Improvements in the stopping power library libdEdx and release of the web GUI dedx.au.dk

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Abstract. Purpose: In ion beam therapy electronic stopping power data enter in different disciplines, e.g., dose planning, dosimetry, and radiobiology. However, relevant stopping power data are only known within an accuracy of 2%-10%. We started the software library project libdEdx to unify data from several well-known stopping power sources into one ready-to-use package being 1) freely available and 2) easy accessible via a web-based front end.

Methods: Currently, stopping power data from PSTAR, ASTAR, MSTAR and ICRU49+73 are implemented along with a version of the Bethe formula. The library is programmed in the language C to provide broad portability and high performance. A clean API provides full access to the underlying functions and thread safety in multi-threaded applications. The possibility to define arbitrary materials complements the list of predefined ICRU materials. Furthermore, we introduced a collection of tools, e.g., inverse stopping power look-up as well as CSDA range calculation and its inverse.

Results: On a standard desktop PC libdEdx calculates 22 million look-ups/sec. A web GUI (available at http://dedx.au.dk) provides easy access to libdEdx and download of stopping data and graphs. For compounds, we observe that stopping power data are robust for variations in the mean excitation potential of the constituents as long as the total mean excitation potential is fixated.

Conclusion: We released libdEdx (version number 1.2.1: http://sf.net/projects/libdedx/) with a web-based GUI. Future development will focus on implementing further stopping powers sources (e.g., for electrons and nuclear stopping) and relativistic effects.

1. Introduction

The energy loss of charged particles has extensively been researched for almost a century. Medical physics rely on electronic stopping powers in several ways. In ion therapy calculations, penetration ranges can be derived in the continuous slowing down approximation (CSDA), but uncertainties in the mean excitation potential lead to range uncertainties [1]. In clinical settings, dose is reported as dose-to-water while Monte Carlo particle transport codes calculate the dose deposited in the simulated medium, which might be different from water. The translation is
done by calculating the stopping power ratio of the two media in the corresponding fluence spectrum. Such a situation arises, e.g., for ionization chamber dosimetry, in the evaluation of beam quality correction factors, where the dose in the ionization chamber wall material is translated to dose-to-water using stopping power ratios, as described in dosimetry protocols such as IAEA TRS-398 [2]. The impact of various stopping power tables in this context was investigated in [3–5]. Furthermore, radiobiology models that describe the response of in vitro cell cultures exposed to ion or neutron radiation rely on stopping powers [6, 7] in similar ways as numerous detector response models [8–11] do.

To date, several stopping power tables and algorithms are available, with various ranges of applicability with respect to ions and target combinations. The aim of the libdEdx project is to provide a unified interface to several stopping power algorithms and tables to enable users to test their specific application against the sensitivity of stopping powers and to easily migrate their code to new stopping power tables if these become available. Additionally, users should be able to conveniently look up stopping powers and particle ranges for various media/ion types using several algorithms and tables by means of a web front end dedx.au.dk.

2. Methods

The computer library libdEdx is coded in ANSI-C for platform independence, targeting, e.g., Windows, Linux/Unix and embedded systems such as mobile phones or dedicated hardware for real time data processing in scientific laboratory environments. libdEdx features two modes of operation, “fast” and “simple”. The “simple” mode is intended for rapid application development and less experienced users. “Fast” mode is meant for CPU bound applications such as Monte Carlo codes. The installer is based on the CMAKE (http://www.cmake.org) build environment which provides a platform independent build system following de-facto standards on Unix/Linux and Windows systems. A single common programming interface (API) provides access to all implemented stopping power tables and algorithms, covering energy ranges from 10 keV/u up to 1 GeV/u. Functions for CSDA range calculation and inverse look-ups are provided as well. The library is extensible with new tables and algorithms providing stopping powers.

So far only electronic mass stopping powers are provided by libdEdx. PSTAR and ASTAR [12] tables handle proton and helium ion stopping powers, respectively, and are identical to those provided by the ICRU 49 report [13] by the International Commission on Radiation Units & Measurements (ICRU). However, libdEdx discriminates between these in case of future updates of PSTAR and ASTAR tables. The National Institute of Standards and Technology (NIST) allows the use of these data tables for free. MSTAR [14] is implemented for heavier ions (from Li to Ar), not covered by PSTAR and ASTAR. The implementation was made in agreement with Helmut Paul, Linz. ICRU 73 [15] tables are provided which also cover heavier ions from Li to Ar. Here, we also included the deprecated first version with the erroneous stopping power table for water to retain full compatibility. In addition, a version of the Bethe formula was implemented, which is sewed with the Lindhard-Scharff formula for low energies (below and around the Bragg peak).

The complete ESTAR [12] material composition list for compounds is included, following the ICRU material number and composition scheme. While this list covers 279 materials PSTAR, ASTAR, MSTAR, and the ICRU tables do only provide stopping powers for selected materials. libdEdx complements this by applying Braggs additivity rule when a compound is requested that is not in the list and all constituents are available. ICRU material definitions provide also mean excitation energies (I-values) which are applied by default for the extended Bethe algorithm. Additionally, I-values can be overridden if requested by the user. For compounds, ICRU 49 rules for gas phase or liquid/solid state apply.

The extended Bethe algorithm is identical to the implementation found in SHIELD-HIT [16–18]. The basis for the algorithm is the original Bethe from 1930 [19] together with
a density correction and a charge scaling function by Hubert et al. [20]. The resulting modified Bethe formula is only applicable for energies above 1 MeV/nucleon. Energies below $\sim 1$ MeV/nucleon are treated in accordance with the Lindhard-Scharff (LS) formula [21]. A result from the LS description is that the stopping power is proportional to the projectile velocity, $S = k\sqrt{E}$, where $k$ is a constant depending on projectile and target charge and $E$ is the energy of the projectile. Instead of calculating $k$ analytically, $k$ is found along the sewing point for the low-energy LS expression and the modified Bethe-equation. The sewing point is determined by the criteria that the combined stopping power function and its first derivative must be continuous, while the low-energy stopping power function must reach zero at $E = 0$. The sewing point is located between the point where the modified Bethe-equation turns negative (which is nonphysical) at low energies, and the global maximum found at slightly higher energies. A cost function for the sewing point is defined as the absolute difference between the first derivative of the low-energy function and the modified Bethe-equation, both evaluated in the sewing point interval. The actual sewing point is the minimum of the cost function, which is found using the golden section search method [22].

For compounds with more than one atomic element, Bragg’s additivity rule,

$$\ln(I_c) = \sum_i w_i \ln(I_i), \quad (1)$$

is applied, where $w_i$ are the individual normalized compound fractions by mass for each constituent $i$. If required, the mean excitation potential of a compound, $I_c$, can be set by the user either by directly specifying $I_c$ or by specifying all $I_i$ for each of the constituents. If only $I_c$ is specified by the user, equation 1 is under-determined. In this case, the default ICRU $I$-values are used for the constituents $I_i$ and a common dimensionless scaling factor $a$ is included so that

$$\ln(I_c) = \sum_i w_i \ln(a I_i), \quad (2)$$

holds. Equation 2 is solved for $a$ and the stopping power for each component is calculated using $aI_i$ instead of $I_i$. Robustness of this method is tested by applying an asymmetric scaling factor $a_i$ for the individual components, where $\max(a_i) = 1.2 \min(a_i)$.

Computation speed of libdEdx was tested on an Intel i7-2670QM CPU with a clock frequency of 2.20 GHz. libdEdx was compiled with GCC-4.7.2 on Debian 7.0 using -O2 optimization. Stopping power for helium ions in water was calculated with ASTAR and five different energy steps are chosen: 0.1, 1, 10, 100 and 200 MeV/nucleon.

Figure 1 illustrates how libdEdx is intended to be used in the "fast" mode. A workspace is allocated holding necessary memory for the data structures. Several material/ion/data set configurations can be set, and stopping powers can be retrieved from each or these configurations. After use, the workspace should be freed again.

3. Results and Discussion

An automated test script for libdEdx has been created that compares values determined by libdEdx with stopping power values taken directly from the corresponding original sources for more than 250 different ion, target and energy configurations. libdEdx reproduces the original sources with an accuracy better than 0.3 %. This test script is shipped with the libdEdx distribution and let the user verify the installation at any time.

The mean execution time for 100 million stopping power look-ups is 4.54 seconds, which corresponds to approximately 22 million look-ups per second making libdEdx attractive for CPU-intensive computations with many calls of stopping power routines.

In the case that an $I$-value for a compound, $I_c$, is specified by the user, the extended Bethe algorithm shows less than 0.1 % deviation between stopping power values obtained either with
Figure 1. Diagram of how libdEdx can be used in the “fast” mode. Boxes with a star in the upper right corner can be invoked multiple times within the same workspace.

a common or with an asymmetric scaling factor $a$ or $a_i$, respectively. This means that even if equation 2 is under-determined, there is only little sensitivity to relative changes of the $I$-values of the constituents, as long as the value of $I_c$ for the compound is fixed.

Generally, the choice of a certain source of stopping powers may introduce a systematic error in a theoretical calculation. One can try to estimate the effect size by comparing to results obtained by applying alternative stopping power tables. The magnitude of deviations between stopping power sources depends on the considered combination of projectile, target, and energy. For instance, the stopping power algorithm implemented in SHIELD-HIT is for most purposes in good agreement with, e.g., ICRU 49, but deviates considerably at low energies for protons on aluminium, as pointed out in [23]. This encourages the use of different stopping power tables. A careful choice of stopping power tables is relevant when calculating, e.g., stopping power ratios which may differ in the order of some percent [5]. And also in the process of determining the quantities dose-to-media and dose-to-water [24, 25] it has been observed that the choice of stopping power tables might give +/- 2% systematic error to calculated dose.

4. Conclusion
libdEdx provides a programming library with a fast, clean and easy to use programming API that gives access to multiple stopping power tables and routines. This enables the user to perform comparative studies and, e.g., to determine uncertainties that arise from the choice of stopping power tables. A web front end to libdEdx is provided at http://dedx.au.dk.

For the future, we would like to include nuclear stopping power tables and implement further algorithms such as ATIMA [26], SRIM/TRIM [27], ESTAR, PASS [28], and possibly also radiative stopping power implementations.

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