

z1	The projectile charge.
b	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).

Returns

The sum of the Bloch, Mott and Ahlen corrections.

Note

The variables lambda and theta0 are free parameters in the Ahlen correction. Theta0 also appears in the Mott correction. Here I have used Ahlen's recommended values, lambda = 1, theta0 = 0.1. An alternative formula, $\theta_0 = \sqrt{\alpha/(\beta\gamma\lambda)}$, is suggested by Waddington, Freier & Fixsen, [26].

Warning

The Mott correction has a severely limited range of validity, especially for high charges. It's so bad it can render the calculation not just inaccurate, but unphysical (dE/dx < 0) below about 10 A MeV for uranium. Ahlen recommends turning the Mott correction off for $Z/\beta > 100$. Here for $Z/\beta > 100$ the Mott correction is given the value at $Z/\beta = 100$. This prescription is given by Waddington, Freier & Fixsen, [26].

Bug Currently, this function is not called by anything.

Definition at line 768 of file crange.c.

6.3.4.3 gsl_complex complex_hyperg (gsl_complex *a*, gsl_complex *b*, gsl_complex *z*)

Confluent hypergeometric function.

Computes the confluent hypergeometric function. All input parameters are complex numbers. Uses the formula:

$$M(a,b,z) = 1 + \sum_{n=1} \frac{(a)_n}{(b)_n} \frac{z^n}{n!},$$

where

$$(x)_n \equiv \frac{\Gamma(x+n)}{\Gamma(x)}$$

is the Pochhammer Symbol.

Parameters

a	First parameter of the hypergeometric function.
b	Second parameter of the hypergeometric function.
z	A complex number.

Returns

The value $M(a,b,z)$, a complex number.

Warning

May not be stable for large values of $|z|$.

Definition at line 267 of file crange.c.

6.3.4.4 gsl_complex complex_lngamma (gsl_complex *z*)

Complex logarithm of the Gamma function.

Computes the fully complex logarithm of the fully complex Gamma function. Works in all portions of the complex plane, including the negative real axis.

Parameters

z	A complex number.

Returns

$\ln\Gamma(z)$, a complex number.

Warning

The Gamma function has poles at all integers <= 0.

Definition at line 299 of file crange.c.

6.3.4.5 double dedx (double *e1*, double *rel0*, double *z0*, double *a1*, short *sswitch*, tdata * *target*)

Computes dE/dx.

This is the core of the whole package, the dE/dx calculator. I have based this largely on the work of Salamon, [20]. Values of certain physical constants have been updated, as well as some of the corrections to the basic stopping power formula.

If the restricted energy loss parameter *rel0* is non-zero, dedx() computes restricted energy loss instead.

The dE/dx calculator includes a number of effects that are controlled by switches encoded in a bit field. Below we describe each bit field and the effect it controls.

- SSWITCH_ND : Density effect version. If this bit is set (which it is by default), a newer version of the density effect is used. See delta() and olddelta() for details.
- SSWITCH_SH : Inner shell correction. The inner shell correction is somewhat problematic. It arises when the projectile velocity is comparable to the velocity of inner shell electrons in the target medium. This is discussed by Fano, [9]. The shell correction can be included explicitly using this formula from Barkas & Berger, [5]. Alternatively, the shell correction can be "hidden" in the logarithmic mean ionization potential. Much more work is required before this topic can be fully understood.
- SSWITCH_LE : Relativistic shell correction. The Leung, or relativistic shell correction is a small effect which is due to relativistic inner shell electrons in very heavy targets. See Leung, [15], and Leung, [16]. SSWITCH_LE has no effect unless SSWITCH_SH is also turned on.
- The Lindhard-Sørensen effect (see lindhard()) is turned on by default. The Bloch, Mott & Ahlen effects are included for historical interestest. Right now these can be turned on by uncommenting a particular section of the code.
- SSWITCH_KI : Ultrarelativistic kinematic correction. This an estimate of the ultrarelativistic kinematic correction from Ahlen, [2]. It corrects to the finite mass (as opposed to size) of the nucleus in relativistic electron-nucleus collisions.
- SSWITCH_RA : Radiative correction. This is the radiative correction discussed in Ahlen, [2]. It arises from bremsstrahlung of scattered electrons in ultrarelativistic collisions. The form here is that of Jankus, [14]. The parameter Q from that paper is here set equal to the geometric mean between the the electron rest energy and $2m_e c^2\gamma$.
- SSWITCH_PA : Slowing due to pair production. This value and the value for the bremsstrahlung correction below are based on the work of Sørensen, [24].
- SSWITCH_BR : Slowing due to projectile bremsstrahlung. This version is that of Sørensen, [24], who has shown that this effect is much smaller than the version suggested by Weaver & Westphal, [27].. This is due to their treatment of the projectile and target nuclei as a point particles. That version appeared in some much older versions of this code, but has been replaced with Sørensen's version. We have not yet updated this code to reflect Sørensen's more recent paper [25].
- SSWITCH_BA : Barkas effect. This is the Barkas correction as calculated in Jackson & McCarthy, [13]. It is multiplied by a factor of two to bring it into agreement with Lindhard, [17]. It is not, however, equal to the results of Lindhard, and more work is needed to decide which, if any, form is correct. The recommended value seems to be the Jackson & McCarthy result multiplied by two. Jackson & McCarthy do not have reliable values of $F(V)$ for $V < 0.8$. For the purposes of the computation, the cut-off is placed at $V = 1.0$. I have followed the convention of Salamon in having the Barkas correction multiply just the "Bethe" portion of the stopping logarithm rather than the whole stopping logarithm. As there is considerable disagreement in the literature about the application of correction, and as changing the convention makes makes a difference of less than 1 A MeV even in calculating the energy of stopping uranium, I have chosen to leave it where it is. Furthermore, I have found that a simple power law V^{-2} is adequate to model Jackson & McCarthy's function for $V > 1.0$, so I have used this instead of the numbers found by reading off one of Jackson & McCarthy's figures (these values are stored in the array fva[10], but only the last value is used).

Parameters

e1	The projectile kinetic energy in A MeV.
rel0	Restricted energy loss parameter in eV.
z0	The projectile charge.
a1	The projectile atomic number.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

dE/dx in units of A MeV g^{-1} cm^2

Definition at line 545 of file crange.c.

6.3.4.6 double delta (double *g*, tdata * *target*)

Computes the density effect.

This function implements the density effect correction as formulated in Sternheimer & Peierls, [22] and as extended in Sternheimer, Berger & Seltzer, [21]. This version can distinguish between solids and gasses, and between metals and insulators. For conducting materials, there is a low-energy density effect.

Parameters

g	Projectile Lorentz factor.
target	A pointer to a TDATA structure.

Returns

The value of the density effect.

Definition at line 657 of file crange.c.

6.3.4.7 double djdx (double *e1*, double *z0*, double *I0*, double *f0*, double *K*, short *sswitch*, tdata * *target*)

Computes primary ionization.

This computes the primary ionization, the number of delta-rays produced per unit length. The formula is based on Bethe [7], as well as Fleischer *et al.*, [10].

Parameters

e1	The projectile kinetic energy in A MeV.
z0	The projectile charge.
I0	The binding energy of outermost electron in eV.
f0	The fraction of electrons in the outermost state.
K	A constant that depends on the target.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

Number of delta-rays per unit length in units of g^{-1} cm^2 .

Bug The parameters needed are not contained in the target table.

Definition at line 437 of file crange.c.

6.3.4.8 double effective_charge (double *z0*, double *e1*, double *z2*, short *sswitch*)

Computes effective projectile charge.

This is the modification of projectile charge due to electron capture. Hubert, Bimbot & Gauvin, [12], give an empirically determined function which depends on the target material. This version is used if SSWITCH_EC is set. Two older versions, from Anthony & Landford, [4], and Pierce & Blann, [19] are also available.

Parameters

z0	The bare projectile charge.

e1	The projectile kinetic energy in A MeV.
z2	The target mean nuclear charge.
sswitch	The switch bit field.

Returns

The effective projectile charge.

Bug The Pierce & Blann formula is not actually available; it is simply commented out.

Definition at line 366 of file crange.c.

6.3.4.9 double energy_table (int *i*)

Returns the energy corresponding to a value in a range table.

This utility returns an energy value from a (virtual) vector containing A logarithmically uniform distribution of energies between a minimum and maximum energy (defined by LOGTENEMIN and LOGTENEMAX), with a number of entries given by MAXE.

Parameters

i	The index of the vector.

Returns

The *i* th energy in A MeV.

Definition at line 1569 of file crange.c.

6.3.4.10 double Fbrems (double *x*)

Compute a mathematical function related to bremsstrahlung.

This function is used in an obsolete version of projectile slowing due to nuclear-nuclear bremsstrahlung. It appears in Heitler's treatment of bremsstrahlung, [11], which was adapted by Weaver & Westphal, [27].

Parameters

x	The input parameter.

Returns

The value of the function.

Bug Currently, this function is unused.

Definition at line 1039 of file crange.c.

6.3.4.11 tdata* find_target (char * *target*, tdata * *extratargets*)

Finds target data corresponding to a target name.

This function returns a pointer to a structure containing the target data corresponding to the input name. There is a built-in list. The built-in list may be added to or overridden by supplying an INI-type file on the command line, which will then be parsed & passed to this function. If the special target name "List" is passed to this function, the built-in list will be printed as an INI-type file.

Parameters

target	The name of a target.
extratargets	A pointer to an array of TDATA structures.

Returns

A pointer to a structure containing the target data. If the name of the target was not found, it will point to a dummy structure.

Definition at line 1596 of file crange.c.

6.3.4.12 short init_switch (char * *switchfile*)

Initializes the value of of the switch bit field.

This utility reads an INI-type file and sets the switch bit field accordingly.

Parameters

switchfile	The name of an INI-type file containing switch configuration.

Returns

The switch bit field.

Warning

If the iniparser library is not found, this function will only return the default value SSWITCH_DEFAULT.

Definition at line 1441 of file crange.c.

6.3.4.13 void init_table (void)

Initialize range-energy tables.

Sets all data in the array of RANGE_TABLE structures trange to zero.

Definition at line 1543 of file crange.c.

6.3.4.14 tdata* init_target (char * *targetfile*)

Read optional target data file.

This utility reads an INI-type file and returns an array of pointers to TDATA structures.

Parameters

targetfile	the name of an INI-type file containing target data.

Returns

A pointer to an array of TDATA structures. This pointer must be free()d!

Warning

If the iniparser library is not found, this function will only return a NULL pointer.

Definition at line 1481 of file crange.c.

6.3.4.15 double lindhard (double *zz*, double *aa*, double *bb*, short *sswitch*)

Compute the Lindhard-Sørensen correction.

This is the Lindhard-Sørensen correction including finite nuclear size effects as described in Lindhard & Sørensen, [18]. The defined variable SSWITCH_NS will turn off the nuclear size effect if it is set to zero. For values of the Lorentz factor above 10/R, where R is the nuclear size divided by the electron Compton wavelength, the correction is set to its asymptotic value which is described by Sørensen, [23]. This also avoids some difficulties with the evaluation of the confluent hypergeometric function (A. H. Sørensen, private communication).

Parameters

zz	The projectile charge.
aa	The projectile atomic mass.
bb	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).
sswitch	The switch bit field.

Returns

The value of the Lindhard-Sørensen correction.

Definition at line 897 of file crange.c.

6.3.4.16 double olddelta (double *g*, tdata * *target*)

Computes an obsolete version of the density effect.

This function implements the density effect correction as originally formulated in Sternheimer & Peierls, [22]. Although it is now obsolete, I have included it here for compatibility with earlier codes.

Parameters

g	Projectile Lorentz factor.
target	A pointer to a TDATA structure.

Returns

The value of the density effect.

Definition at line 692 of file crange.c.

6.3.4.17 void print_target (tdata * *target*)

Prints a target table entry in INI format.

This utility prints a TDATA structure in INI format.

Parameters

target	A pointer to a TDATA structure.

Definition at line 1677 of file crange.c.

6.3.4.18 double qrange (double *e*, double *z1*, double *a1*, short *sswitch*, tdata * *target*)

Computes total range by direct integration of dE/dx.

This function computes total range by direct integration of the dedx() function. It does not create a range table or do table interpolation.

Parameters

e	Initial energy in A MeV.
z1	Projectile charge.
a1	Projectile mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

Total range in g cm^{-2} .

Bug Currently, this function isn't called by anything.

Definition at line 1183 of file crange.c.

6.3.4.19 double range (double *e*, double *z1*, double *a1*, short *sswitch*, tdata * *target*, int * *tno*)

Computes total range given initial energy.

This function computes total range given initial energy. The technique is quite clever, in that if from one call to the next, the projectile and target material parameters do not change, the calculation of range is performed by table interpolation rather than direct integration. The savings in calculation time can be enormous. However, the range of valid energies is limited by the size of the table. The function dE/dx is evaluated at most of the energies defined by the function energy_table(). Results are stored in the RANGE_TABLE array trange. The size of trange (set by MAXAB) is arbitrary and should be set to whatever is most useful. Certainly it should be no smaller than the number of target materials being used.

Parameters

e	Initial projectile kinetic energy in A MeV.
z1	Projectile charge.
a1	Projectile atomic mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.
tno	A pointer to the index of the most recently generated or used table.

Returns

Projectile range in g cm^{-2} .

Definition at line 1086 of file crange.c.

6.3.4.20 double relbloch (double *z12*, double *b1*, double *lambda*, double *theta0*)

Compute the relativistic Bloch correction.

This is the relativistic Bloch (or Ahlen) correction of Ahlen, [3]. The evaluation of this correction has been enormously simplified by the use of fully complex arithmetic.

Parameters

z12	The projectile charge.
b1	The projectile velocity in units of the speed of light (*i.e.* $\beta = v/c$).

lambda	A free parameter, described in bma().
theta0	A free parameter, described in bma().

Returns

The value of the relativistic Bloch correction.

Definition at line 838 of file crange.c.

6.3.4.21 double renergy (double *e*, double *r0*, double *z1*, double *a1*, short *sswitch*, tdata * *target*)

Extract energies from range tables.

This function extracts energies from a range table by table interpolation. It calls range() to initialze the range table or to find the correct table if it has already been computed.

Parameters

e	Projectile kinetic energy [A MeV].
r0	Range [g cm^{-2}].
z1	Projectile charge.
a1	Projectile atomic mass.
sswitch	The switch bit field.
target	A pointer to a TDATA structure.

Returns

The final energy of the projectile.

Definition at line 1348 of file crange.c.

6.3.4.22 void run_range (FILE * *finput*, FILE * *foutput*, short *sswitch*, tdata * *extratargets*)

Parses and executes the task list.

This utility function steps through the range, energy and dE/dx tasks specified in the input data file. The tasks are denoted by a single letter:

- *r* compute ranges
- *e* compute energies
- *d* compute dE/dx
- *j* compute dJ/dx (primary ionization)

The task letter should be followed by the energy (or range) at which to compute range (or energy), the charge and mass of the particle, and the name of the target material. Names of target materials can be found in the target.ini file. Target material names may be up to NAMEWIDTH characters in length and should contain no whitespace.

Parameters

finput	An open file pointer containing the task list.
foutput	An open file pointer to write results to.
sswitch	The switch bit field.
extratargets	A pointer to an array of TDATA structures.

Bug The primary ionization parameters are currently hard-coded.

Definition at line 1396 of file crange.c.

6.3.5 Variable Documentation

6.3.5.1 range_table trange[MAXAB]

The range-energy table.

This external variable contains the range-energy tables.

Definition at line 166 of file crange.h.

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