`libAmTrack` Manual

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Contents

Chapter 1

Introduction

`libAmTrack` is a library of computational routines for the prediction of solid state detector response and radiobiological effectiveness in proton and ion beams. In this field, `libAmTrack` focusses on methods that are based on widely used amorphous track models (ATMs) rather than for example microdosimetry models.

Direct comparisons between ATMs are usually hampered by the lack of knowledge on the details of the modelling and computational procedures. We believe that this hinders a wider application of ATMs and the advance towards a better accurracy of their predictions.

The `libAmTrack` project has therefore been started with the intention to provide an open-source, freely available, and comprehensive code for the community. Written in ANSI C, it is designed to be used independent of which platform the user is working on. Furthermore, the idea behind organizing `libAmTrack` as a library is that the user can access its functionality from whatever software tools they are using, e.g. MatLab, R, S-Plus etc.

The organization and documentation of the code – albeit still far from being perfect – should help to use `libAmTrack` for educational purposes as well.

1.1 Amorphous track models

ATMs (in a slightly confusing manner also referred to as 'track structure models') disregard the stochastic energy deposition pattern by secondary electrons around the track of heavy charged particles (protons or ions, HCPs) considering only the averaged dose d as a function of distance r from the trajectory, i.e. the radial dose distribution (Fig. 1.1). Their second important assumption is that – since photons deposit their energy eventually by electrons as well – local radiation effects are supposed to be the same for photons and HCPs. Thus, the detector response to irradiation with particles of type T and energy E can be predicted from the homogenous bulk photon dose response $S_X(D)$ of the detector system and the spatial deposition of local dose $d(x, y)$ as calculated from the fluences $\Phi(E, T)$ of the particle field. Despite many simplifications, ATMs are reasonably successful in predicting the response for a variety of physical detectors and biological systems [1, 2, 3, 4].

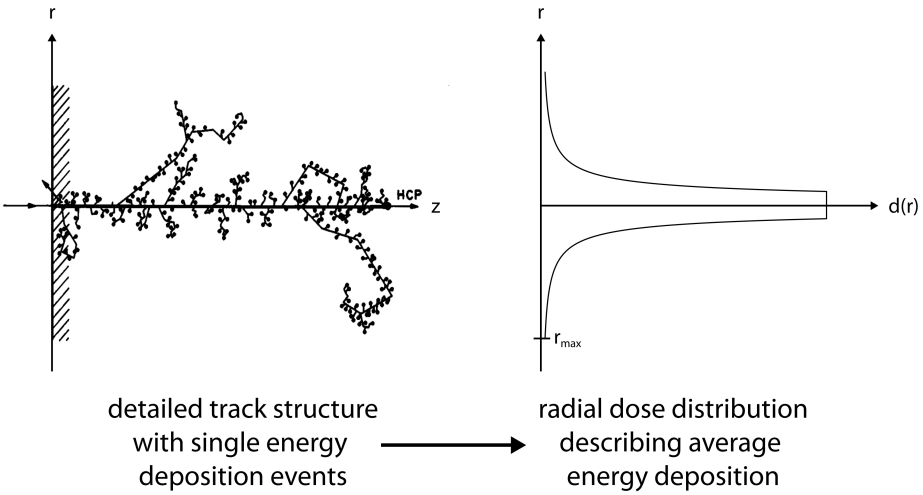

Figure 1.1: Amorphization of the detailed track structure.

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Chapter 2

Installation

The libAmTrack project is hosted at libamtrack.sourceforge.net using svn version control. Regularily, release versions are published.

2.1 Installing GNU Scientific Library (GSL)

A prerequsit for using libAmTrack is GSL (http://www.gnu.org/software/gsl/) as libAmTrack uses many of its numerical functions.

- For most Linux distributions you can install GSL from repositories. Make sure that the GSL path is added to the library path. If you want to or have to compile libAmTrack yourself you will have to install the header files for GSL, too, i.e. the developer version.
- For Windows there is a port available (http://gnuwin32.sourceforge.net/packages/gsl.htm). To work correctly, it is necessary that the binary files (libgsl.dll and libgslcblas.dll) are placed in the same directory as libamtrack.dll.

2.2 Installing libAmTrack binaries (for Windows only)

The easiest way to get libAmTrack is to download the latest compiled version.

2.3 Installing libAmTrack from latest released source code

2.4 Installing libAmTrack working version

2.4.1 Using Eclipse IDK

!repository at: https://libamtrack.svn.sourceforge.net/svnroot/libamtrack !SVNKit instead of subversion (JavaHL!) !Proxy for private IPs !GSL path for windows (GCC linker - libraries (gsl, gslcblas), library path (normally C:/Programs/GnuWin32/bin), GCC compiler - include path (normally C:/Programs/GnuWin32/include))

2.4.2 Using gcc only

svn co https://libamtrack.svn.sourceforge.net/svnroot/libamtrack libamtrack

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Chapter 3

libAmTrack methods

3.1 Introduction

'Methods' are the top-level routines in `libAmTrack`. From the physical parameters describing a HCP field they compute the predicted RE or RBE. In order to do so, the user has to both chose

- method independent settings, such as the radiation field, RDD, ER, gamma model and
- method specific setting, e.g. the binning width to be used.

Methods are implemented in the `Amtrack.c` and make use of all other subordinate routines. At the moment, four methods are available, Tab. 3.1 gives an overview. All methods apply to slice of a homogenous detector being infinitesimally small in z direction[1], i.e. in direction of the beam. The latter is supposed to be perfectly parallel and homogenous in fluence with respect to x and y (Fig. 3.1.

All methods share the following input parameters:

`n`	number of components in mixed field (long integer)
`E_MeV_u[]`	the kinetic energy per nucleon for each component (array of double, size `n`)
`particle_no[]`	the particle id number for each component, see ref. for more details (array of long, size `n`)
`fluence_cm2[]`	the fluence (in cm^{-2}) or the dose (in Gy), if negative, for each component (array of double, size `n`)
`material_no`	the material id number (long integer)
`rdd_model`	the radial dose distribution id number, see 4 for details (long)
`rdd_parameters[]`	parameters for the given RDD, see 4 for details (array of long, size depending on RDD model)
`er_model`	the electron range id number, see 5 for details (long)
`gamma_model`	the photon response id number, see 6 for details (long)
`gamma_parameters[]`	parameters for the given RDD, see 6 for details (array of long, size depending on GR model)

[1] Or a slice of the detector with finite size in z but with crucial parameters, such as LET, fluence etc. not changing significantly over Δz

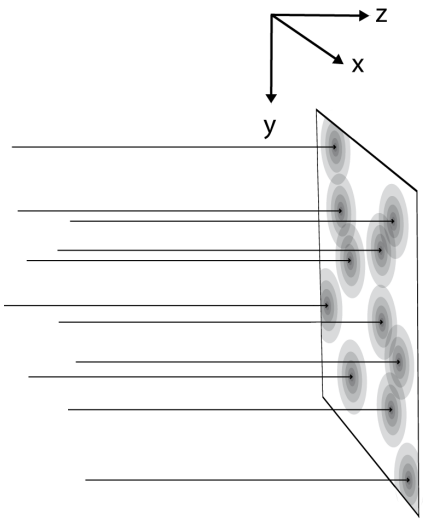

Figure 3.1: Coordinate definition in `libAmTrack`

All methods need in addition an array to return their results:

`results[]`	the particle id number for each component (array of long, size 10)

3.2 The grid summation method (GSL)

This is the most straight-forward approach: particles are sampled according to their relative fluence and local doses $d(x, y)$ — and therefore local response $s(x, y) = S_X(d(x, y))$ — are computed on a Cartesian grid ('checkerboard') by attributing the corresponding $d_{E,T}(r)$ to the sampled particle (FIGURE?). The detector is thought to be homogenous, perpendicular to the beam in (x, y), and of negligible thickness Δz. The relative efficiency η can then be estimated by averaging the local response s over all grid elements:

$$\eta(\phi(E,T)) = \frac{S_{HCP}}{S_X(D)} = \frac{\langle s \rangle}{S_X(\langle d \rangle)} \tag{3.1}$$

Although conceptually straightforward, GSM can be very time-consuming, esp. in the case of higher fluences and particle energies (e.g. $E_{\text{proton}} > 20$ MeV) with many contributions to a single voxel. Furthermore, the procedure has to be repeated many times in order to converge — or a large detector grid has to be simulated.

3.3 The compound Poisson process methods (CPP)

To overcome the limitations of GSM calculating the local dose distibution as a spatial deposition pattern $d(x, y)$, we consider a representative point P (FIGURE?). The cumulative distribution function $F(d)$ of local dose d in P depends on the macroscopic fluence ϕ (and dose D, resp.) and the microscopic pattern around a track as expressed by $d(r)$. Then, one can state:

Name	Description	Reference
Ion-Gamma-Kill (IGK)	Get activation cross-section by fusing photon response (activation probability) and RDD, get particle response by cross-section and fluence (ion-kill, intratrack action), for multi-hit systems and lower LET consider also intertrack action (gamma kill).	[2]
Grid summation (GSM)	Throw of particle tracks on a Cartesian grid for local dose, apply photon response for local response, then average response.	[3]
Compound Poisson processes using successive convolution (CPP-SC, SPIFF)	Derive local dose frequency distribution analytically from RDD for single particle case, assume none or one-impact situation for low fluence, convolute resulting distribution with itself until desired high fluence / dose is reached, apply photon response.	[5]
Compound Poisson processes using statistical sampling (CPP-SS, SPISS)	Derive local dose frequency distribution analytically from RDD for single particle case as for SPIFF. But then use statistical sampling to add single impact doses according to relative fluences in the particle field.	[5]

Table 3.1: Methods implemented in `libAmTrack`.

- r_{max} is the maximum delta electron range in the field, so P is only influenced by tracks within a circle C of radius r_{max} around P (FIGURE?).
- All tracks in C are contributing to d and their number n is Poisson distributed with mean $\mu = \phi \cdot \pi r_{max}^2$.
- Let F_n be the cumulative distribution function of the local dose in the case of exactly n tracks. For a single track traversing C, we readily have the cumulative single impact distribution

$$F_1(d) = 1 - \frac{R(d)^2}{r_{max}^2}, \tag{3.2}$$

  with $R(d) = D^{-1}(r)$ (FIGURE?).
- In the case of n tracks in C, d is the sum of n independent and identically distributed single track doses, so F_n can be expressed as the n-fold convolution of F_1:

$$F_n = \underbrace{F_1 * \ldots * F_1}_{n \text{ times}} \tag{3.3}$$

- As n is Poisson distributed, F is the distribution function of a compound Poisson process:

$$F(d) = e^{-\mu} \sum_{i=1}^{\infty} \frac{\mu^i}{i!} F_i(d) \tag{3.4}$$

- The derivative $f(d)$ of $F(d)$ can then be eventually used to compute the macroscopic HCP detector response as the expected local response $\langle s \rangle$:

$$\langle s \rangle = \int_0^{\max(d)} S_X(d) f(d) \, \mathrm{d}d, \tag{3.5}$$

  and used in Eq. (3.1) to get the η. A similar procedure for $\langle d \rangle$ provides a quality check as it has to meet D.

This description enables F to be determined from the explicitly given distribution function F_1 in the case of monoenergetic particle fields. It can easily be extended to mixed particle fields by using the adjusted F_1 from Eq.(3.6) in Eq.(3.3) with $p_{E,T}$ being the relative fluence and $R_{E,T}$ the inverse radial dose distribution for the composing particles

$$F_1(d) = 1 - \sum_{E,T} p_{E,T} \cdot \frac{R_{E,T}(d)^2}{\hat{r}_{max}^2}, \tag{3.6}$$

where $\hat{r}_{max} = max(r_{max}(E,T))$.

It should be stressed that the presented approach is in no way limited to handle extended targets despite the point nature of P as the averaging across the target is already contained in $D(r)$ (for the difference between point and extended target distributions, see [1, 6]). While the computation of detector response from the local dose distribution $F(d)$ is trivial, the numerical calculation of $F(d)$ itself can, however, be cumbersome.

3.3.1 Computation using statistical sampling (CPP-SS)

One way to approximate $F(d)$ is the following:

The implementation of this approach in `libAmTrack` is named SPISS, which is explained below.

3.3.2 Accelerated computation using successive convolution (CPP-SC)

An approximation method for the rapid computation of compound Poisson processes was introduced by Kellerer [7]. It makes use of the fact that the distribution $f(d;\mu)$ can be obtained by a convolution operation:

$$f(d;\mu) = \int_0^d f(d-t;\mu/2) \cdot f(t;\mu/2) dt \tag{3.7}$$

One can chose a $\mu_{start} << 1$ with $\mu = 2^m \cdot \mu_{start}$ so that multiple events can be neglected and therefore $f(d;\mu_{start})$ consists, in good approximation, of two components only, namely the probability of no track in C ($d = 0$)

$$e^{-\mu_{start}} \approx (1 - \mu_{start}) = \hat{f}_0 \tag{3.8}$$

and of the density related to a single track

$$\hat{f}_1 \approx \mu_{start} \cdot f_1(d). \tag{3.9}$$

Performing m successive convolutions on these two components, i.e. replacing

$$\hat{f}_0 \text{ by } \hat{f}_0^2 \tag{3.10}$$

and

$$\hat{f}_1 \text{ by } 2 \cdot \hat{f}_0 \cdot \hat{f}_1 + \hat{f}_1 * \hat{f}_1 \tag{3.11}$$

will eventually yield $f(d)$. For obscure reasons, the implementation of this approach in `libAmTrack` is named SPIFF.

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Chapter 4

Radial dose distributions

One of the most disputed submodels in AT modelling is the parametrization of the distribution of radial dose around the particle tracks ('radial dose distribution', RDD). Up to now, `libAmTrack` can use the RDDs given in Tab. 4 and Fig. 4.1.

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Name	Expression	Reference
Test	$d(r) = c \cdot \Theta(-r_{max})$	*simple step function*
Katz (point target)	$d(r) = \frac{N_e \cdot e^4}{m_e c^2} \cdot \frac{1}{\rho_m} \cdot \frac{z^2}{\beta^2} \cdot \frac{1}{\alpha} \cdot \frac{1}{r^2} \cdot (1 - \frac{r}{r_{max}})^{\alpha} = d_{point}(r)$	[8]
Katz (extended target)	$d(r) = \frac{1}{A} \int_{\lvert r-a_0 \rvert}^{\lvert r+a_0 \rvert} 2 \cdot \Phi \cdot \hat{r} \cdot d_{point}(\hat{r}) \cdot d\hat{r}$	[9]
Site	$d(r) = \begin{cases} c & \text{if } r < a_0, \\ d_{point}(r) & \text{otherwise.} \end{cases}$	[10]
Geiß	$d(r) = \begin{cases} c & \text{if } r < a_0, \\ \frac{c}{r^2} & \text{if } a0 \leq r \leq r_{max} \\ 0 & \text{if } r > r_{max} \end{cases}$	[3]

Table 4.1: RDDs implemented in `libAmTrack`.

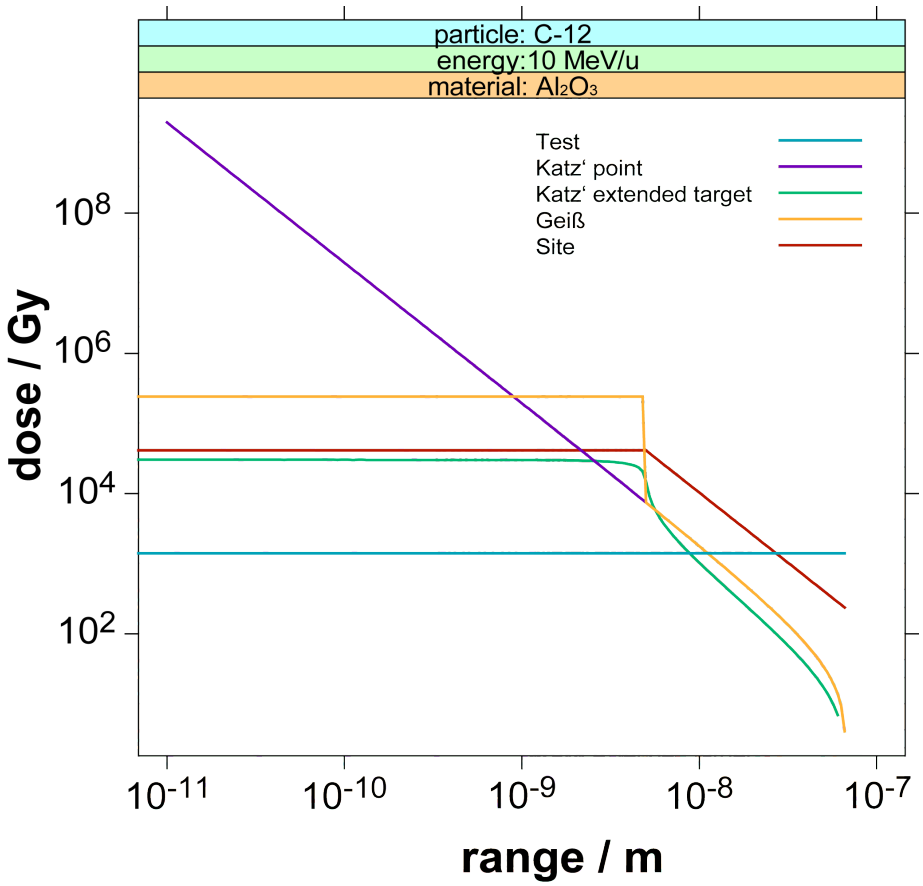

Figure 4.1: Radial dose distribution submodels available in `libAmTrack`

Chapter 5

Electron range relation

The submodels of electron-range relation determining the width of the particle tracks (Tab. 5 and Fig. 5.1) – their differences can be up to two orders of magnitude at the upper end of the range of clinically used energies.

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Name	Expression	Reference
Butts and Katz	$r_{max}/(\mathrm{g{\cdot}cm^{-2}}) = 10^{-6} \cdot w/\mathrm{keV}$, with $w/\mathrm{keV} = 2 \cdot m_e \cdot ((\frac{E}{E_0})^2 + 2(\frac{E}{E_0})$	[11]
Waligórski	$r_{max}/(\mathrm{g{\cdot}cm^{-2}}) = 6 \cdot 10^{-6} \cdot (w/\mathrm{keV})^{\alpha}$, with $\alpha = 1.079 (w < 1\ \mathrm{keV})$ or 1.667 (otherwise)	[12]
Geiss	$r_{max}/\mathrm{cm} = 4 \cdot 10^{-5} \cdot (E/\mathrm{MeV})^{1.5} \cdot \frac{\rho_{material}}{\rho_{water}}$	[13]
Scholz	$r_{max}/\mu\mathrm{m} = 0.05 \cdot 10^{-5} \cdot (E/\mathrm{MeV})^{1.7} \cdot \frac{\rho_{material}}{\rho_{water}}$	[14]

Table 5.1: ERs implemented in `libAmTrack`.

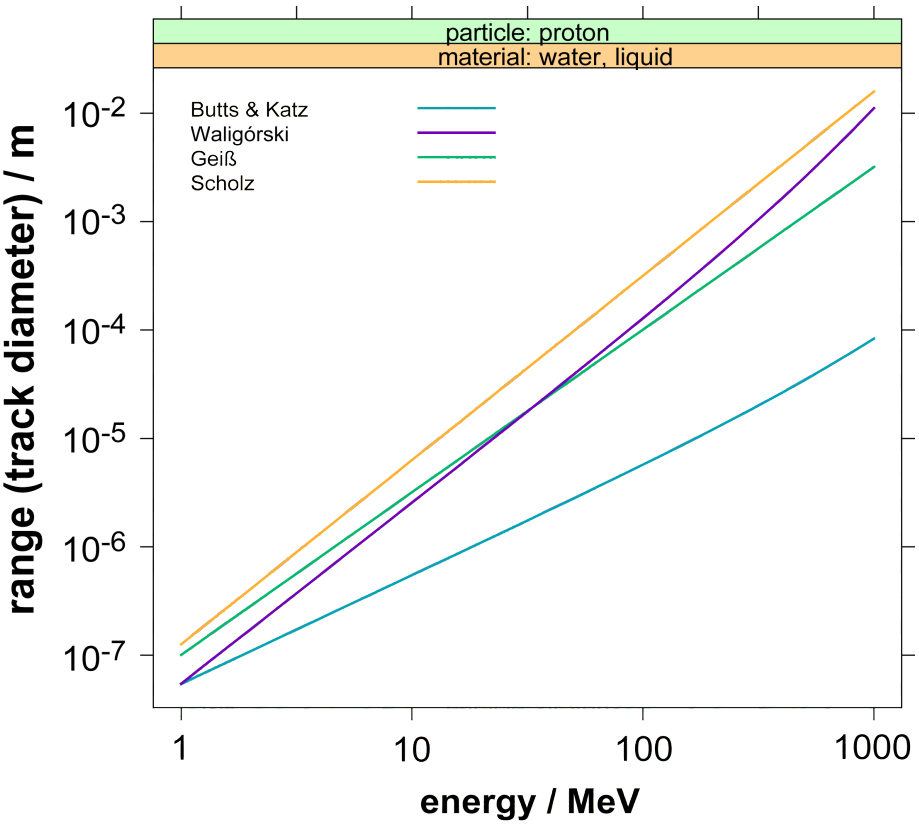

Figure 5.1: Electron-range submodels available in `libAmTrack`.

Chapter 6

Photon response models

For the actual computation of HCP response, several photon-response relations are found in libamtrack (Tab. **??** and and Fig. 6.1). Again, they can almost freely combined with the ATMs (an important exception still being IGK which is bound to a general hit/target response).

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Name	Expression	Reference
Test	$S(D) = a \cdot D + b$	*simple linear function*
General hit/target	$S(D) = (1 - sum_{k=0}^{c-1} \frac{(D/D_0)^k}{k!} \cdot e^{-(D/D_0)})^m$	[15]
Radioluminescence	$S(D) = \begin{cases} c_1 \cdot D + c_2 \cdot D^2 & \text{if } D < D_{sat}, \\ c_3 + c_4 \cdot D & \text{if } D \geq D_{sat}, \end{cases}$	[16], [17]
Exp.-saturation	$S(D) = c \cdot (1 - e^{-D/D_0})$	*simplified case of the general hit/target model*
Linear-quadratic	$S(D) = e^{-\alpha \cdot D - \beta \cdot D^2}$	[18]

Table 6.1: Photons response models implemented in `libAmTrack`.

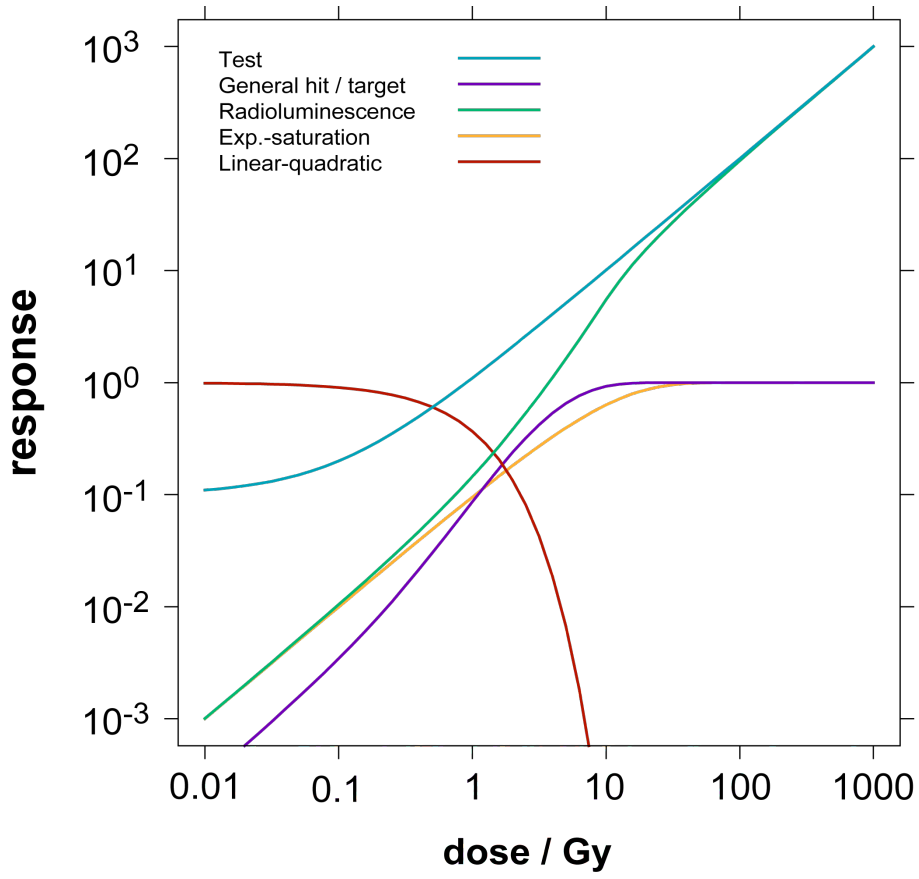

Figure 6.1: Photon-responses available in `libAmTrack`.

Chapter 7

Physics routines

`libAmTrack` contains a number of auxiliary routines handling the physics of ion beams needed. These routines can be used independently from the efficiency methods. They are implemented in `AT_PhysicsRoutines.c` and are described in detail in this.

7.1 AT_beta_from_E

Computes the relativistic speed $\beta = \frac{v}{c}$ from a particle's kinetic energy using

$$\beta = \sqrt{1 - \frac{1}{\frac{E}{1.0079 \cdot m_p}}} \tag{7.1}$$

Note that this relation is independent from the particle mass.

Single version:

`E_MeV_u`	the kinetic energy per nucleon (double)

Multi version:

`n`	array size (long integer)
`E_MeV_u`	the kinetic energy per nucleon (array of double, size `n`)
`beta`	array for results (array of double, size `n`)

7.2 AT_effective_charge_from_beta

Computes the effective charge of a travelling HCP as a function of its relativistic speed. Due to charge pick-up slower particle might not be fully stripped. Here, the Barkas (ref.?) equation is used:

$$Z_{eff} = Z \cdot (1 - e^{-125 \cdot \frac{\beta}{Z^{2/3}}}) \tag{7.2}$$

Single version:

`beta`	relativistic speed (double)
`Z`	charge (long integer)

Multi version:

`n`	array size (integer)
`beta`	relativistic speed (array of double, size `n`)
`Z`	charge (array of long integer, size `n`)
`effective_charge`	relativistic speed (array of double, size `n`)

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Chapter 8

Wrapper

8.1 R

8.2 Java

8.3 Python - pyamtrack

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Chapter 9

List of symbols

β	relativistic speed [1]
E	kinetic energy per nucleon [MeV/u]
T	total kinetic energy [MeV]
m_p	proton mass [938.272029 MeV/c^2]
Z	charge [elemental unit]
Z_{eff}	effective charge [elemental unit]

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