

Package ‘libamtrack’

January 27, 2015

Version 0.5.5

Date 2014-07-07

Title Computational routines for proton and ion radiotherapy

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Depends R (>= 2.11.0)

SystemRequirements Gnu Scientific Library version >= 1.8

Suggests lattice

Description This package is the R interface to the open-source, ANSI C library libamtrack (<http://libamtrack.dkfz.org>). libamtrack provides computational routines for the prediction of detector response and radiobiological efficiency in heavy charged particle beams. It is designed for research in proton and ion dosimetry and radiotherapy. libamtrack also provides many auxiliary physics routines for proton and ion beams. Original package and C-to-R conversion routines developed by Felix A. Klein.

URL libamtrack.dkfz.org

License GPL (>= 3)

Repository CRAN

Repository/R-Forge/Project libamtrack

Repository/R-Forge/Revision 7

Repository/R-Forge/DateTimeStamp 2014-07-07 15:02:12

Date/Publication 2014-07-08 07:49:26

NeedsCompilation yes

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libamtrack-package *libamtrack package*

Description

This package is the R interface to the open-source, ANSI C library libamtrack. libamtrack provides computational routines for the prediction of detector response and relative biological efficiency in heavy charged particle beams. It is designed for research in proton and ion dosimetry and radiotherapy. libamtrack also provides many auxiliary physics routines for proton and ion beams. Please note that libamtrack is still under heavy development and so is the R interface. Function can be unstable especially when arguments are pushed out of their scope. If you experience any trouble your feed back is very appreciated: <s.greilich@dkfz.de>.

Details

Package:	libamtrack
Version:	0.5.5 (Violet Wombat)
Date:	2014-07-07
Depends:	R (>= 2.12.0)
Suggests:	lattice
SystemRequirements:	gsl (optionally: cernlib to enable energy loss distributions)
License:	GPL (version 3 or later)

FUNCTION INDEX: Efficiency / RBE routines: These functions compute the relative efficiency / RBE of a mixed particle field according to a specific amorphous track model flavour and physics

AT.run.GSM.method	Grid-summation ('checkerboard') method
AT.run.IGK.method	Ion-gamma-kill ('Katz') method
AT.run.CPPSC.method	Compound-Poison process with successive convolutions (CPP-SC, 'SPIFF') method
AT.CPPSC.alpha.and.beta	Alpha, beta for ion beams as predicted by CPP-SC method

Track-structure routines: These functions handle underlying physic used in amorphous track modeling:

AT.D.RDD.Gy	Dose distribution around a particle track
AT.r.RDD.m	Inverse dose distribution around a particle track
AT.max.electron.ranges.m	Maximum electron range / track width
AT.gamma.response	Gamma / X ray response of a system
AT.inverse.gamma.response	Inverse Gamma / X ray response of a system

SPC routines: These functions provide an interface to spectral depth data:

<code>AT.SPC.read</code>	Read in spc data from file
<code>AT.SPC.spectrum.at.depth.step</code>	Extract spectrum at given depth step
<code>AT.SPC.spectrum.at.depth.g.cm2</code>	Extract spectrum at given depth (will use closest step)
<code>AT.SPC.tapply</code>	Applies a function to all depths of spc data

FLUKA routines: These function provide an interface to FLUKA output files:

<code>AT.FLUKA.read.USRBIN.mesh</code>	Reads USRBIN output (Cartesian mesh, also for multiple runs)
<code>AT.FLUKA.read.USRBIN.regs</code>	Reads USRBIN output (regions, also for multiple runs).
<code>AT.FLUKA.read.USRTRACK</code>	Reads USRTRACK output (energy spectra, also for multiple runs)
<code>AT.FLUKA.particle.name.to.libamtrack.particle.name</code>	Converts FLUKA particle names to libamtrack conventions.

Physics routines: These functions handle the physics of proton and ion beams needed in libamtrack. Stopping-power routines:

<code>AT.Stopping.Power.keV.um</code>	Unrestricted LET / Stopping power
<code>AT.Stopping.Power.MeV.cm2.g</code>	Unrestricted LET per mass / mass stopping power
<code>AT.stopping.power.ratio</code>	Computes stopping power ratios, also for mixed fields
<code>TODO:</code>	Re-enable CSDA functions
<code>AT.WEPL.Bethe</code>	Water equivalent path length from Bethe range

Mean LET / energy in mixed fields routines:

<code>AT.fluence.weighted.LET.MeV.cm2.g</code>	Computes fluence-weighted LET
<code>AT.dose.weighted.LET.MeV.cm2.g</code>	Computes dose-weighted LET
<code>AT.fluence.weighted.E.MeV.u</code>	Computes fluence-weighted mean energy
<code>AT.dose.weighted.E.MeV.u</code>	Computes dose-weighted mean energy

Dose / fluence conversions:

<code>AT.dose.Gy.from.fluence.cm2</code>	Compute dose(s) for given fluence(s) and particle(s)
<code>AT.fluence.cm2.from.dose.Gy</code>	Compute fluence(s) given dose(s) and particle(s)
<code>AT.total.D.Gy</code>	Computes total dose for a mixed field
<code>AT.total.fluence.cm2</code>	Computes total fluence for a mixed field

Beam related routines:

<code>AT.beam.par.technical.to.physical</code>	For double Gaussian beam, converts FWHM and particle number into fluence and sigma
<code>AT.beam.par.physical.to.technical</code>	Inverse, converts fluence and sigma width into FWHM and particle number

Misc physics routines:

<code>AT.momentum.MeV.c.u.from.E.MeV.u</code>	Momentum from kinetic energy
<code>AT.E.MeV.u.from.momentum.MeV.c.u</code>	Kinetic energy from momentum
<code>AT.effective.charge.from.E.MeV.u</code>	Effective charge of an ion depending on its kinetic energy

AT.max.E.transfer.MeV	Max energy transferred from an ion to secondary electrons
AT.mean.number.of.tracks.contrib	Mean number of tracks that desposit dose in a representative point
AT.Rutherford.SDCS	Rutherford cross section of energy transferred to sec. electrons
AT.beta.from.E	Relativistic beta of an ion with
AT.E.from.beta	Kinetic energy for given beta
AT.gamma.from.E	Relativistic gamma of an ion

Other routines:

AT.particle.name.from.particle.no	Converts particle index numbers into particle names
AT.particle.no.from.particle.name	Converts particle names into particle index numbers
AT.particle.no.from.Z.and.A	Returns particle index number for given mass and atomic number
AT.A.from.particle.no	Returns mass number for given particle number
AT.Z.from.particle.no	Returns atomic number for given particle number
AT.nuclear.spin.from.particle.no	Returns nuclear spin for given particle number
AT.electron.density.m3	Returns electron density from average Z and A
AT.electron.density.m3.from.material.no	Returns electron density for given material
AT.material.name.from.material.no	Converts material index numbers into material names
AT.material.no.from.material.name	Converts material names into material index numbers
AT.electron.density.m3.from.composition	Computes electron density from material composition
AT.average.A.from.composition	Computes average mass number from material composition
AT.average.Z.from.composition	Computes average atomic number from material composition
AT.effective.Z.from.composition	Computes effective atomic number from material composition
AT.I.eV.from.composition	Computes average I value from material composition
AT.set.user.material	Sets properties of user defined material (CAVE: only valid until library is f
AT.set.user.material.from.composition	Sets properties of user defined material from elemental composition (CAV
AT.get.materials.data	Returns properties of pre-defined materials

Helper routines shipped with libamtrack:

AT.add.leading.zeros	Adds leading zeros to a character string representing a number
AT.add.trailing.zeros	Adds trailing zeros to a character string representing a number

Author(s)

C2R autoconversion developed by: Felix Klein <fklein@embl.de> Package maintainer: Steffen Greilich <s.greilich@dkfz.de>

References

Greilich, Grzanka, Bassler, Andersen and Jakel, Amorphous track models: A numerical comparison study, doi:10.1016/j.radmeas.2010.05.039

See Also

<http://libamtrack.dkfz.org>


```

er.model          = df$er.model[i],
stopping.power.source.no
= 0)[[1]]        # use PSTAR data
}
xyplot( log10(D.Gy) ~ log10(r.m)|particle.name,
# Plot
df,
type          = 'l',
groups       = E.MeV.u,
auto.key     = TRUE)[c(2,1)]

#####
##### 3. DETECTOR EFFICIENCY #####
cat("Compute the relative efficiency of Alanine in 10 MeV protons\n")
cat("Waligorskis version of the Katz' model\n")
AT.run.IGK.method( particle.no          = 1001,
# namely protons with
E.MeV.u                                = 10,
# 10 MeV/u
fluence.cm2.or.dose.Gy                 = c(-1.0),
# delivering 1 Gy
material.no                             = 5,
# i.e. Alanine
rdd.model                               = 4,

# Katz parametrization of radial dose distribution with simplified extended
# targets
rdd.parameter                          = c(5e-8,1e-10),
# with 50 nm target size and 1e-10 dose minimum
er.model                                = 2,
# Butts&Katz parametrization of track radius
gamma.model                             = 2,
# Use general target/hit model but here...
gamma.parameters                        = c(1,500,1,1,0),
# ...as exponential saturation with characteristic dose 500 Gy
saturation.cross.section.factor        = 1.4,
# factor to take 'brush' around track into account
write.output                            = TRUE,
# write a log file
stopping.power.source.no                = 0)
# use PSTAR data

```

AT.A.from.particle.no *ATA.from.particle.no*

Description

Returns mass number for given particle number

Usage

```
AT.A.from.particle.no(particle.no)
```

Arguments

particle.no particle index number (array of size n) (see also [particle.no](#)).

Value

A mass number (array of size n)
return return

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L53

AT.add.leading.zeros *AT.add.leading.zeros*

Description

Adds leading zeros to a number and represent it in a string of fixed length.

Usage

```
AT.add.leading.zeros( x, digits = 5)
```

Arguments

x number
digits length of resulting string. Should be larger than $\log_{10}(x)$.

Value

Character string with digits characters.

Examples

```
# Represent 99 as '00099'  
AT.add.leading.zeros(x = 99, digits = 5)
```

`AT.add.trailing.zeros` *AT.add.trailing.zeros*

Description

Adds trailing zeros to a number and represent it in a string of fixed length.

Usage

```
AT.add.trailing.zeros( x, digits = 5)
```

Arguments

<code>x</code>	number
<code>digits</code>	length of resulting string.

Value

Character string with `digits` characters.

Examples

```
# Represent 99.1 as '99.100'  
AT.add.trailing.zeros(x = 99.1, digits = 5)
```

`AT.atomic.weight.from.element.acronym`
AT.atomic.weight.from.element.acronym

Description

Returns atomic weight for given elemental symbols

Usage

```
AT.atomic.weight.from.element.acronym(acronym)
```

Arguments

<code>acronym</code>	elemental symbols (array of size n).
----------------------	--------------------------------------

Value

<code>atomic.weight</code>	corresponding A (array of size n)
<code>status</code>	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L391

AT.atomic.weight.from.Z
AT.atomic.weight.from.Z

Description

Returns atomic weight for given Z

Usage

AT.atomic.weight.from.Z(Z)

Arguments

Z atomic number (array of size n).

Value

atomic.weight atomic weight (array of size n)
return return

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L109

AT.average.A.from.composition
AT.average.A.from.composition

Description

Computes the average mass number for a given material composition

Usage

AT.average.A.from.composition(A, weight.fraction)

Arguments

A mass numbers of constituents (array of size n).
weight.fraction relative fractions of weight of constituents (array of size n).

Value

average.A average A

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L386

AT.average.Z.from.composition
AT.average.Z.from.composition

Description

Computes the average atomic number for a given material composition

Usage

AT.average.Z.from.composition(Z, weight.fraction)

Arguments

Z atomic numbers of constituents (array of size n).
weight.fraction relative fractions of weight of constituents (array of size n).

Value

average.Z average Z

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L403

AT.beam.par.physical.to.technical
AT.beam.par.physical.to.technical

Description

Converts physical beam parameters of a symmetric, double lateral Gaussian shape beam, i.e. central (=peak) fluence and width (= 1 standard deviation) to technical, accelerator parameters, i.e. total number of particles and FWHM

Usage

```
AT.beam.par.physical.to.technical(fluence.cm2, sigma.cm)
```

Arguments

fluence.cm2	fluence in beam center (array of size n).
sigma.cm	beam width stdev (array of size n).

Value

N	resulting absolute particle numbers (array of size n)
FWHM.mm	resulting FWHMs (in mm) (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L371

Examples

```
# Technical parameters for a double Gaussian beam
# of Carbon ions at 270 MeV/u in water with
# 0.5 cm sigma width and 1 Gy in the peak
AT.beam.par.physical.to.technical( fluence.cm2 = AT.fluence.cm2.from.dose.Gy(
  E.MeV.u      = 270,

  D.Gy         = 1.0,

  particle.no  = AT.particle.no.from.particle.name("12C"),

  material.no  = AT.material.no.from.material.name("Water, Liquid"),

  stopping.power.source.no = 0),

  sigma.cm    = 0.5)
```

AT.beta.from.E	<i>AT.beta.from.E</i>
----------------	-----------------------

Description

Returns relativistic speed for many particles

Usage

AT.beta.from.E(E.MeV.u)

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
---------	---

Value

beta	vector of relative particle speed $\beta = v/c$ (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L34

Examples

```
# Compute beta between 1 and 1000 MeV/u:
AT.beta.from.E( E.MeV.u      = c(1,10,100,1000))
```

AT.Bethe.mean.energy.loss.MeV	<i>AT.Bethe.mean.energy.loss.MeV</i>
-------------------------------	--------------------------------------

Description

Computes the mean energy loss in a slab of material using the Bethe formula for many particles according to ICRU49 BUT WITHOUT shell, Bloch or Barkas correction! No effective projectile charge is considered!

Usage

AT.Bethe.mean.energy.loss.MeV(E.MeV.u, particle.no, material.no, slab.thickness.um)

Arguments

<code>E.MeV.u</code>	energies of particle per nucleon (see also E.MeV.u).
<code>particle.no</code>	particle indices (see also particle.no).
<code>material.no</code>	material index (see also material.no).
<code>slab.thickness.um</code>	slab thickness in um.

Value

<code>result</code>	result
---------------------	--------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L281

`AT.characteristic.single.scattering.angle`
AT.characteristic.single.scattering.angle

Description

Returns characteristic single scattering angles `chi_c`

Usage

`AT.characteristic.single.scattering.angle(E.MeV.u, particle.charge.e, target.thickness.cm, element.acronym)`

Arguments

<code>E.MeV.u</code>	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
<code>particle.charge.e</code>	vector of charge numbers of particle (array of size n).
<code>target.thickness.cm</code>	vector of thicknesses of target material in cm (array of size n).
<code>element.acronym</code>	vector of elemental symbols of target material (array of size n).

Value

<code>chi.c</code>	vector of characteristic single scattering angles in rad (array of size n)
<code>status</code>	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L34

AT.characteristicple.scattering.angle

AT.characteristicple.scattering.angle

Description

Returns characteristic multiple scattering angles Theta_M

Usage

```
AT.characteristicple.scattering.angle(E.MeV.u, particle.charge.e,
target.thickness.cm, element.acronym)
```

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
particle.charge.e	vector of charge numbers of particle (array of size n).
target.thickness.cm	vector of thicknesses of target material in cm (array of size n).
element.acronym	vector of elemental symbols of target material (array of size n).

Value

Theta.M	vector of characteristic multiple scattering angles in rad (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L181

 AT.CPPSC.alpha.and.beta

AT.CPPSC.alpha.and.beta

Description

Returns alpha and beta for an ion survival curve predicted by the CPPSC model. The arguments are directly passed on to the `AT.run.CPPSC.method` routine, some are provided default values here to simplify the use. !! THIS ROUTINE IS LIMITED TO THE LIN-QUAD MODEL BUT SHOULD BE GENERALIZED FOR ANY GAMMA REPNSE, BOTH IN TERMS OF INPUT X RAY PARAMETERS *AND* OF RETURNED (FITTED) ION PARAMETERS!! Cave: Even if input X ray response is LQ with cut dose, the resulting LQ will be purely linear-quadratic without high-dose linear characteristic.

Usage

```
AT.CPPSC.alpha.and.beta(E.MeV.u, particle.no, fluence.cm2.or.dose.Gy,
  material.no, RDD.model, RDD.parameters, ER.model, gamma.model,
  gamma.parameters, N2 = 20, fluence.factor = 1.0, write.output = FALSE,
  shrink.tails = TRUE, shrink.tails.under = 1e-30, adjust.N2 = TRUE)
```

Arguments

E.MeV.u	Energy
particle.no	Particle index
fluence.cm2.or.dose.Gy	Mean dose - will be varied for survival / response in a range 0.1x-10x.
material.no	Material index
RDD.model	RDD index
RDD.parameters	RDD parameters
ER.model	ER index
gamma.model	gamma model index, must be LQ = 5
gamma.parameters	gamma parameters, here alpha, beta, Dcut
N2	defaulted
fluence.factor	defaulted
write.output	defaulted
shrink.tails	defaulted
shrink.tails.under	defaulted
adjust.N2	defaulted

Value

List with following items

alpha	alpha for ion response curve
beta	beta for ion response curve
df	data frame with complete ion response curve as computed to find alpha and beta including residuals fo that fit.

Examples

```
# None yet
```

AT.D.RDD.Gy

AT.D.RDD.Gy

Description

Returns local dose as a function of distance `r_m` for a given radial dose distribution model

Usage

```
AT.D.RDD.Gy(r.m, E.MeV.u, particle.no, material.no, rdd.model,
rdd.parameter, er.model, stopping.power.source.no)
```

Arguments

<code>r.m</code>	distance [m] (array of size n).
<code>E.MeV.u</code>	particle (ion) energy per nucleon [MeV/u] (single number, no mixed fields) (see also E.MeV.u).
<code>particle.no</code>	particle code number (single number, no mixed fields) (see also particle.no).
<code>material.no</code>	material code number (single number, no mixed fields) (see also material.no).
<code>rdd.model</code>	radial dose distribution model index (see also rdd.model).
<code>rdd.parameter</code>	radial dose distribution model parameters (array of size 4).
<code>er.model</code>	electron range / track with model index (see also er.model).
<code>stopping.power.source.no</code>	TODO (see also stopping.power.source.no).

Value

<code>D.RDD.Gy</code>	dose [Gy] (array of size n)
<code>status</code>	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_RDD.c#L474

Examples

```

# Compute dose in several distances of an 100 MeV/u neon ion in water
# according to 'Site' parametrization
AT.D.RDD.Gy(  r.m           = 10^(-9:-4),
              E.MeV.u      = 100,
              particle.no   = 10020,
              material.no   = 1,
              rdd.model     = 4,
              rdd.parameter = c(5e-8, 1e-10),
              er.model      = 2,
              stopping.power.source.no = 0)

# Compare the Geiss parametrization of RDD for protons and Carbon ions at
# different energies:
require(lattice)
df <- expand.grid( E.MeV.u      = 10^seq(0, 3, length.out = 4),
                  particle.no   = c(1001,6012),
                  # protons and carbons
                  r.m           = 10^seq(-9, -2, length.out = 100),
                  # from 1 nm to 1 cm in 100 steps
                  material.no   = 2,
                  # Aluminium Oxide
                  rdd.model     = 3,
                  # Geiss parametrization
                  rdd.parameter = 5e-8,
                  # Fixed core size of 50 nm
                  er.model      = 4,
                  # Geiss track width parametrization
                  D.Gy          = 0)

# For later use
ii <- df$particle.no == 1001
# Add particle names
df$particle.name <- "Carbon-12"
df$particle.name[ii] <- "Protons"
for (i in 1:nrow(df)){
  # Loop through particles/energies
  df$D.Gy[i] <- AT.D.RDD.Gy( r.m           = df$r.m[i],
                            E.MeV.u      = df$E.MeV.u[i],
                            particle.no   = df$particle.no[i],
                            material.no   = df$material.no[i],
                            rdd.model     = df$rdd.model[i],
                            rdd.parameter = df$rdd.parameter[i],
                            er.model      = df$er.model[i],
                            stopping.power.source.no = 0)$D.RDD.Gy
}
xyplot( log10(D.Gy) ~ log10(r.m)|particle.name,
        # Plot
        df,
        type      = 'l',
        groups    = E.MeV.u,

```

```
auto.key = TRUE)[c(2,1)]
```

AT.density.g.cm3.from.element.acronym

AT.density.g.cm3.from.element.acronym

Description

Returns the elemental densities in g/cm³ for given elemental symbols

Usage

```
AT.density.g.cm3.from.element.acronym(acronym)
```

Arguments

acronym elemental symbols (array of size n).

Value

density corresponding elemental densities in g/cm³ (array of size n)

status status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L419

AT.dose.Gy.from.fluence.cm2

AT.dose.Gy.from.fluence.cm2

Description

Returns dose in Gy for each given particle

Usage

```
AT.dose.Gy.from.fluence.cm2(E.MeV.u, particle.no, fluence.cm2,  
material.no, stopping.power.source.no)
```

Arguments

E.MeV.u	energy of particles in the mixed particle field (array of size n) (see also E.MeV.u).
particle.no	type of the particles in the mixed particle field (array of size n) (see also particle.no).
fluence.cm2	fluence for each particle type (array of size n).
material.no	material index (see also material.no).
stopping.power.source.no	stopping power source index (see also stopping.power.source.no).

Value

dose.Gy	be allocated by the user which will be used to return the results (array of size n)
---------	---

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L297

Examples

```
# Compute dose from protons, He-3, C-12 and O-16 at
# same energy and fluence in air
AT.dose.Gy.from.fluence.cm2( E.MeV.u      = c(10, 10, 10, 10),
                             fluence.cm2 = c(1e7, 1e7, 1e7, 1e7),
                             particle.no  = c(1001, 2003, 6012, 8016),
                             material.no  = 7,
                             stopping.power.source.no = 0)
```

AT.dose.weighted.E.MeV.u

AT.dose.weighted.E.MeV.u

Description

Computes the dose-weighted average energy of a particle field Needed by SuccessiveConvolutions

Usage

```
AT.dose.weighted.E.MeV.u(E.MeV.u, particle.no, fluence.cm2,
                        material.no, stopping.power.source.no)
```

Arguments

E.MeV.u	energy of particles in the mixed particle field (array of size <code>number.of.field.components</code>) (see also <code>E.MeV.u</code>).
particle.no	particle index (array of size <code>number.of.field.components</code>) (see also <code>particle.no</code>).
fluence.cm2	fluences of particles in the mixed particle field (array of size <code>number.of.field.components</code>).
material.no	material index (see also <code>material.no</code>).
stopping.power.source.no	TODO (see also <code>stopping.power.source.no</code>).

Value

dose-weighted dose-weighted

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L536

Examples

```
# fluence- and dose-weighted mean energy for a simple mixed field
# of high and low (99/1) energy protons
AT.fluence.weighted.E.MeV.u( E.MeV.u      = c(100, 1),
                             fluence.cm2  = c(99e8, 1e8))
AT.dose.weighted.E.MeV.u( E.MeV.u      = c(100, 1),
                          particle.no   = c(1001, 1001),
                          fluence.cm2   = c(99e8, 1e8),
                          material.no   = 1,                               # water
                          stopping.power.source.no = 0)
```

AT.dose.weighted.LET.MeV.cm2.g

AT.dose.weighted.LET.MeV.cm2.g

Description

Computes the dose-weighted average LET of a particle field

Usage

```
AT.dose.weighted.LET.MeV.cm2.g(E.MeV.u, particle.no, fluence.cm2,
                               material.no, stopping.power.source.no)
```

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size `number.of.field.components`) (see also `E.MeV.u`).

particle.no particle index (array of size `number.of.field.components`) (see also `particle.no`).

fluence.cm2 fluences of particles in the mixed particle field (array of size `number.of.field.components`).

material.no material index (see also `material.no`).

stopping.power.source.no TODO (see also `stopping.power.source.no`).

Value

dose-weighted dose-weighted

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L610

Examples

```
# fluence- and dose-weighted LET for a simple mixed field
# of high and low (99/1) energy protons
AT.fluence.weighted.LET.MeV.cm2.g( E.MeV.u      = c(100, 5),
                                   particle.no   = c(1001, 1001),
                                   fluence.cm2   = c(99e8, 1e8),
                                   material.no    = 1,                               # water
                                   stopping.power.source.no = 0)
AT.dose.weighted.LET.MeV.cm2.g( E.MeV.u      = c(100, 5),
                                 particle.no   = c(1001, 1001),
                                 fluence.cm2   = c(99e8, 1e8),
                                 material.no    = 1,                               # water
                                 stopping.power.source.no = 0)
```

AT.E.from.beta

AT.E.from.beta

Description

Returns energy per nucleon of particle with relativistic speed beta

Usage

AT.E.from.beta(beta)

Arguments

beta vector of relative particle speed beta = v/c (array of size n).

Value

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L71

Examples

```
# Compute energies for betas between 0.1 and 0.99:
AT.E.from.beta( beta = c(0.1, 0.1*(1:9), 0.99))
```

```
AT.E.MeV.u.from.momentum.MeV.c.u
      AT.E.MeV.u.from.momentum.MeV.c.u
```

Description

Returns energy per nucleon for particles with given momentum per nucleon

Usage

```
AT.E.MeV.u.from.momentum.MeV.c.u(momentum.MeV.c.u)
```

Arguments

momentum.MeV.c.u	vector of particle momenta per nucleon [MeV/c], (array of size n).
------------------	--

Value

E.MeV.u	vector of energies of particle per nucleon [MeV], (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L112

Examples

```
# Get kinetic energy for a 502 MeV/c antiproton beam (CERN AD/ACE experiment):
AT.E.MeV.u.from.momentum.MeV.c.u( momentum.MeV.c.u = 502)
```

 AT.effective.charge.from.E.MeV.u

AT.effective.charge.from.E.MeV.u

Description

Effective charge according to Barkas-Bethe-approximation: for particles with given kinetic energy per nucleon

Usage

```
AT.effective.charge.from.E.MeV.u(E.MeV.u, particle.no)
```

Arguments

`E.MeV.u` vector of energies of particle per nucleon [MeV] (array of size `n`) (see also [E.MeV.u](#)).

`particle.no` type of the particles in the mixed particle field (array of size `n`) (see also [particle.no](#)).

Value

`effective.charge` Effective charge according to Barkas-Bethe-approximation (array of size `n`)

`status` status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L149

Examples

```
# Charge pick-up of several nuclids depending on ion energy
require(lattice)
df <- data.frame( E.MeV.u      = 10^seq(-1, 2, length.out = 50),
                  particle.name = c("1H", "3He", "6Li", "12C",
                  "16O"),
                  effective.charge = 0)

for(i in 1:nrow(df)){
  df$effective.charge[i] <- AT.effective.charge.from.E.MeV.u( E.MeV.u      =
df$E.MeV.u[i],
                                                              particle.no =
AT.particle.no.from.particle.name(df$particle.name[i])[1])
}
xyplot( effective.charge ~ log10(E.MeV.u),
        df,
        type      = 'l',
        groups    = particle.name,
```

```

auto.key = list( space = 'right', points = FALSE, lines = TRUE),
xlab     = 'kinetic energy / (MeV/u)',
ylab     = 'effective charge',
panel    = function(...){
            panel.grid(-1,-1)
            panel.xyplot(...)},
scales   = list( x = list( at      = -1:2,
                           labels = c("0.1", "1", "10", "100")))

```

AT.effective.collision.number

AT.effective.collision.number

Description

Returns effective collision numbers `exp_b`

Usage

```
AT.effective.collision.number(E.MeV.u, particle.charge.e,
target.thickness.cm, element.acronym)
```

Arguments

`E.MeV.u` vector of energies of particle per nucleon [MeV] (array of size `n`) (see also [E.MeV.u](#)).

`particle.charge.e` vector of charge numbers of particle (array of size `n`).

`target.thickness.cm` vector of thicknesses of target material in cm (array of size `n`).

`element.acronym` vector of elemental symbols of target material (array of size `n`).

Value

`exp.b` vector of effective collision numbers (array of size `n`)

`status` status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L101

AT.effective.Z.from.composition

AT.effective.Z.from.composition

Description

Computes the effective atomic number for a given material composition

Usage

AT.effective.Z.from.composition(Z, weight.fraction,
electron.densities.cm3, exponent)

Arguments

Z	atomic numbers of constituents (array of size n).
weight.fraction	relative fractions of weight of constituents (array of size n).
electron.densities.cm3	if not zero, weight fractions will additionally include electron densities per volume (array of size n).
exponent	exponent for additivity rule reflecting the photon energy regime (usually 3.5 at ~ 100 kV).

Value

effective.Z effective Z

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L420

AT.electron.density.m3

AT.electron.density.m3

Description

Returns electron density from average A and Z

Usage

AT.electron.density.m3(density.g.cm3, average.A, average.Z)

Arguments

density.g.cm3 material density in g/cm3 (array of size n).
average.A average mass number (array of size n).
average.Z average atomic number (array of size n).

Value

electron.density.m3
electron density in 1/m3 (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L350

AT.electron.density.m3.from.composition
AT.electron.density.m3.from.composition

Description

Computes the electron density for a given material composition

Usage

AT.electron.density.m3.from.composition(density.g.cm3, Z, A,
weight.fraction)

Arguments

density.g.cm3 physical density (in g per cm3) of material.
Z atomic numbers of constituents (array of size n).
A mass numbers of constituents (array of size n).
weight.fraction relative fractions of weight of constituents (array of size n).

Value

electron.density.m3
electron density per m3

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L364

AT.electron.density.m3.from.material.no
AT.electron.density.m3.from.material.no

Description

Get electron density [1/m3] for materials

Usage

AT.electron.density.m3.from.material.no(material.no)

Arguments

material.no material indices (array of size n) (see also [material.no](#)).

Value

electron.density.m3
 electron densities per m3 (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L327

AT.element.acronym.from.Z
AT.element.acronym.from.Z

Description

Returns elemental symbols for given Z

Usage

AT.element.acronym.from.Z(Z)

Arguments

Z atomic numbers (array of size n).

Value

acronym corresponding elemental symbols (array of size n)
 status status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L355

AT.energy.loss.distribution
AT.energy.loss.distribution

Description

Computes the energy loss distribution Uses Landau, Vavilov or Gauss depending on kappa parameter No effective projectile charge is considered!

Usage

```
AT.energy.loss.distribution(energy.loss.keV, E.MeV.u, particle.no,  
material.no, slab.thickness.um)
```

Arguments

energy.loss.keV	energy loss (array of size n).
E.MeV.u	energy of particle per nucleon (see also E.MeV.u).
particle.no	particle index (see also particle.no).
material.no	material index (see also material.no).
slab.thickness.um	slab thickness in um.

Value

fDdD	(array of size n)
------	-------------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L437

AT.energy.loss.FWHM *AT.energy.loss.FWHM*

Description

Computes the width of the energy loss distribution Uses Landau, Vavilov or Gauss depending on kappa parameter No effective projectile charge is considered!

Usage

AT.energy.loss.FWHM(E.MeV.u, particle.no, material.no,
slab.thickness.um)

Arguments

E.MeV.u energy of particle per nucleon (see also [E.MeV.u](#)).
particle.no particle index (see also [particle.no](#)).
material.no material index (see also [material.no](#)).
slab.thickness.um
 slab thickness in um.

Value

result result

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L683

AT.energy.loss.mode *AT.energy.loss.mode*

Description

Computes the most probable energy loss Uses Landau, Vavilov or Gauss depending on kappa parameter No effective projectile charge is considered!

Usage

AT.energy.loss.mode(E.MeV.u, particle.no, material.no,
slab.thickness.um)

Arguments

E.MeV.u energy of particle per nucleon (see also [E.MeV.u](#)).
particle.no particle index (see also [particle.no](#)).
material.no material index (see also [material.no](#)).
slab.thickness.um
 slab thickness in um.

Value

result result

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L658

AT.energy.stragglng.after.slab.E.MeV.u
 AT.energy.stragglng.after.slab.E.MeV.u

Description

Get energy spread of an ion beam after traversing a material slab according to Bohr's classical theory. Bohr, N. (1915), Phil. Mag. 30, 581ff, see also Evans, R.D. (1955), The atomic nucleus, McGraw Hill, New York, p. 661 Please note that the effective charge is assumed to be constant over the material slab If this is not the case you should apply this routine multiple times to subslices

Usage

AT.energy.stragglng.after.slab.E.MeV.u(E.MeV.u, particle.no,
material.no, slab.thickness.m, initial.sigma.E.MeV.u)

Arguments

E.MeV.u vector of energies of particle per nucleon [MeV] (array of size n) (see also [E.MeV.u](#)).
particle.no type of the particles in the mixed particle field (array of size n) (see also [particle.no](#)).
material.no index number for slab material (see also [material.no](#)).
slab.thickness.m
 thickness of slab in m.
initial.sigma.E.MeV.u
 energy spread - 1 sigma - before traversing the slab - can be 0 (array of size n).

Value

sigma.E.MeV.u energy spread - 1 sigma - after traversing the slab (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L271

AT.energy.straggling.MeV2.cm2.g

AT.energy.straggling.MeV2.cm2.g

Description

Get energy spread with depth according to Bohr's classical theory Bohr, N. (1915), Phil. Mag. 30, 581ff, see also Evans, R.D. (1955), The atomic nucleus, McGraw Hill, New York, p. 661 In the literature dsE^2dz is often given in units ergs²/cm. Here we report it mass-normalized MeV²*cm²/g Since the effective charge of the particle enters the equation, particle types and energies have to be given The equation is however limited to energies > 10 MeV/u and not too heavy ions TODO: add William extension for relativistic effects (Williams, E.J. (1945), Revs. Mod. Phys. 17, 217ff)

Usage

AT.energy.straggling.MeV2.cm2.g(E.MeV.u, particle.no, material.no)

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
particle.no	type of the particles in the mixed particle field (array of size n) (see also particle.no).
material.no	index number for slab material (see also material.no).

Value

dsE²dz.MeV².cm².g

Increase of energy straggling variance $\sigma.E^2$ per unit length of material (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L254

AT.fluence.cm2.from.dose.Gy
AT.fluence.cm2.from.dose.Gy

Description

Returns fluence in 1/cm2 for each given particle

Usage

AT.fluence.cm2.from.dose.Gy(E.MeV.u, particle.no, D.Gy, material.no,
 stopping.power.source.no)

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size n) (see also [E.MeV.u](#)).
 particle.no type of the particles in the mixed particle field (array of size n) (see also [particle.no](#)).
 D.Gy dose / Gy for each particle type (array of size n).
 material.no material index (see also [material.no](#)).
 stopping.power.source.no
 TODO (see also [stopping.power.source.no](#)).

Value

fluence.cm2 to be allocated by the user which will be used to return the results (array of size
 n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L327

AT.fluence.weighted.E.MeV.u
AT.fluence.weighted.E.MeV.u

Description

Computes the fluence-weighted average energy of a particle field Needed by SuccessiveConvolutions

Usage

AT.fluence.weighted.E.MeV.u(E.MeV.u, fluence.cm2)

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size `number.of.field.components`)
 (see also `E.MeV.u`).

fluence.cm2 fluences of particles in the mixed particle field (array of size `number.of.field.components`).

Value

average.E.MeV.u
 average.E.MeV.u

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L514

Examples

```
# fluence- and dose-weighted mean energy for a simple mixed field
# of high and low (99/1) energy protons
AT.fluence.weighted.E.MeV.u( E.MeV.u      = c(100, 1),
                             fluence.cm2  = c(99e8, 1e8))
AT.dose.weighted.E.MeV.u( E.MeV.u      = c(100, 1),
                          particle.no    = c(1001, 1001),
                          fluence.cm2    = c(99e8, 1e8),
                          material.no    = 1,                               # water
                          stopping.power.source.no = 0)
```

AT.fluence.weighted.LET.MeV.cm2.g
 AT.fluence.weighted.LET.MeV.cm2.g

Description

Computes the fluence-weighted average LET of a particle field

Usage

```
AT.fluence.weighted.LET.MeV.cm2.g(E.MeV.u, particle.no, fluence.cm2,
material.no, stopping.power.source.no)
```

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size `number.of.field.components`)
 (see also `E.MeV.u`).

particle.no particle index (array of size `number.of.field.components`) (see also `particle.no`).

fluence.cm2 fluences of particles in the mixed particle field (array of size `number.of.field.components`).

material.no material index (see also `material.no`).

stopping.power.source.no
 TODO (see also `stopping.power.source.no`).

Value

```
fluence-weighted
           fluence-weighted
```

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L574

Examples

```
# fluence- and dose-weighted LET for a simple mixed field
# of high and low (99/1) energy protons
AT.fluence.weighted.LET.MeV.cm2.g( E.MeV.u      = c(100, 5),
                                   particle.no   = c(1001, 1001),
                                   fluence.cm2   = c(99e8, 1e8),
                                   material.no    = 1,                               # water
                                   stopping.power.source.no = 0)
AT.dose.weighted.LET.MeV.cm2.g( E.MeV.u      = c(100, 5),
                                 particle.no   = c(1001, 1001),
                                 fluence.cm2   = c(99e8, 1e8),
                                 material.no    = 1,                               # water
                                 stopping.power.source.no = 0)
```

```
AT.FLUKA.particle.name.to.libamtrack.particle.name
           AT.FLUKA.particle.name.to.libamtrack.particle.name
```

Description

Converts FLUKA style particle names to libamtrack convention.

Usage

```
AT.FLUKA.particle.name.to.libamtrack.particle.name(
  FLUKA.particle.names)
```

Arguments

```
FLUKA.particle.names
           vector of strings containing the FLUKA-style particle names
```

Details

FLUKA particle names relating to all particle with a specific Z, e.g. LI* or H*, will be translated to the 'even' isotope $A = 2*Z$. The only exception is H* which will be replaced by 1H. For example, LI* → 6Li, C* → 12C, BE* → 8Be. This is a pure convention and does not necessarily represent the most prominent isotope. For most computations which only rely on Z it is, however, valid.

Value

Character string vector with libamtrack-style particle names.

Examples

```
AT.FLUKA.particle.name.to.libamtrack.particle.name( FLUKA.particle.names =
  c("H*", "B*", "B10", "C12", "BE7", "U238") )
```

```
AT.FLUKA.read.USRBIN.mesh
```

```
AT.FLUKA.read.USRBIN.mesh
```

Description

Reads USRBIN output for Cartesian mesh, also for multiple output files from cluster runs. As USRBIN (mesh) scores energy deposited per unit volume per primary weight (GeV/cm3), the density as to be given for dose computation.

Usage

```
AT.FLUKA.read.USRBIN.mesh(exp.name, number.of.runs, unit, data.source =
  'local', density.g.cm3 = 1.0)
```

Arguments

exp.name	Experiment name, i.e. name of input file (without '.inp' extension)
number.of.runs	Number of output files from parallel (cluster) runs.
unit	FLUKA output unit number
data.source	'local' if output files are from a local machine, 'condor' if from condor cluster, 'condor_cleaned' if from condor cluster with clean option (-c) in rcf luka.py
density.g.cm3	Physical density of material in mesh, needed for computation of dose.

Value

Data frame with deposited energy, deposited dose (and in case of multiple runs estimate of their standard deviation) for each mesh cell.

Examples

```
# None yet, requires FLUKA output file
```

```
AT.FLUKA.read.USRBIN.regs
    AT.FLUKA.read.USRBIN.regs
```

Description

Reads USRBIN output for a series of regions, also for multiple output files from cluster runs. As USRBIN (regions, option 12.0) scores energy deposited per primary weight (GeV), both the region volume(s) and density(ies) have to be given for dose computation.

Usage

```
AT.FLUKA.read.USRBIN.regs(exp.name, number.of.runs, unit, data.source =
    'local', vol.cm3 = NULL, density.g.cm3 = NULL)
```

Arguments

<code>exp.name</code>	Experiment name, i.e. name of input file (without '.inp' extension)
<code>number.of.runs</code>	Number of output files from parallel (cluster) runs.
<code>unit</code>	FLUKA output unit number
<code>data.source</code>	'local' if output files are from a local machine, 'condor' if from condor cluster, 'condor_cleaned' if from condor cluster with clean option (-c) in <code>rcfluka.py</code>
<code>vol.cm3</code>	Volume of regions, either single value (will be applied to all regions) or vector of length matching the number of regions (individual volume for each region).
<code>density.g.cm3</code>	Physical density of regions, either single value (will be applied to all regions) or vector of length matching the number of regions (individual density for each region).

Value

Data frame with deposited energy, deposited dose (and in case of multiple runs estimate of their standard deviation) for each region.

Examples

```
# None yet, requires FLUKA output file
```

AT.FLUKA.read.USRTRACK

AT.FLUKA.read.USRTRACK

Description

Reads USRTRACK output (for energy spectra scoring using flusw.SPC.f) for a series of regions, also for multiple output files from cluster runs (using rcfuka.py). USRTRACK scores the fluence per primary weight per bin width(cm-2/GeV) but only if the correct volume of the corresponding regions is given in the FLUKA input card! AT.FLUKA.read.USRTRACK will however out the absolute fluence for each energy bin (in cm-2) as this can be directly used by libamtrack.

Usage

```
AT.FLUKA.read.USRTRACK(exp.name, number.of.runs, unit, data.source =  
'local', compress = TRUE)
```

Arguments

exp.name	Experiment name, i.e. name of input file (without '.inp' extension)
number.of.runs	Number of output files from parallel (cluster) runs.
unit	FLUKA output unit number
data.source	'local' if output files are from a local machine, 'condor' if from condor cluster, 'condor_cleaned' if from condor cluster with clean option (-c) in rcfuka.py
compress	If TRUE, all entries with zero fluence will be removed from resulting data frame in order to save memory.

Value

Data frame with midpoints and widths of energy bins, particle index no `particle.no`, and fluence (absolute [cm-2], i.e. not normalized to bin width!) for each region.

Examples

```
# None yet, requires FLUKA output file
```

AT.gamma.from.E	<i>AT.gamma.from.E</i>
-----------------	------------------------

Description

Returns relativistic gamma

Usage

```
AT.gamma.from.E(E.MeV.u)
```

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
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Value

gamma	vector of results (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L52

Examples

```
# Compute mass in MeV/c2 for a proton with 1-1000 MeV kinetic energy:
938.3 * AT.gamma.from.E( E.MeV.u = 10^(0:3))$gamma
```

AT.gamma.response	<i>AT.gamma.response</i>
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Description

Returns a system (detector or cells) response for given doses according to the chosen gamma response model

Usage

```
AT.gamma.response(d.Gy, gamma.model, gamma.parameter, lethal.event.mode)
```

Arguments

d.Gy doses in Gy (array of size number.of.doses).
 gamma.model gamma response model index.
 gamma.parameter vector holding necessary parameters for the chose gamma response model (array of size 9).
 lethal.event.mode if true computation is done in lethal event mode.

Value

S gamma responses (array of size number.of.doses)

Examples

```
# Show the gamma response of two Al203 detectors (A & B) and two protocols
# ('peak' and 'total')

# parametrized in two components (single hit/single target and two hit/single
# target)
# as measured and published by Edmund et al., NIM B 262 (2007), 261-275
require(lattice)
# Compute 100 points between 0.1 and 25 Gy
# General hit/target model
d.Gy <- 10^seq(from = log10(0.1), to = log10(25),
  length.out = 100)
gamma.model <- 2
# Probe A, 'peak'
R <- 1
Smax <- 0.81e6
k1 <- Smax * (R / 100)
k2 <- Smax * (1 - R / 100)
gamma.parameter.peak.A <- c( k1 = k1, D01 = 0.36, c1 = 1, m1 = 1,
  k2 = k2, D02 = 3.06, c2 = 2, m2 = 1,
  0)
# Probe A, 'total'
R <- 33
Smax <- 6.2e6
k1 <- Smax * (R / 100)
k2 <- Smax * (1 - R / 100)
gamma.parameter.total.A <- c( k1 = k1, D01 = 1.13, c1 = 1, m1 = 1,
  k2 = k2, D02 = 1.77, c2 = 2, m2 = 1,
  0)
# Probe B, 'peak'
R <- 13
Smax <- 2.84e6
k1 <- Smax * (R / 100)
k2 <- Smax * (1 - R / 100)
gamma.parameter.peak.B <- c( k1 = k1, D01 = 4.15, c1 = 1, m1 = 1,
  k2 = k2, D02 = 5.14, c2 = 2, m2 = 1,
```

```

    0)
# Probe B, 'total'
R <- 44
Smax <- 27.6e6
k1 <- Smax * (R / 100)
k2 <- Smax * (1 - R / 100)
gamma.parameter.total.B <- c( k1 = k1, D01 = 2.90, c1 = 1, m1 = 1,
                             k2 = k2, D02 = 4.66, c2 = 2, m2 = 1,
                             0)
vecA <- AT.gamma.response( d.Gy          = d.Gy,
                           gamma.model   = gamma.model,
                           gamma.parameter = gamma.parameter.peak.A,
                           lethal.event.mode = FALSE)$response
vecB <- AT.gamma.response( d.Gy          = d.Gy,
                           gamma.model   = gamma.model,
                           gamma.parameter = gamma.parameter.total.A,
                           lethal.event.mode = FALSE)$response
vecC <- AT.gamma.response( d.Gy          = d.Gy,
                           gamma.model   = gamma.model,
                           gamma.parameter = gamma.parameter.peak.B,
                           lethal.event.mode = FALSE)$response
vecD <- AT.gamma.response( d.Gy          = d.Gy,
                           gamma.model   = gamma.model,
                           gamma.parameter = gamma.parameter.total.B,
                           lethal.event.mode = FALSE)$response

# Compose data frame
df <- data.frame( d.Gy   = rep( d.Gy, 4),
                  S      = c(vecA, vecB, vecC, vecD ),
                  which  = rep( c( rep("peak", length(d.Gy)),
                                   rep("total", length(d.Gy))), 2),
                  probe  = c( rep("probe A", 2 * length(d.Gy)),
                               rep("probe B", 2 * length(d.Gy))))
# Plot
xyplot( log10(S) ~ log10(d.Gy)|probe,
        df,
        groups = which,
        type = 'l',
        lwd = 2,
        ylim = log10(c(1e3, 4e7)),
        ylab = list( "OSL response", cex = 1.2),
        xlim = log10(c(0.1, 25)),
        xlab = list( "dose / Gy", cex = 1.2),
        scales = list( x = list( at      = log10(c(1,10,20)),
                                labels = as.character(c(1,10,20))),
                       y = list( at      = c(4,5,6,7),
                                labels = 10^(c(4,5,6,7))))),
        aspect = 2.5)

```

Description

Returns material data for list of materials

Usage

```
AT.get.materials.data(material.no)
```

Arguments

`material.no` material indices (array of size `number.of.materials`) (see also [material.no](#)).

Value

<code>density.g.cm3</code>	material density in g/cm ³ (array of size <code>number.of.materials</code>)
<code>I.eV</code>	mean ionization potential in eV (array of size <code>number.of.materials</code>)
<code>alpha.g.cm2.MeV</code>	fit parameter for power-law representation of <code>stp.power/range/E</code> -dependence (array of size <code>number.of.materials</code>)
<code>p.MeV</code>	fit parameter for power-law representation of <code>stp.power/range/E</code> -dependence (array of size <code>number.of.materials</code>)
<code>m.g.cm2</code>	fit parameter for the linear representation of fluence changes due to nuclear interactions based on data from Janni 1982 (array of size <code>number.of.materials</code>)
<code>average.A</code>	average mass number (array of size <code>number.of.materials</code>)
<code>average.Z</code>	average atomic number (array of size <code>number.of.materials</code>)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L238

AT.Highland.angle *AT.Highland.angle*

Description

Returns Highland angles Theta0

Usage

```
AT.Highland.angle(E.MeV.u, particle.charge.e, l.over.lR)
```

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
particle.charge.e	vector of charge numbers of particle (array of size n).
l.over.lR	vector of thicknesses of target material in radiation lengths (array of size n).

Value

Theta0	vector of Highland angles in rad (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L345

AT.I.eV.from.composition

AT.I.eV.from.composition

Description

Computes the I value for a given material composition

Usage

AT.I.eV.from.composition(Z, A, weight.fraction)

Arguments

Z	atomic numbers of constituents (array of size n).
A	mass numbers of constituents (array of size n).
weight.fraction	relative fractions of weight of constituents (array of size n).

Value

I.eV	I value in eV
------	---------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L452

AT.I.eV.from.element.acronym
AT.I.eV.from.element.acronym

Description

Returns the I values in eV for given elemental symbol

Usage

AT.I.eV.from.element.acronym(acronym)

Arguments

acronym elemental symbols (array of size n).

Value

I corresponding I values in eV (array of size n)
status status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L448

AT.inverse.gamma.response
AT.inverse.gamma.response

Description

Computes the inverse gamma response, i.e. the dose for a given response. !!THIS WORKS UPTONOW FOR THE LIN-QUAD-MODEL ONLY, BUT SHOULD BE DEVELOPED TO A GENERAL ROUTINE!!

Usage

AT.inverse.gamma.response(surv, alpha, beta)

Arguments

surv Response (survival)
alpha Alpha parameter in (1/Gy)
beta Beta parameter in (1/Gy²)

Value

Dose in Gy

Examples

```
# Compute dose for 10% survival for HSG cells
AT.inverse.gamma.response( surv = 0.1, alpha = 0.2, beta = 0.05)
```

AT.kappa	<i>AT.kappa</i>
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Description

Computes the kappa criterium for the energy loss distribution according to Seltzer & Berger No effective projectile charge is considered!

Usage

```
AT.kappa(E.MeV.u, particle.no, material.no, slab.thickness.um)
```

Arguments

E.MeV.u	energy of particle per nucleon (see also E.MeV.u).
particle.no	particle index (see also particle.no).
material.no	material index (see also material.no).
slab.thickness.um	slab thickness in um.

Value

result	result
--------	--------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L294

AT.lambda.from.energy.loss
AT.lambda.from.energy.loss

Description

Computes the lambda parameter for the Vavilov distribution acc. to Seltzer & Berger No effective projectile charge is considered!

Usage

AT.lambda.from.energy.loss(energy.loss.keV, E.MeV.u, particle.no,
 material.no, slab.thickness.um)

Arguments

energy.loss.keV	energy loss (array of size n).
E.MeV.u	energy of particle per nucleon (see also E.MeV.u).
particle.no	particle index (see also particle.no).
material.no	material index (see also material.no).
slab.thickness.um	slab thickness in um.

Value

lambda.V	(array of size n)
----------	-------------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L309

AT.Landau.PDF *AT.Landau.PDF*

Description

Compute Landau distribution using CERNLIB (G115)

Usage

AT.Landau.PDF(lambda)

Arguments

lambda lambda (array of size n).

Value

density resulting density (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L41

`AT.material.name.from.material.no`

AT.material.name.from.material.no

Description

Returns material name(s) for given material index number(s)

Usage

`AT.material.name.from.material.no(material.no)`

Arguments

material.no material index number(s) (see also [material.no](#)).

Value

material.name material name(s) (see also [material.name](#)).

Examples

```
# Get material names for all predefined materials
AT.material.name.from.material.no( material.no = 1:25)
```

```
AT.material.no.from.material.name
    AT.material.no.from.material.name
```

Description

Returns material name(s) for given material index number(s)

Usage

```
AT.material.no.from.material.name(material.name)
```

Arguments

material.name material name(s) (see also [material.name](#)).

Value

material.no material index number(s) (see also [material.no](#)).

Examples

```
# Get material index numbers for three materials of which one is not
# implemented
AT.material.no.from.material.name( material.name = c("Water, Liquid",
  "PMMA", "Squirrel liver pudding"))
```

```
AT.max.E.transfer.MeV AT.max.E.transfer.MeV
```

Description

Kinetic energy maximally transferred from an ion to an electron in a collision - relativistic or non-relativistic

Usage

```
AT.max.E.transfer.MeV(E.MeV.u)
```

Arguments

E.MeV.u energies of particle per nucleon [MeV/u]; if positive, the computation will be relativistic; if negative, the classic formular will be used (array of size n) (see also [E.MeV.u](#)).

Value

```
max.E.transfer.MeV
                maximal energies transferred (array of size n)

status          status
```

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L209

Examples

```
# Plot maximum energy transferred in a collision in the range from 1 to 1000
# MeV
# (this is independent of the ion type!) and compare the classical with
# the relativistic approach
require(lattice)
E.MeV.u    <- 10^seq(0, 3, length.out = 50)
df         <- data.frame( E.MeV                = E.MeV.u,
                        max.E.keV.classical    = AT.max.E.transfer.MeV(-1.0
* E.MeV.u)$max.E.transfer.MeV * 1000,
                        max.E.keV.relativistic =
AT.max.E.transfer.MeV(E.MeV.u)$max.E.transfer.MeV * 1000)
plot1 <- xyplot( log10(max.E.keV.relativistic) ~ log10(E.MeV),
                df,
                type      = 'o',
                xlab      = list('ion kinetic energy', font = 4),
                ylab      = list('maximum electron energy (relativistic)',
font = 4),
                scales   = list( x = list( at = 0:3, labels = c("1 MeV/u",
"10 MeV/u", "100 MeV/u", "1 GeV/u")),
                                y = list( at = 1:3, labels = c("10 keV",
"100 keV", "1 MeV"))))
plot2 <- xyplot( log10(max.E.keV.classical) ~ log10(max.E.keV.relativistic),
                df,
                type      = 'l',
                col       = 'red',
                lwd       = 2,
                xlab      = 'maximum electron energy (relativistic) / keV',
                ylab      = 'maximum electron energy (classical) / keV',
                xlim      = c(0, 4),
                ylim      = c(0, 4),
                scales    = list( at = 1:3, labels = c("10", "100", "1000")),
                panel     = function(...){
                            panel.grid(-1, -1)
                            panel.abline(a = 0, b = 1, lty = 2, col =
'grey')
                            panel.xyplot(...))
plot(plot1, split = c(1, 1, 2, 1))
plot(plot2, split = c(2, 1, 2, 1), newpage = FALSE)
```

 AT.max.electron.ranges.m

AT.max.electron.ranges.m

Description

Returns the maximum electron range (track radius) in m for a given parametrization

Usage

```
AT.max.electron.ranges.m(E.MeV.u, material.no, er.model)
```

Arguments

E.MeV.u	kinetic energy for particles in the given field (array of size number.of.particles) (see also E.MeV.u).
material.no	material index (see also material.no).
er.model	electron-range model index (see also er.model).

Value

```
max.electron.range.m
    electron range (track radius) in m (array of size number.of.particles)
```

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_ElectronRange.c#L135

Examples

```
# Compute the electron range in PMMA for the Tabata parametrization between
# 0.3 keV and 30 MeV
AT.max.electron.ranges.m( E.MeV.u    = 0.3 * 10^(-4:2),
                          material.no = 4,
                          er.model    = 7)
```

AT.mean.number.of.tracks.contrib
AT.mean.number.of.tracks.contrib

Description

Computes the number of track contributing to a representative point in a mixed field

Usage

```
AT.mean.number.of.tracks.contrib(E.MeV.u, particle.no, fluence.cm2,
    material.no, er.model,
    stopping.power.source.no)
```

Arguments

E.MeV.u	energy of particles in the mixed particle field (array of size number.of.field.components) (see also E.MeV.u).
particle.no	particle index (array of size number.of.field.components) (see also particle.no).
fluence.cm2	fluences of particles in the mixed particle field (array of size number.of.field.components).
material.no	material index (see also material.no).
er.model	chosen electron-range-model (see also er.model).
stopping.power.source.no	TODO (see also stopping.power.source.no).

Value

resulting	resulting
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See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L700

AT.Moliere.function.f0
AT.Moliere.function.f0

Description

Returns values f0(red_Theta) of the first Moliere function

Usage

```
AT.Moliere.function.f0(red.Theta)
```

Arguments

red.Theta reduced angle variable.

Value

first first

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L219

AT.Moliere.function.f1

AT.Moliere.function.f1

Description

Returns values f1(red_Theta) of the second Moliere function

Usage

AT.Moliere.function.f1(red.Theta)

Arguments

red.Theta reduced angle variable.

Value

second second

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L231

 AT.Moliere.function.f2

AT.Moliere.function.f2

Description

Returns values f2(red_Theta) of the third Moliere function

Usage

AT.Moliere.function.f2(red.Theta)

Arguments

red.Theta reduced angle variable.

Value

third third

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L255

 AT.momentum.MeV.c.u.from.E.MeV.u

AT.momentum.MeV.c.u.from.E.MeV.u

Description

Returns relativistic momenta per nucleon for particles with given kinetic energy

Usage

AT.momentum.MeV.c.u.from.E.MeV.u(E.MeV.u)

Arguments

E.MeV.u kinetic energy per nucleon (array of size n) (see also [E.MeV.u](#)).

Value

momentum.MeV.c momentum per nucleon (array of size n)

return return

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L242

Examples

```
# Relation between kinetic proton energy and momentum
# in relativistic and non-relativistic regime
require(lattice)
E.MeV.u <- 10^seq(-2, 5, length.out = 100)
df <- data.frame( E.MeV      = E.MeV.u,
                  p.MeV.c    =
    AT.momentum.MeV.c.u.from.E.MeV.u(E.MeV.u)$momentum.MeV.c)
xyplot( log10(p.MeV.c) ~ log10(E.MeV),
        df,
        type = 'l',
        xlab = 'proton kinetic energy / MeV',
        ylab = 'proton momentum / (MeV/c)',
        panel = function(...){
            panel.abline(a = 0, b = 1, lty = 2, col = 'grey')
            panel.xyplot(...)}

```

AT.nuclear.spin.from.particle.no

AT.nuclear.spin.from.particle.no

Description

Returns nuclear spin from particle no

Usage

```
AT.nuclear.spin.from.particle.no(particle.no)
```

Arguments

particle.no particle index number (array of size n) (see also [particle.no](#)).

Value

I	nuclear spin (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L184

`AT.particle.name.from.particle.no`
AT.particle.name.from.particle.no

Description

Returns particle name(s) for given particle index number(s)

Usage

`AT.particle.name.from.particle.no(particle.no)`

Arguments

`particle.no` particle name(s) (see also [particle.no](#)).

Value

`particle.name` particle index number(s) (see also [particle.name](#)).

Examples

```
# Get particle index names for some nuclides
AT.particle.name.from.particle.no( particle.no = c(1001, 6012))
```

`AT.particle.no.from.particle.name`
AT.particle.no.from.particle.name

Description

Returns particle index number(s) for given particle names(s)

Usage

`AT.particle.no.from.particle.name(particle.name)`

Arguments

`particle.name` particle name(s) (see also [particle.name](#)).

Value

`particle.no` particle index number(s) (see also [particle.no](#)).

Examples

```
# Get particle names for some nuclides
AT.particle.no.from.particle.name( particle.name = c("1H", "2H", "3He",
"12C", "16O","238U"))
```

```
AT.particle.no.from.Z.and.A
      AT.particle.no.from.Z.and.A
```

Description

Returns particle index number from given A and Z

Usage

```
AT.particle.no.from.Z.and.A(Z, A)
```

Arguments

Z	atomic numbers (array of size n).
A	mass number (array of size n).

Value

particle.no	corresponding particle index numbers (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L34

AT.r.RDD.m

AT.r.RDD.m

Description

Returns distance as a function of dose

Usage

```
AT.r.RDD.m(D.RDD.Gy, E.MeV.u, particle.no, material.no, rdd.model,
rdd.parameter, er.model, stopping.power.source.no)
```

Arguments

D.RDD.Gy	dose [Gy] (array of size n).
E.MeV.u	particle (ion) energy per nucleon [MeV/u] (see also E.MeV.u).
particle.no	particle code number (see also particle.no).
material.no	material code number (see also material.no).
rdd.model	Radial Dose Distribution model code number (see also rdd.model).
rdd.parameter	Radial Dose Distribution model parameters vector (array of size 4).
er.model	delta electron range model code number (see also er.model).
stopping.power.source.no	TODO (see also stopping.power.source.no).

Value

r.RDD.m	distance [m] (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_RDD.c#L645

AT.reduced.target.thickness

AT.reduced.target.thickness

Description

Returns reduced target thicknesses B

Usage

```
AT.reduced.target.thickness(E.MeV.u, particle.charge.e,
    target.thickness.cm, element.acronym)
```

Arguments

E.MeV.u	vector of energies of particle per nucleon [MeV] (array of size n) (see also E.MeV.u).
particle.charge.e	vector of charge numbers of particle (array of size n).
target.thickness.cm	vector of thicknesses of target material in cm (array of size n).
element.acronym	vector of elemental symbols of target material (array of size n).

Value

B vector of reduced target thicknesses (array of size n)
 status status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L147

AT.run.CPPSC.method *AT.run.CPPSC.method*

Description

Computes HCP response and relative efficiency/RBE using compound Poisson processes and successive convolutions (CPP_SC, the SPIFF algorithm)

Usage

```
AT.run.CPPSC.method(E.MeV.u, particle.no, fluence.cm2.or.dose.Gy,
  material.no, stopping.power.source.no,
  rdd.model, rdd.parameters, er.model, gamma.model, gamma.parameters,
  N2, fluence.factor, write.output, shrink.tails, shrink.tails.under,
  adjust.N2, lethal.events.mode)
```

Arguments

E.MeV.u particle energy for each component in the mixed particle field [MeV/u] (array of size [number.of.field.components](#)) (see also [E.MeV.u](#)).

particle.no particle type for each component in the mixed particle field (array of size [number.of.field.components](#)) (see also [particle.no](#)).

fluence.cm2.or.dose.Gy
 if positive, particle fluence for each component in the mixed particle field [1/cm2];
 if negative, particle dose for each component in the mixed particle field [Gy] (array of size [number.of.field.components](#)) (see also [fluence.cm2.or.dose.Gy](#)).

material.no index number for detector material (see also [material.no](#)).

stopping.power.source.no
 TODO (see also [stopping.power.source.no](#)).

rdd.model index number for chosen radial dose distribution (see also [rdd.model](#)).

rdd.parameters parameters for chosen radial dose distribution (array of size 4).

er.model index number for chosen electron-range model (see also [er.model](#)).

gamma.model index number for chosen gamma response.

gamma.parameters
 parameters for chosen gamma response (array of size 9).

N2	number of bins per factor of two for the dose scale of local dose histogram.
fluence.factor	factor to scale the fluences / doses given in fluence.cm2.or.dose.Gy with.
write.output	if true, a log-file is written to SuccessiveConvolutions.txt in the working directory.
shrink.tails	if true, tails of the local dose distribution, contributing less than shrink.tails.under are cut.
shrink.tails.under	limit for tail cutting in local dose distribution.
adjust.N2	if true, N2 will be increase if necessary at high fluence to ensure sufficient local dose histogram resolution.
lethal.events.mode	if true, computations are done for dependent subtargets.

Value

N2	number of bins per factor of two for the dose scale of local dose histogram
relative. efficiency	particle response at dose D / gamma response at dose D
d.check	sanity check: total dose (in Gy) as returned by the algorithm
S.HCP	absolute particle response
S.gamma	absolute gamma response
mean.number.of.tracks.contrib	mean number of tracks contributing to representative point
start.number.of.tracks.contrib	low fluence approximation for mean number of tracks contributing to representative point (start value for successive convolutions)
n.convolution	number of convolutions performed to reach requested dose/fluence
lower.Jensen.bound	lower bound for Jensen's inequality
upper.Jensen.bound	upper bound for Jensen's inequality

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_Algorithms_CPP.c#L34

Examples

```
# Compute the relative efficiency of an Alanine detector in a mixed
# carbon / proton field
AT.run.CPPSC.method( particle.no           = c(6012, 1001,
  1001),          # namely carbon, protons, and protons with
                  E.MeV.u                 = c(270, 270, 5),

# 270 MeV/u (primary Carbon, 270 MeV/u and 5 MeV/u (fast and slow proton
```

```

# component)
      fluence.cm2.or.dose.Gy           = c(1e8, 1e9, 1e7),
# and their corresponding fluences
      material.no                       = 5,
# i.e. Alanine
      rdd.model                         = 3,
# simple 'Geiss' parametrization of radial dose distribution
      rdd.parameter                     = 50e-9,
# with 50 nm core radius
      er.model                          = 4,
# M. Scholz' parametrization of track radius
      gamma.model                       = 2,
# General hit/target X ray response, but
      gamma.parameters                  = c(1,500,1,1,0),

# as simple single exponential saturation (one hit, one target), saturation
# dose 500 Gy
      N2                                = 10,
# ten bins per factor 2 for internal local dose histogramming
      fluence.factor                     = 1.0,
# can be used to easily scale total fluence (historical)
      write.output                       = TRUE,
# write a log file
      shrink.tails                       = TRUE,
# cut tails of local dose distribution, if...
      shrink.tails.under                 = 1e-30,
# ... they contribute less then 1e-30 to first moment of histogram
      adjust.N2                          = TRUE,
# perform rebinning if local dose distribution becomes too narrow
      lethal.events.mode                 = FALSE,
# use independent subtargets
      stopping.power.source.no           = 0)

```

AT.run.GSM.method *AT.run.GSM.method*

Description

Computes HCP response and relative efficiency/RBE using summation of tracks on a Cartesian grid (the GSM algorithm). Be aware that this routine can take considerable time to compute depending on the arguments, esp. for higher energy (>10 MeV/u) particles. It is therefore advantageous to test your settings with a low number of runs first.

Usage

```

AT.run.GSM.method(E.MeV.u, particle.no, fluence.cm2.or.dose.Gy,
  material.no, stopping.power.source.no,
  rdd.model, rdd.parameters, er.model, gamma.model, gamma.parameters,
  N.runs, write.output, nX, voxel.size.m, lethal.events.mode)

```

Arguments

E.MeV.u	particle energy for each component in the mixed particle field [MeV/u] (array of size <code>number.of.field.components</code>) (see also <code>E.MeV.u</code>).
particle.no	particle type for each component in the mixed particle field (array of size <code>number.of.field.components</code>) (see also <code>particle.no</code>).
fluence.cm2.or.dose.Gy	if positive, particle fluence for each component in the mixed particle field [1/cm ²]; if negative, particle dose for each component in the mixed particle field [Gy] (array of size <code>number.of.field.components</code>) (see also <code>fluence.cm2.or.dose.Gy</code>).
material.no	index number for detector material (see also <code>material.no</code>).
stopping.power.source.no	TODO (see also <code>stopping.power.source.no</code>).
rdd.model	index number for chosen radial dose distribution (see also <code>rdd.model</code>).
rdd.parameters	parameters for chosen radial dose distribution (array of size 4).
er.model	index number for chosen electron-range model (see also <code>er.model</code>).
gamma.model	index number for chosen gamma response.
gamma.parameters	parameters for chosen gamma response (array of size 9).
N.runs	number of runs within which track positions will be resampled.
write.output	if true, a protocol is written to SuccessiveConvolutions.txt in the working directory.
nX	number of voxels of the grid in x (and y as the grid is quadratic).
voxel.size.m	side length of a voxel in m.
lethal.events.mode	if true, allows to do calculations for cell survival.

Value

relative.efficacy	particle response at dose D / gamma response at dose D
d.check	sanity check: total dose (in Gy) as returned by the algorithm
S.HCP	absolute particle response
S.gamma	absolute gamma response
n.particles	average number of particle tracks on the detector grid
sd.relative.efficacy	standard deviation for relative.efficacy
sd.d.check	standard deviation for d.check
sd.S.HCP	standard deviation for S.HCP
sd.S.gamma	standard deviation for S.gamma
sd.n.particles	standard deviation for n.particles

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_Algorithms_GSM.c#L277

Examples

```
# Compute the relative efficiency of an Alanine detector
# in a proton field
AT.run.GSM.method( # protons
                  particle.no           = 1001,
                  # with 10 MeV/u
                  E.MeV.u               = 10,
                  # delivering 1 Gy
                  fluence.cm2.or.dose.Gy = c(-1.0),
                  # i.e. Alanine
                  material.no           = 5,

                  # simple 'Geiss' parametrization of radial dose distribution
                  rdd.model              = 3,
                  # with 50 nm core radius
                  rdd.parameter          = 50e-9,
                  # M. Scholz' parametrization of track radius
                  er.model               = 4,
                  # Use exponential saturation
                  gamma.model            = 4,
                  # max. response normalized to 1, saturation dose 500 Gy
                  gamma.parameters      = c(1,500),
                  # resample 1000 times
                  N.runs                 = 1000,
                  # write a log file
                  write.output           = TRUE,
                  # use a 10x10 grid
                  nX                      = 10,
                  # with 5 nm voxel size
                  voxel.size.m           = 5e-9,
                  # use independent subtargets
                  lethal.events.mode     = FALSE,
                  # and PSTAR stopping powers
                  stopping.power.source.no = 0)
```

AT.run.IGK.method

AT.run.IGK.method

Description

Computes HCP response and relative efficiency/RBE using Katz' Ion-Gamma-Kill approach according to Waligorski, 1988

Usage

```
AT.run.IGK.method(E.MeV.u, particle.no, fluence.cm2.or.dose.Gy,
  material.no, stopping.power.source.no,
  rdd.model, rdd.parameters, er.model, gamma.model, gamma.parameters,
  saturation.cross.section.factor, write.output)
```

Arguments

E.MeV.u	particle energy for each component in the mixed particle field [MeV/u] (array of size number.of.field.components) (see also E.MeV.u).
particle.no	particle type for each component in the mixed particle field (array of size number.of.field.components) (see also particle.no).
fluence.cm2.or.dose.Gy	if positive, particle fluence for each component in the mixed particle field [1/cm ²]; if negative, particle dose for each component in the mixed particle field [Gy] (array of size number.of.field.components) (see also fluence.cm2.or.dose.Gy).
material.no	index number for detector material (see also material.no).
stopping.power.source.no	stopping power source number (PSTAR,...) (see also stopping.power.source.no).
rdd.model	index number for chosen radial dose distribution (see also rdd.model).
rdd.parameters	parameters for chosen radial dose distribution (array of size 4).
er.model	index number for chosen electron-range model (see also er.model).
gamma.model	index number for chosen gamma response.
gamma.parameters	parameters for chosen gamma response (array of size 9).
saturation.cross.section.factor	scaling factor for the saturation cross section.
write.output	if true, a protocol is written to a file in the working directory.

Value

relative. efficiency	particle response at dose D / gamma response at dose D
S.HCP	absolute particle response
S.gamma	absolute gamma response
sI.cm2	resulting ion saturation cross section in cm ²
gamma.dose.Gy	dose contribution from gamma kills
P.I	ion kill probability
P.g	gamma kill probability

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_Algorithms_IGK.c#L34

Examples

```

# Compute the relative efficiency of an Alanine detector in a mixed
# carbon / proton field
AT.run.IGK.method( particle.no           = 1001,
                  # namely protons with
                  E.MeV.u               = 10,
                  # 10 MeV/u
                  fluence.cm2.or.dose.Gy = c(-1.0),
                  # delivering 1 Gy
                  material.no           = 5,
                  # i.e. Alanine
                  rdd.model             = 4,

# Katz parametrization of radial dose distribution with simplified extended
# targets
                  rdd.parameter         = c(5e-8,1e-10),
                  # with 50 nm target size and 1e-10 dose minimum
                  er.model              = 2,
                  # Butts&Katz parametrization of track radius
                  gamma.model          = 2,
                  # Use general target/hit model but here...
                  gamma.parameters     = c(1,500,1,1,0),
                  # ...as exponential saturation with characteristic dose 500 Gy
                  saturation.cross.section.factor = 1.4,
                  # factor to take 'brush' around track into account
                  write.output         = TRUE,
                  # write a log file
                  stopping.power.source.no = 0)

```

AT.Rutherford.SDCS *AT.Rutherford.SDCS*

Description

Computes the Rutherford single differential cross section for the energy spectrum of secondary electrons produced by an HCP

Usage

AT.Rutherford.SDCS(E.MeV.u, particle.no, material.no, T.MeV)

Arguments

E.MeV.u	energy of particle per nucleon (see also E.MeV.u).
particle.no	particle index (see also particle.no).
material.no	material index (see also material.no).
T.MeV	electron energies (array of size n).

Value

dsdT.m2.MeV	Rutherford SDCS for given electron energies (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L50

AT.scattering.angle.distribution
AT.scattering.angle.distribution

Description

Returns scattering angle distribution f(Theta) The distribution is not normalized because the energy loss in the target is not considered.

Usage

```
AT.scattering.angle.distribution(E.MeV.u, particle.charge.e,
    target.thickness.cm, element.acronym, Theta)
```

Arguments

E.MeV.u	energy of particle per nucleon [MeV] (see also E.MeV.u).
particle.charge.e	charge number of particle.
target.thickness.cm	thickness of the target material in cm.
element.acronym	elemental symbol of target material (array of size PARTICLE.NAME.NCHAR).
Theta	vector of polar angles in rad (array of size n).

Value

distribution	vector of scattering angle distribution values (array of size n)
status	status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L285

AT.screening.angle *AT.screening.angle*

Description

Returns screening angles `chi_a`

Usage

`AT.screening.angle(E.MeV.u, particle.charge.e, element.acronym)`

Arguments

`E.MeV.u` vector of energies of particle per nucleon [MeV] (array of size n) (see also [E.MeV.u](#)).

`particle.charge.e` vector of charge numbers of particle (array of size n).

`element.acronym` vector of elemental symbols of target material (array of size n).

Value

`chi.a` vector of screening angles in rad (array of size n)

`status` status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_MultipleCoulombScattering.c#L70

AT.set.user.material *AT.set.user.material*

Description

Initializes user defined material. The material can then be used with material index number 0. !Be aware! that is definition is only valid during run-time. When the library is reloaded, the default settings are restored and the material is removed.

Usage

`AT.set.user.material(density.g.cm3, I.eV, average.A, average.Z)`

Arguments

density.g.cm3	physical density in g per cm3.
I.eV	I value in eV.
average.A	average mass number.
average.Z	average atomic number.

Value

status	material defined successfully if zero
--------	---------------------------------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L479

AT.set.user.material.from.composition

AT.set.user.material.from.composition

Description

Initializes user defined material from composition data. The material can then be used with material index number 0. !Be aware! that is definition is only valid during run-time. When the library is reloaded, the default settings are restored and the material is removed.

Usage

```
AT.set.user.material.from.composition(density.g.cm3, Z, A,
weight.fraction)
```

Arguments

density.g.cm3	physical density (in g per cm3) of material.
Z	atomic numbers of constituents (array of size n).
A	mass numbers of constituents (array of size n).
weight.fraction	relative fractions of weight of constituents (array of size n).

Value

status	material defined successfully if zero
--------	---------------------------------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataMaterial.c#L494

AT.SPC.convert.to.DDD *AT.SPC.convert.to.DDD*

Description

Converts spectral fluence data differential in depth and energy (spc) into a depth-dose. It also allows for the export of TRiP98 compatible DDD files. The routine calls AT.SPC.read so if you experience problems, please check if additional arguments for AT.SPC.read are needed (via '...'). For the DDD format, see M. Kramer's TRiP98 documentation: <http://bio.gsi.de/DOCS/TRiP98BEAM/DOCS/trip98fmtddd.html>.

Usage

```
AT.SPC.convert.to.DDD(file.name.spc, file.name.ddd = NULL, endian =
  'little', plot = TRUE, write = TRUE, ...)
```

Arguments

file.name.spc	path and file name for spc data
file.name.ddd	path and file name for ddd data, if not given file.name.spc will be used but with *.ddd extension (only applicable if write = TRUE)
endian	endianess of spc data, see also AT.SPC.read
plot	if true, the resulting depth-dose curve will be plotted, e.g. for error-checking
write	if true, the resulting depth-dose curve will be exported in TRiP98 format
...	additional arguments for the AT.SPC.read routine

Value

A data frame containing the depth-dose curve

AT.SPC.export.DEDX *AT.SPC.export.DEDX*

Description

Creates stopping power data tables from libamtrack and exports them in TRiP98 compatible format. For the DEDX format, see M. Kramer's TRiP98 documentation: <http://bio.gsi.de/DOCS/TRiP98BEAM/DOCS/trip98fmtdedx.html>. N.B. check the resulting data carefully for NAs, as not all stopping power data sources might cover the energy grid requested.

Usage

```
AT.SPC.export.DEDX(stopping.power.source.no, file.name.DEDX = NULL,
  element.names = NULL, energy.MeV.u = NULL, plot = TRUE, write = TRUE)
```

Arguments

stopping.power.source.no	index of stopping power data source, see also stopping.power.source.no .
file.name.DEDX	path and file name for DEDX data, if not given libamtrack.dedx will be used.
element.names	elements to be used (see particle.no), if not given the ICRU49/73 elements H...Ar will be used.
energy.MeV.u	energy grid, if not given the ICRU49/73 standard (0.025...1000 MeV/u in 51 steps) will be used.
plot	if true, the resulting data will be plotted.
write	if true, the resulting data will be exported in TRiP98 format.

Value

A data frame containing the stopping power data

AT.SPC.get

AT.SPC.get

Description

Returns interpolated spc data. Needs list of spc files as input which is obtained by [AT.SPC.get.list](#).
 TODO: use path.to.files here alternative argument and call AT.SPC.get.list internally.

Usage

```
AT.SPC.get(spc.list, energy.MeV.u)
```

Arguments

spc.list	data frame with spc file information as returned by AT.SPC.get.list
energy.MeV.u	requested beam energy, has to be within energy grid covered by spc.list

Value

list with spc data equivalent to those returned by [AT.SPC.read](#).

Examples

```
## Download data from libamtrack homepage
##
## To read a simple SPC file, use AT.SPC.read
##

# To get SPC data for arbitrary energy, you first have to make libamtrack aware
## of the appropriate SPC files:
#
```

```

# spc.list <- AT.SPC.get.list(path.to.files,...) where 'path.to.files'
# should point to spc files

#                               OF ONE KIND, i.e. same
# projectile, target, active/passive
#                               # but different energies

# N.B.: This routine can also be used to browser spc files and check their
# integrity
##
## Using the returned list, you can get spc data for any energy in between
#

# spc <- AT.SPC.get(spc.list, energy = ...) This will can AT.SPC.read
# and AT.SPC.interpolate
#
## returns a list in which the actual data are found in spc$spc
## which can then used in spc related routines, e.g.
## AT.SPC.tapply, AT.SPC.convert.to.DDD, etc.
##
## A spectrum at arbitraty can be obtain by using the data in spc$spc
## with AT.SPC.spectrum.at.depth.g.cm2

```

AT.SPC.get.list *AT.SPC.get.list*

Description

Returns filenames and essential information (energy, projectile etc.) of all spc files that are found at a user-proveded location. Needed by [AT.SPC.get](#).

Usage

```
AT.SPC.get.list(path.to.files, endian = "little")
```

Arguments

`path.to.files` absolute path to spc files, including wildcard, e.g. *.active*.spc
`endian` byte-order of the spc file to read, "big" (AIX) or "little" (Linux, VMS, etc., default). Only necessary if flavour = 'vanilla'

Value

A dataframe with path and file names, number of depth steps, projectile, target, beam energy, peak position.

Examples

```

## Download data from libamtrack homepage
##
## To read a simple SPC file, use AT.SPC.read
##

# To get SPC data for arbitrary energy, you first have to make libamtrack aware
## of the appropriate SPC files:
#

# spc.list <- AT.SPC.get.list(path.to.files,...) where 'path.to.files'
# should point to spc files

#                                     OF ONE KIND, i.e. same
# projectile, target, active/passive   # but different energies

# N.B.: This routine can also be used to browser spc files and check their
# integrity
##
## Using the returned list, you can get spc data for any energy in between
#

# spc <- AT.SPC.get(spc.list, energy = ...) This will can AT.SPC.read
# and AT.SPC.interpolate
#
## returns a list in which the actual data are found in spc$spc
## which can then used in spc related routines, e.g.
## AT.SPC.tapply, AT.SPC.convert.to.DDD, etc.
##
## A spectrum at arbitrary can be obtain by using the data in spc$spc
## with AT.SPC.spectrum.at.depth.g.cm2

```

AT.SPC.interpolate *AT.SPC.interpolate*

Description

Interpolates between two spc files.

Usage

```
AT.SPC.interpolate(spc.lower, spc.upper, energy.MeV.u)
```

Arguments

spc.lower	spc data (read by AT.SPC.read) with lower bracketing energy.
spc.upper	spc data (read by AT.SPC.read) with upper bracketing energy.
energy.MeV.u	energy of interpolated spc data

Value

list equivalent to those returned by AT.SPC.read.

Examples

```
## Download data from libamtrack homepage
##
## To read a simple SPC file, use AT.SPC.read
##

# To get SPC data for arbitrary energy, you first have to make libamtrack aware
## of the appropriate SPC files:
#

# spc.list <- AT.SPC.get.list(path.to.files,...) where 'path.to.files'
# should point to spc files

#                                     OF ONE KIND, i.e. same
# projectile, target, active/passive   # but different energies

# N.B.: This routine can also be used to browser spc files and check their
# integrity
##
## Using the returned list, you can get spc data for any energy in between
#

# spc <- AT.SPC.get(spc.list, energy = ...) This will can AT.SPC.read
# and AT.SPC.interpolate
#
## returns a list in which the actual data are found in spc$spc
## which can then used in spc related routines, e.g.
## AT.SPC.tapply, AT.SPC.convert.to.DDD, etc.
##
## A spectrum at arbitrary can be obtain by using the data in spc$spc
## with AT.SPC.spectrum.at.depth.g.cm2
```

AT.SPC.read

AT.SPC.read

Description

Read a spc-formatted data file with energy-fluence in n depth steps. For original TRiP format definition by M. Kraemer, please see <http://bio.gsi.de/DOCS/TRiP98BEAM/DOCS/trip98fmtspc.html> and Kraemer and Scholz, Treatment planning for heavy-ion radiotherapy: calculation and optimization of biologically effective dose, Phys. Med. Biol. 45 (2000) 3319-3330. Please note that the user has to take care of picking the spc-file for the projectile and target material desired. Presently, two versions of the reader exists: a slower but stable R version ('vanilla') and a faster but still buggy C version. IMPORTANT: SPC files report DIFFERENTIAL fluences dN/dE per

primary particle, i.e. normalized by the energy bin. This reader converts them to ABSOLUTE fluences by multiplying dE. This facilitates e.g. summation to get the total fluence etc. but produces funny results when ABSOLUTE fluences are plotted. Also, SPCs only contain the left limit of the energy bins. This reader also reports the energy bin midpoint which is more reasonable e.g. for the computation of mean dE/dx etc. Please note that the "compress" statement has been depreciated due to preparation for C translation of spc handling.

Usage

```
AT.SPC.read( file.name, flavour, endian, mean, header.only = FALSE)
```

Arguments

file.name	name of spc-file to be read (with extension).
flavour	'vanilla' (default) to use stable R version.
endian	byte-order of the spc file to read, "big" (AIX) or "little" (Linux, VMS, etc., default). Only necessary if flavour = 'vanilla'
mean	method for computing bin midpoints, "geometric" or "arithmetic" (default).
header.only	if true, only information on spc file but no data will be read.

Value

A list with (1) the 'spc' data frame with the following columns

depth.step	Index number of depth step (one-based)
depth.g.cm2	Depth in g/cm2
particle.no	Particle index number (see also(particle.no)).
E.low.MeV.u	Energy bin lower limit in MeV/u (see also(E.MeV.u)).
E.mid.MeV.u	Energy bin mid in MeV/u (see also(E.MeV.u)).
E.high.MeV.u	Energy bin upper limit in MeV/u (see also(E.MeV.u)).
dE.MeV.u	Energy bin width in MeV/u
dN.dE.per.MeV.u.per.primary	Fluence differential in energy (bin width) per primary.
N.per.primary	Fluence per primary.

and (2) variables containing information as beam energy, peak position, projectile and target material.

See Also

[AT.SPC.tapply](#) for more example to derive quantities from spc-data.


```

FUN =
AT.dose.weighted.LET.MeV.cm2.g,
    additional.arguments =
list(c("material.no", "AT.material.no.from.material.name('Water, Liquid)'),
FALSE),

c("stopping.power.source.no", "0", FALSE)))$returnValue
df.total$fLET.MeV.cm2.g <- AT.SPC.tapply( spc = spc,
INDEX =
"depth.g.cm2",
FUN =
AT.fluence.weighted.LET.MeV.cm2.g,
    additional.arguments =
list(c("material.no", "AT.material.no.from.material.name('Water, Liquid)'),
FALSE),

c("stopping.power.source.no", "0", FALSE)))$returnValue
df.total$Mean.E.C.MeV.u <- AT.SPC.tapply( spc =
spc[spc$particle.no == 6012,],
INDEX =
"depth.g.cm2",
FUN =
AT.dose.weighted.E.MeV.u,
    additional.arguments =
list(c("material.no", "AT.material.no.from.material.name('Water, Liquid)'),
FALSE),

c("stopping.power.source.no", "0", FALSE)))$returnValue
xyplot( D.Gy ~ depth.g.cm2,
df.total,
grid = TRUE,
type = 'o',
ylab = 'total dose / Gy',
xlab = 'depth / (g/cm2)')
xyplot( LET.MeV.cm2.g + fLET.MeV.cm2.g ~ depth.g.cm2,
df.total,
type = 'o',
main = 'Fluence (fLET) and dose (LET) weighted LET',
grid = TRUE,
auto.key = list(space = 'right', lines = TRUE, points = FALSE),
ylab = 'LET / (MeV*cm2/g)',
xlab = 'depth / (g/cm2)')
xyplot( Mean.E.C.MeV.u ~ depth.g.cm2,
df.total,
type = 'o',
grid = TRUE,
main = file.name,
ylab = 'Average kinetic energy of C / (MeV/u)',
xlab = 'depth / (g/cm2)')

## End(Not run)

```

AT.SPC.spectrum.at.depth.g.cm2
AT.SPC.spectrum.at.depth.g.cm2

Description

Returns spectrum from spc data in given depth step.

Usage

AT.SPC.spectrum.at.depth.g.cm2(spc, depth.g.cm2)

Arguments

spc	spc data
depth.g.cm2	depth the spectrum should be taken at (up to now, the data from the closest depth step will be taken)

Value

A data frame with the following columns (ready to use in most libamtrack functions):

E.MeV.u	Energy [MeV/u] - mid point of bin
particle.no	Particle index number
fluence.cm2	Fluence for each bin

See Also

Uses [AT.SPC.spectrum.at.depth.step](#). spc data should be read in by [AT.SPC.read](#).

Examples

None yet.

AT.SPC.spectrum.at.depth.step
AT.SPC.spectrum.at.depth.step

Description

Returns spectrum from spc data in given depth step.

Usage

AT.SPC.spectrum.at.depth.step(spc, depth.step)

Arguments

spc	spc data
depth.step	depth step the spectrum should be taken from (if outside data scope an error message will be issued)

Value

A data frame with the following columns (ready to use in most libamtrack functions):

E.MeV.u	Energy [MeV/u] - mid point of bin
particle.no	Particle index number
fluence.cm2	Fluence for each bin

See Also

Use [AT.SPC.spectrum.at.depth.g.cm2](#) to get spectrum at given depth. spc data should be read in by [AT.SPC.read](#).

Examples

```
# None yet.
```

AT.SPC.tapply

AT.SPC.tapply

Description

Similar to R's tapply this applies a function to cells defined by indices in a spc data object

Usage

```
AT.SPC.tapply( spc, INDEX, FUN, mixed.field.arguments = list(E.MeV.u =
  "E.mid.MeV.u", fluence.cm2 = "N.per.primary", particle.no = "particle.no"),
  additional.arguments = NULL, names.results = NULL)
```

Arguments

spc	spc data as returned by AT.SPC.read
INDEX	vector of column names in spc data that should be used as indices (indicating the cells).
FUN	Function to be applied - preferably this is a libamtrack function obeying the standard naming of mixed field variables number.of.field.components and material.no . Additional arguments to FUN can be passed using ...)

mixed.field.arguments

Named list containing the variables necessary to describe a mixed field (energy, fluence, particle type). The defaults are set to correspond to the column names used in `AT.SPC.read`. The user can change the list referring to other columns (of same length), e.g. when having multiplied the fluence per primary in the spc to get a realistic dose.

additional.arguments

Optional additional arguments to FUN. This should be a list with a three-entry vector for each argument. The first entry is the argument name, the second the value, the third indicated if it should be applied cell-wise (if TRUE). For example: the primitive R function to evaluate the mean energy per cell: `mean(x)`: `additional.arguments = list(c("x", "E.MeV.u", TRUE))` Or to pass the material.no (same for all cells): `additional.arguments = list(c("material.no", "1", FALSE))`

names.results optional vector with names for the returned values of FUN

Value

A data frame with the following columns:

index.columns Columns for indices given in INDEX to be looped over

results[] Additional columns containing the returned values from FUN

Examples

```
## Not run:
# Load required libraries
require(libamtrack)
require(lattice)
# Use example data set
file.name      <- system.file("extdata",
  "libamtrack.12C.H2O.active3.MeV27000.zip", package = "libamtrack")
endian         <- c("big", "little")[2]
# Read in spc data, we use old style R reader, so endianness has to be given
spc           <- AT.SPC.read ( file.name = file.name,
                              endian    = endian,
                              flavour   = "vanilla")$spc
# Translate particle numbers in particle names (looks better)
spc$particle.name <- AT.particle.name.from.particle.no(particle.no =
  spc$particle.no)
spc$particle.name <- factor(spc$particle.name)

# Compute and plot dose per primary with depth from spc data
df1 <- AT.SPC.tapply( spc           = spc,
                      INDEX        = "depth.g.cm2",
                      FUN          = AT.total.D.Gy,
                      additional.arguments = list( c("material.no", "1",
FALSE),
                      # Water

c("stopping.power.source.no", "0", FALSE)), # PSTAR
                      names.results = "D.Gy")
xyplot( D.Gy ~ depth.g.cm2,
```



```

        df1,
        type = "o",
grid = TRUE,
        ylab = "dose per primary / Gy",
        xlab = "depth / (g/cm2)")
# Compute and plot dose (1 Gy entrance) with depth from spc data
# To do so, first the fluence per primary has to be scaled and then

# AT.SPC.tapply has to be referred to the new non-standard column (default:
# fluence.cm2 = "N.per.primary")
fluence.factor <- 1.0 / df1$D.Gy[1]
# factor between dose per primary (from above) and 2 Gy
spc$fluence.cm2 <- spc$N.per.primary * fluence.factor
df2 <- AT.SPC.tapply( spc                = spc,
  INDEX          = "depth.g.cm2",
  FUN            = AT.total.D.Gy,
  mixed.field.arguments = list( fluence.cm2 = "fluence.cm2",
                                E.MeV.u    = "E.mid.MeV.u",
                                particle.no = "particle.no"),
  additional.arguments = list( c("material.no",
                                "1",
                                FALSE), # Water
                                c("stopping.power.source.no",
                                "0", FALSE)), # PSTAR
  names.results    = "D.Gy")
xyplot( D.Gy ~ depth.g.cm2,
        df2,
        type = "o",
col = "red",
        grid = TRUE,
ylab = "dose / Gy",
        xlab = "depth / (g/cm2)")

# Compute and plot the dose with depth, but differentiate contribution
# from individual particle species
# Also: use nicer (human-readable) code for material
df3 <- AT.SPC.tapply( spc                = spc,
  INDEX          = c("depth.g.cm2", "particle.name"),
  FUN            = AT.total.D.Gy,
  additional.arguments = list(c("material.no",
                                "AT.material.no.from.material.name('Water,
Liquid')",
                                FALSE),
                                c("stopping.power.source.no",
                                "0",
                                FALSE)),
  names.results    = "D.Gy")
xyplot( log10(D.Gy) ~ depth.g.cm2,
        df3,
        groups      = particle.name,
        type        = 'o',
        grid        = TRUE,

```

```
auto.key = list(space = 'right'),
ylab     = "log10( dose per primary / Gy )",
xlab     = 'depth / (g/cm2)')

## End(Not run)
```

AT.Stopping.Power.keV.um

AT.Stopping.Power.keV.um

Description

Main access method to stopping power data - multiple field

Usage

```
AT.Stopping.Power.keV.um(stopping.power.source.no, E.MeV.u,
particle.no, material.no)
```

Arguments

`stopping.power.source.no`
(see also [stopping.power.source.no](#)).

`E.MeV.u` (array of size `number.of.particles`) (see also [E.MeV.u](#)).

`particle.no` (array of size `number.of.particles`) (see also [particle.no](#)).

`material.no` (see also [material.no](#)).

Value

`Stopping.Power.keV.um`
(array of size `number.of.particles`)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataStoppingPower.c#L265

AT.Stopping.Power.MeV.cm2.g
AT.Stopping.Power.MeV.cm2.g

Description

Main access method to stopping power data - multiple field

Usage

AT.Stopping.Power.MeV.cm2.g(stopping.power.source.no, E.MeV.u,
particle.no, material.no)

Arguments

stopping.power.source.no
(see also [stopping.power.source.no](#)).

E.MeV.u (array of size number.of.particles) (see also [E.MeV.u](#)).

particle.no (array of size number.of.particles) (see also [particle.no](#)).

material.no (see also [material.no](#)).

Value

Stopping.Power.MeV.cm2.g
(array of size number.of.particles)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataStoppingPower.c#L247

AT.stopping.power.ratio
AT.stopping.power.ratio

Description

Computes the stopping power ratio for a material and a reference material. In case of mixed particle fields, the stopping power ratios of individual components are weighted by their respective fluences. Thus, this routines computes the ration of fluence-weighted stopping powers, NOT of dose-weighted stopping powers.

Usage

```
AT.stopping.power.ratio(E.MeV.u, particle.no, fluence.cm2, material.no,
  reference.material.no,
  stopping.power.source.no)
```

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size `number.of.field.components`) (see also `E.MeV.u`).

particle.no particle index (array of size `number.of.field.components`) (see also `particle.no`).

fluence.cm2 fluences of particles in the mixed particle field (array of size `number.of.field.components`).

material.no material index (see also `material.no`).

reference.material.no
 material index of reference material.

stopping.power.source.no
 TODO (see also `stopping.power.source.no`).

Value

stopping stopping

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L657

Examples

```
require(lattice)
df <- expand.grid( particle.name      = "1H",
  # Define parameter space:
  particle.energy.MeV.u = 10^seq(-1, 3,
  length.out = 500),          # 1 nuclid, energy between 0.1 and 1000 MeV/u,
  material.name         = c("Air", "PMMA",
  "Aluminum Oxide"),        # and three materials
  stopping.power.ratio = 0)
df$particle.no <- AT.particle.no.from.particle.name(df$particle.name)
df$material.no <- AT.material.no.from.material.name(df$material.name)
material.no.water <- AT.material.no.from.material.name("Water, Liquid")
for (i in 1:nrow(df)){
  df$stopping.power.ratio[i] <- AT.stopping.power.ratio( E.MeV.u
    = df$particle.energy.MeV.u[i],

  particle.no      = df$particle.no[i],

  fluence.cm2     = 1,
  # does not have any meaning here as monoenergetic beams are assumed

  material.no     = df$material.no[i],
```

```

reference.material.no = material.no.water,

stopping.power.source.no = 0)
}
xyplot( stopping.power.ratio ~ log10(particle.energy.MeV.u)|particle.name,
        df,
        groups      = material.name,
        type         = "l",
        layout       = c(1,1),
        aspect       = 1,
        as.table     = TRUE,
        auto.key     = list( columns = 3, points = FALSE, lines = TRUE),
        xlab         = list( "energy / (MeV/u)", cex = 1.25),
        ylab         = list( "stopping power ratio\nwith respect to water",
cex = 1.25),
        main         = list("stopping powers based on PSTAR data", cex =
1.0),
        panel       = function(...){
                        panel.grid(h = -1, v = -1)
                        panel.abline(h = 1.0)
                        panel.xyplot(...)
                        },
        between     = list( x = .5),
        scales      = list( x = list( at      = log10(c(.1, 1, 10,
100, 1000)),
                                labels  = c(".1", "1", "10",
"100", "1000"),
                                cex    = 1.0))
)

```

AT.total.D.Gy

AT.total.D.Gy

Description

Computes the total dose of a mixed particle field

Usage

```
AT.total.D.Gy(E.MeV.u, particle.no, fluence.cm2, material.no,
stopping.power.source.no)
```

Arguments

E.MeV.u	energy of particles in the mixed particle field (array of size number.of.field.components) (see also E.MeV.u).
particle.no	particle index (array of size number.of.field.components) (see also particle.no).
fluence.cm2	fluences of particles in the mixed particle field (array of size number.of.field.components).

material.no material index (see also [material.no](#)).
 stopping.power.source.no
 TODO (see also [stopping.power.source.no](#)).

Value

total.dose.Gy total.dose.Gy

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L457

Examples

```
# Compute dose of monoenergtic high energy
# and a mixed (99/1) field of high and low
# energy protons in water at same fluence
AT.total.D.Gy( E.MeV.u      = 100,
               particle.no = 1001,
               fluence.cm2 = 100e8,
               material.no = 1,
               stopping.power.source.no = 0)
AT.total.D.Gy( E.MeV.u      = c(100, 5),
               particle.no = c(1001, 1001),
               fluence.cm2 = c(99e8, 1e8),
               material.no = 1,
               stopping.power.source.no = 0)
```

AT.total.fluence.cm2 *AT.total.fluence.cm2*

Description

Computes the total fluence of a mixed particle field

Usage

```
AT.total.fluence.cm2(E.MeV.u, particle.no, D.Gy, material.no,
                    stopping.power.source.no)
```

Arguments

E.MeV.u energy of particles in the mixed particle field (array of size [number.of.field.components](#)) (see also [E.MeV.u](#)).

particle.no particle index (array of size [number.of.field.components](#)) (see also [particle.no](#)).

D.Gy doses of particles in the mixed particle field (array of size [number.of.field.components](#)).

material.no material index (see also [material.no](#)).

stopping.power.source.no
 TODO (see also [stopping.power.source.no](#)).

Value

```
total.fluence.cm
total.fluence.cm
```

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_PhysicsRoutines.c#L485

Examples

```
# Compute total fluence in a
# and a mixed field of
# high and low energy protons
# that deliver the same dose to water
AT.total.fluence.cm2( E.MeV.u      = c(100, 5),
                    particle.no = c(1001, 1001),
                    D.Gy        = c(1, 1),
                    material.no = 1,
                    stopping.power.source.no = 0)
```

```
AT.translate.dose.into.DSB.distribution
AT.translate.dose.into.DSB.distribution
```

Description

Converts a local dose into a DSB distribution assuming Poissonian rule for creation.

Usage

```
AT.translate.dose.into.DSB.distribution(f.d.Gy, f.dd.Gy, f,
enhancement.factor, DSB.per.Gy.per.domain,
domains.per.nucleus, write.output)
```

Arguments

f.d.Gy	bin midpoints for f (array of size n.bins.f).
f.dd.Gy	bin widths for f (array of size n.bins.f).
f	dose frequency (array of size n.bins.f).
enhancement.factor	dose enhancement factor (array of size n.bins.f).
DSB.per.Gy.per.domain	number of DSBs per domain per Gy.
domains.per.nucleus	number of domains in nucleus.
write.output	if true, a log file will be written ("dose.to.DSBs.log") containing the DBS distribution.

Value

<code>total.pDSBs</code>	probability sum of DSB probability (quality check, has to be ~1)
<code>total.nDSBs</code>	number of DSBs in nucleus
<code>number.of.iDSBs</code>	number of isolated DSBs in nucleus
<code>number.of.cDSBs</code>	number of complex DSBs in nucleus
<code>avg.number.of.DSBs.in.cDSBs</code>	average number of DSBs in complex DSBs

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_SuccessiveConvolutions.c#L1123

AT.Vavilov.energy.loss.distribution

AT.Vavilov.energy.loss.distribution

Description

Computes the energy loss Vavilov distribution acc. to Seltzer & Berger No effective projectile charge is considered!

Usage

```
AT.Vavilov.energy.loss.distribution(energy.loss.keV, E.MeV.u,
particle.no, material.no, slab.thickness.um)
```

Arguments

<code>energy.loss.keV</code>	energy loss (array of size n).
<code>E.MeV.u</code>	energy of particle per nucleon (see also E.MeV.u).
<code>particle.no</code>	particle index (see also particle.no).
<code>material.no</code>	material index (see also material.no).
<code>slab.thickness.um</code>	slab thickness in um.

Value

`fDdD` (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L403

 AT.Vavilov.PDF

AT.Vavilov.PDF

Description

Compute Vavilov distribution using CERNLIB (G116)

Usage

AT.Vavilov.PDF(lambda.V, kappa, beta)

Arguments

lambda.V	lambda (array of size n).
kappa	straggling parameter.
beta	relativistic speed, between 0 and 1.

Value

density	resulting density (array of size n)
---------	-------------------------------------

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_EnergyLoss.c#L32

 AT.WEPL.Bethe

AT.WEPL.Bethe

Description

Computes the water equivalent path length (WEPL) using the Bethe formula

Usage

AT.WEPL.Bethe(E.MeV.u, particle.no, material.no, slab.thickness.m)

Arguments

E.MeV.u	energy of particle per nucleon (array of size n) (see also E.MeV.u).
particle.no	particle index (array of size n) (see also particle.no).
material.no	material index (see also material.no).
slab.thickness.m	thickness of slab of material different than water, in meter.

Value

WEPL resulting water equivalent path length (array of size n)

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataRange.c#L202

AT.Z.from.element.acronym

AT.Z.from.element.acronym

Description

Returns Z for given elemental symbols

Usage

AT.Z.from.element.acronym(acronym)

Arguments

acronym elemental symbols (array of size n).

Value

Z corresponding Z (array of size n)

status status

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L326

AT.Z.from.particle.no *AT.Z.from.particle.no*

Description

Returns atomic number for given particle number

Usage

AT.Z.from.particle.no(particle.no)

Arguments

particle.no particle index number (array of size n) (see also [particle.no](#)).

Value

Z atomic number (array of size n)
return return

See Also

View the C source code here: http://sourceforge.net/apps/trac/libamtrack/browser/trunk/src/AT_DataParticle.c#L81

E.MeV.u *Ion energy values*

Description

In libamtrack, the kinetic energy for particles is usually given in Megaelectronvolt per nucleon (MeV/u). For therapeutical beam these are usually in range between approx. 1 MeV/u and 500 MeV/u. Please note, that simply the number of nucleons is used, not the actual mass of the nucleon (amu) for a specific nuclid. So, for example for U-238 with 100 MeV/u the total kinetic energy is 23.8 GeV.

er.model *Electron-range models*

Description

In libamtrack, there are currently seven parametrizations of the maximal distance electrons travel from the center of a particle track as a function of the primary particle's energy. They are referred to using sequential positive integer numbers (see details).

Details

er.model	description
1	A simple test function (constant range)
2	Parametrization proposed by Butts and Katz (Butts & Katz, 1972)
3	Parametrization proposed by M. Waligorski (Waligorski, 1985)
4	Parametrization proposed by O. Geiss (Geiss, 1997)
5	Parametrization proposed by M. Scholz (Scholz, 1997)
6	Parametrization proposed by J. Edmund (Edmund et al., 2007)
7	Parametrization proposed by Tabata (Tabata, 1972)

See Also

More information on the electron-range models, especially the explicit formulas used, valid energy ranges and references to literature are found in the libamtrack reference manual (<http://libamtrack.dkfz.org/libamtrack/images/3/31/LibamtrackReferenceManual.pdf>).

fluence.cm2.or.dose.Gy

Fluence and dose as equivalent input parameters

Description

Many functions in libamtrack can take either the fluence or the dose as an argument. For a specific nuclid and energy they can be converted into each other (see also `AT.dose.Gy()` and `AT.fluence.cm2()`). As both can only be positive, the argument `fluence.cm2.or.dose.Gy` will be interpreted as fluence [1/cm2] if positive and as dose [Gy] if given as negative value.

- `fluence.cm2.or.dose.Gy <- 1e7` means fluence = 1e7 / cm2
- `fluence.cm2.or.dose.Gy <- -10` means dose = 10 Gy

gamma.model

Gamma (X ray) response models

Description

In libamtrack, there are currently six parametrizations of the gamma / X ray response of a system. They are referred to using sequential positive integer numbers (see details).

Details**The implemented gamma models are:**

gamma.model	description
1	A simple test function (constant over entire track width/electron range)
2	Generalized hit/target model
3	Radioluminescence response
4	Simple exponential saturation (special case of 2: one hit / one target)
5	Linear-quadratic model
6	Mejdahl's TLD response for LiF as used by Geiss et al. (1998)

The corresponding gamma parameters are:

gamma.model	gamma.parameters[1]	gamma.parameters[2]	gamma.parameters[3]	gamma.parameters[4]	gamma.parameters[5]
1	NA	NA	NA	NA	NA
2	rel. response	characteristic dose [Gy]	hittedness	multiplicity	0 to 1
3	max. response	transition dose [Gy]	dynamic	NA	NA
4	max. response	characteristic dose [Gy]	NA	NA	NA
5	alpha [1/Gy]	beta[1/Gy ²]	transition dose [Gy]	NA	NA
6	const	k1	a1	k2	a2

The corresponding default/example values are:

gamma.model	gamma.parameters[1]	gamma.parameters[2]	gamma.parameters[3]	gamma.parameters[4]	gamma.parameters[5]
1	NA	NA	NA	NA	NA
2	1.0	10.0	1	1	0
3	1e6	20.0	6.0	NA	NA
4	1e6	10.0	NA	NA	NA
5	0.2	0.018	30.0	NA	NA
6	6e3	0.59	5e-4	0.41	2e-4

See Also

More information on models, especially the explicit formulas used, valid energy ranges and references to literature are found in the libamtrack reference manual (<http://libamtrack.dkfz.org/libamtrack/images/3/31/LibamtrackReferenceManual.pdf>).

material.name	<i>Material naming convention</i>
---------------	-----------------------------------

Description

Currently seven predefined materials exist in libamtrack. They are referred to using sequential positive integer numbers (see also [particle.no](#)) but carry also a name, preferably the NIST name. When referring to a material by name, make sure that the spelling (incl. cases) is correct.

Details

The predefined materials in libamtrack are:

material.no	material.name
1	"Water, Liquid"
2	"Aluminum Oxide"
3	"Aluminum"
4	"PMMA"
5	"Alanine"
6	"Lithium Fluoride"
7	"Air"

material.no	<i>Material indexing convention</i>
-------------	-------------------------------------

Description

Currently seven predefined materials exist in libamtrack. They are referred to using sequential positive integer numbers (see details). The material definition follows largely the pstar and astar definitions of NIST (<http://physics.nist.gov/cgi-bin/Star/compos.pl?ap>). `material.no = 0` points in contrast to a material defined by the user during run-time. This feature is still under development and not available yet.

Details

The predefined materials in libamtrack are:

material.no	material
1	Water, Liquid
2	Aluminum Oxide (Al ₂ O ₃)
3	Aluminum
4	PMMA (Polymethylmethacrylate, Perspex, Plexiglass, [C ₅ H ₈ O ₂] _n)
5	Alanine
6	Lithium Fluoride (LiF)
7	Air (dry, at sea level)
8	Silicon
9	Copper

See Also

You can use `AT.material.name.from.material.no` and `AT.material.no.from.material.name` to convert material names into material indices and vice versa. `AT.get.materials.data` will return all available data for a predefined material.

 number.of.field.components

Handling of mixed particle fields

Description

Many functions in libamtrack offer the possibility to consider mixed particle fields. These fields are composed from a finite number of specific nuclids defined by `particle.no`. All particles of an individual component are supposed to have exactly the same energy (given by `particle.no`), without spread. Thus an energy distribution has to be describe in discrete energy steps. Below is a compilation of the arguments a mixed field is described by. Depending on the function all or a subset are necessary. If arrays of length $>$ `number.of.field.components` are entered, the additional data will be ignored. If array hold too few data, the computation will not be executed.

Arguments

<code>number.of.field.components</code>	A variable describing how many components are used for the field. This also dictates the array lengths of all following variables.
<code>E.MeV.u</code>	Particle energies (array of size <code>number.of.field.components</code> , see also E.MeV.u)
<code>particle.no</code>	Particle type indices (array of size <code>number.of.field.components</code>), see also particle.no
<code>fluence.cm2.or.dose.Gy</code>	Fluences (if positive), or doses (if negative, array of size <code>number.of.field.components</code>), see also fluence.cm2.or.dose.Gy

 particle.name

Particle naming convention

Description

The particle naming system in libamtrack works as follows: a particle is identified by a character string consisting of the mass number A and the abbreviation of the element (identifying the atomic number Z).

Details

- For a proton `particle.name` is '1H'.
- For deuterium `particle.name` is '2H'.
- For He-4 `particle.name` is '4He'.
- For C-12 `particle.name` is '12C'.
- For a U-238 `particle.name` is '238U'.

particle.no *Particle indexing convention*

Description

The particle indexing system in libamtrack works as follows: for a particle with atomic number Z and mass number A the index is `particle.no = 1000 * Z + A`. This ensures uniqueness for all particle types used in libamtrack. Also, an extension to anti-protons or ions could be made using negative numbers.

Details

- For a proton ($Z=1, A=1$) `particle.no` is 1001.
- For deuterium ($Z=1, A=2$) `particle.no` is 1002.
- For He-4 ($Z=2, A=4$) `particle.no` is 2004.
- For C-12 ($Z=6, A=12$) `particle.no` is 6012.
- For a U-238 ($Z=92, A=238$) `particle.no` is 92238.

See Also

You can use `AT.particle.name.from.particle.no` and `AT.particle.no.from.particle.name` to convert particle names into particle indices and vice versa.

rdd.model *Radial dose distribution (rdd) models*

Description

In libamtrack, there are currently seven parametrizations of distribution of local dose around particle track as a function of the primary particle's energy and type. They are referred to using sequential positive integer numbers (see details).

Details

The implemented rdd models are:

rdd.model	description
1	A simple test function (constant over entire track width/electron range)
2	Point target rdd proposed by Butts and Katz (Butts & Katz, 1969)
3	Simplified extended target rdd proposed by O. Geiss (Geiss, 1997)
4	Simplified extended target rdd proposed by Katz (Katz et al., 1972)
5	Point target rdd proposed by Cucinotta (Cucinotta, XXXX)
6	Extended target rdd proposed by Katz (Katz, XXXX)
7	Extended target rdd proposed by Cucinotta (Cucinotta, XXXX)

The corresponding rdd parameters are:

rdd.model	rdd.parameters[1]	rdd.parameters[2]	rdd.parameters[3]
1	NA	NA	NA
2	minimal radius (integration limit) [m]	lower dose cut-off [Gy]	NA
3	core diameter/target size [m]	NA	NA
4	core diameter/target size [m]	lower dose cut-off [Gy]	NA
5	minimal radius (integration limit) [m]	lower dose cut-off [Gy]	NA
6	minimal radius (integration limit) [m]	core diameter/target size [m]	lower dose cut-off [Gy]
7	minimal radius (integration limit) [m]	core diameter/target size [m]	lower dose cut-off [Gy]

The corresponding default values are:

rdd.model	rdd.parameters[1]	rdd.parameters[2]	rdd.parameters[3]
1	NA	NA	NA
2	1e-10	1e-10	NA
3	5e-8	NA	NA
4	5e-8	1e-10	NA
5	5e-11	1e-10	NA
6	1e-10	1e-8	1e-10
7	5e-11	1e-8	1e-10

See Also

More information on the radial dose distribution models, especially the explicit formulas used, valid energy ranges and references to literature are found in the libamtrack reference manual (<http://libamtrack.dkfz.org/libamtrack/images/3/31/LibamtrackReferenceManual.pdf>).

stopping.power.source.no

Sources of stopping power data

Description

In libamtrack, there are currently four stopping power data sources. They are referred to using sequential positive integer numbers (see details). Please note, that not all sources can be used for every material. The most versatile, but also inaccurate source in the context is the Bethe formular.

Details**The stopping power sources are:**

stopping.power.source.no	description
0	Tabulated data from NIS T's PSTAR code, for other ions scales by the square of the effective charge
1	Analytical Bethe formular, including density effect
2	Tabulated data from the SHIELD-HIT code, generate with an extended Bethe-Bloch approach
3	Tabulated data from ICRU49 (H, He) and ICRU73, for liquid water only. N.B. the I value incorrect

See Also

More information, especially the explicit formulas used, valid energy ranges and references to literature are found in the libamtrack reference manual (<http://libamtrack.dkfz.org/libamtrack/images/3/31/LibamtrackReferenceManual.pdf>).

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