A Fast and compact approximation of energy loss fluctuation for Monte Carlo simulation of charged particles transport.

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Abstract: A simple and fast functional model is proposed to approximate energy loss distributions of charged particles crossing slabs of matter. The most accepted physical models for treating this problem was created by Landau and later improved by Vavilov. Both models depend on complex functional forms with exact solutions that are, by far, too CPU intensive to be directly included in existing Monte Carlo codes. Several authors have proposed approximations with varying degree of accuracy and performance. This paper presents a compact and efficient form that approximates with enough accuracy the Vavilov distribution and its extreme cases of Landau and Gaussian shapes. Our functional form could be interpreted as a generalization of the basic Gaussian distribution. Some parameter fits are illustrated with various test cases. Our model also represents a simple functional form to use for regression analysis with experimental energy loss data.

Introduction: While crossing a slab of matter a charged particle suffers inelastic interactions and releases energy to the medium. Due to the random nature of those interactions, the resulting energy of the particle emerging at the end of the slab exhibits a probability distribution. Two basic models representing such distributions are in common use inside Monte Carlo (MC) codes: Landau [1] and Vavilov [2].

For a MC code to be used in radiotherapy planning, the need of fast convergence is paramount. In order to be fast, electron transport codes implement condensed history steps to avoid the simulation of billions of interactions per particle history. On the other hand, condensed history simulations alone is less realistic than individual simulation of interactions. As an alternative, most MC uses condensed history steps representing the vast majority of the events but interactions involving high energy transfer are treated individually. Those events over a defined energy threshold are usually called “catastrophic” and its physics is simulated explicitly. Events considered as catastrophic are knocked-on electrons and bremsstrahlung. The introduction of catastrophic events in a code generates some degree of energy loss straggling for the particle, but this fluctuation represents only the extreme cases of fluctuations. All other energy loss fluctuations below the energy threshold are not treated individually and should be included with one of the models by Landau or Vavilov.

The Landau distribution depends on the universal Landau function:

$$\phi(\lambda)=\frac{1}{2\pi i}\int_{c+i\infty}^{c-i\infty} exp(ulnu+\lambda u)du \qquad\qquad c\geq 0$$

The validity of Landau’s theory depends on some restrictions. One of its restrictions conflicts with MC codes including catastrophic events over a cut-off energy: there is no upper limit for the maximum energy loss for a single interaction in Landau’s model ($E_S = \infty$).

The Vavilov distribution is more realistic because it contains a maximum limit to the energy transfer in a single interaction (E_S).

$$f(x,\Delta)=\frac{1}{i2\pi}\int_{q-i\infty}^{q+i\infty}\exp\left\{p\Delta-x\int_0^{E_S}\omega(E)\ (1-\exp(-pE))dE\right\}dp$$

Where x is the path length of the particle and Δ is the actual energy loss over the condensed history step.

It is useful to describe the energy loss fluctuation as a function of a parameter **K** defined as:

$$K = \xi / E_S$$

K is proportional to the ratio of mean energy loss to the maximum allowed energy transfer in a single interaction.

The parameter K could take values in the interval $(0,..,\infty)$. If $K \to 0$, it means that E_S is very high compared to the mean energy loss. If $K \to \infty$, it means that E_S is very low compared to the mean energy loss. For $K \to 0$, the Vavilov distribution should reproduces Landau's shape. On the other hand, if for $K \to \infty$, the distribution became symmetric and identical to a Normal distribution.

Analytic solutions for Landau and Vavilov are too complex and time-consuming for use in MC simulation [3]. Several approaches have being proposed to alleviate the time-consumption impact on MC codes [4, 5, 6, 7].

A possible approach is the use of pre-generated tabulated distributions. This approach has several drawbacks. While it is a reasonable solution for Landau's distribution function, it is too costly to implement for all possible variation of the ***K*** parameter in Vavilov's distribution. An additional performance consideration is that searching into many tables at different address into RAM forces the continuous flush of processor's internal cache, which translate into serious performance penalization in modern superscalar CPUs.

Some authors have used rational functions approximations dividing the distributions in subintervals for better agreement [5]. A clever approach by Chibani proposed the use of the lognormal distribution [6, 7]. The use of Edgeworth expansion is a well-known method to correct a Gaussian distribution and has also being investigated [11].

METHOD

Both, Landau and Vavilov, are skewed distributions, but there is a resemblance between those distributions and the normal distribution. Modifications of the normal distribution have been used to skew the original shape of the function, as in the case of the human longevity distribution [7].

Our proposed model for the probability distribution function, representing Landau and Vavilov is:

$$f(x) = N * \mathrm{e}^{-\left(\frac{x'}{a+b*x'+c*x'^2}\right)^2} \qquad \text{equ.1}$$

where

$$x' = x - u \qquad \text{equ.2}$$

The proposed model has five parameters for fitting the shape of any energy fluctuation distribution, from the ideal Landau case to Vavilov, including the extreme case of a "pure" Gaussian form.

The parameter ***u*** is a translation governing the distribution mean, ***N*** is a normalization or scale factor and the other three parameters adjust the variance and skewness of the resulting distribution.

The parameters of the proposed model were fitted to analytical solutions of Landau and Vavilov. A non-linear regression method was implemented for fitting the parameters. A different set of the five parameters should be fitted for any value of ***K*** and particle speed in the Vavilov distribution function.

The Landau's distribution was generated implementing the solutions by Börsch-Supan [3]. Our results were compared with those published [3] before its use. The exact implementation of Landau demonstrated that was too time consuming for inclusion in MC codes.

Our Vavilov exact solution was based on the original paper [2], complemented with some ideas presented by Seltzer and Berger [7]. Our implementation is improved because we used a better approximations of the sine and cosine integrals, based in the Padé approximants for the argument in the range [0..4] and the use of Chebyshev-Padé expansions of the auxiliary functions for arguments x > 4.0 [9,10]. Our sine and cosine integral are accurate to better than 10^{-16} for the whole range. As expected, the computation time for exact Vavilov is exceedingly large for direct inclusion in MC codes.

Results and discussion.

Figure 1 presents a plot of Landau distribution based on the evaluation method by Börsch-Supan[3].

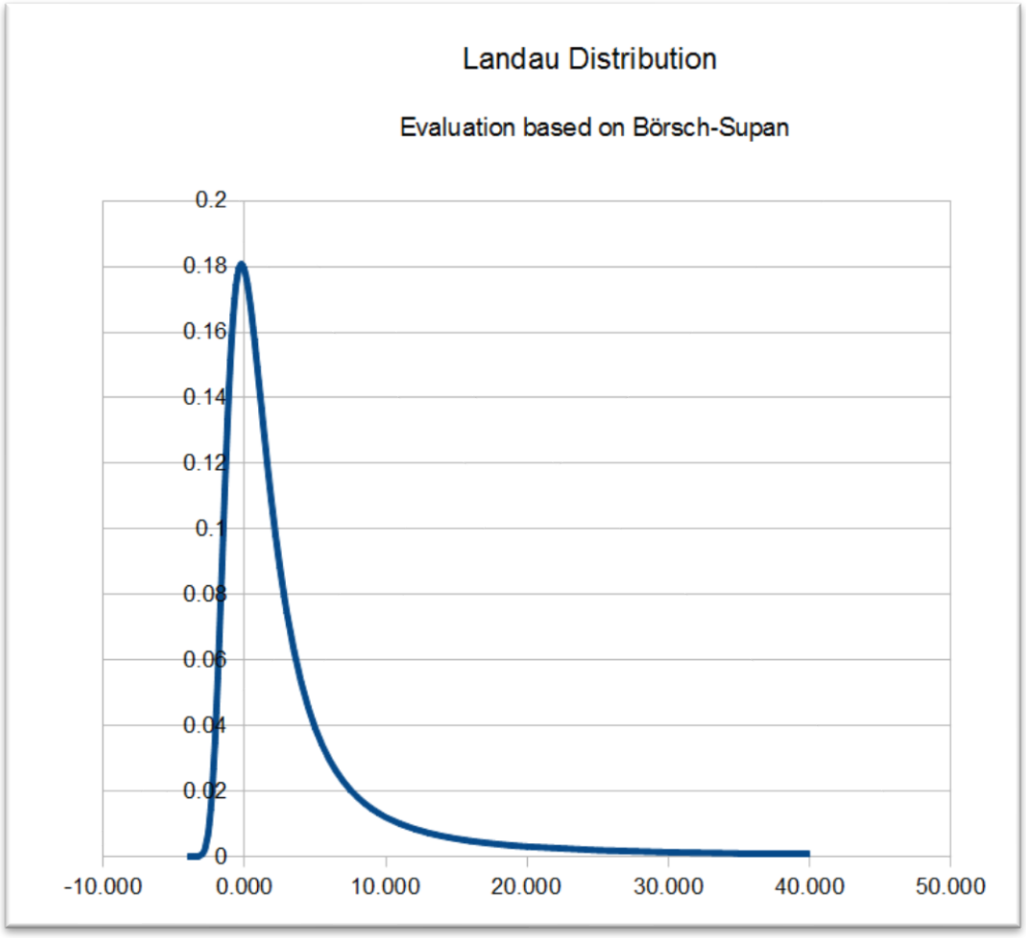

Fig. 1

Figure 2 presents the overlaid plot of Börsch-Supan and the fitting model evaluation. The blue curve is Börsch-Supan while the fitting model is red. The optimum parameters were: N=0.179159, u = 0.390788, A = 2.202571, B = -0.223021, C=-0.000175. Only a few traces of the red curve are visible because of the remarkable proximity between the exact distribution and the proposed approximation.

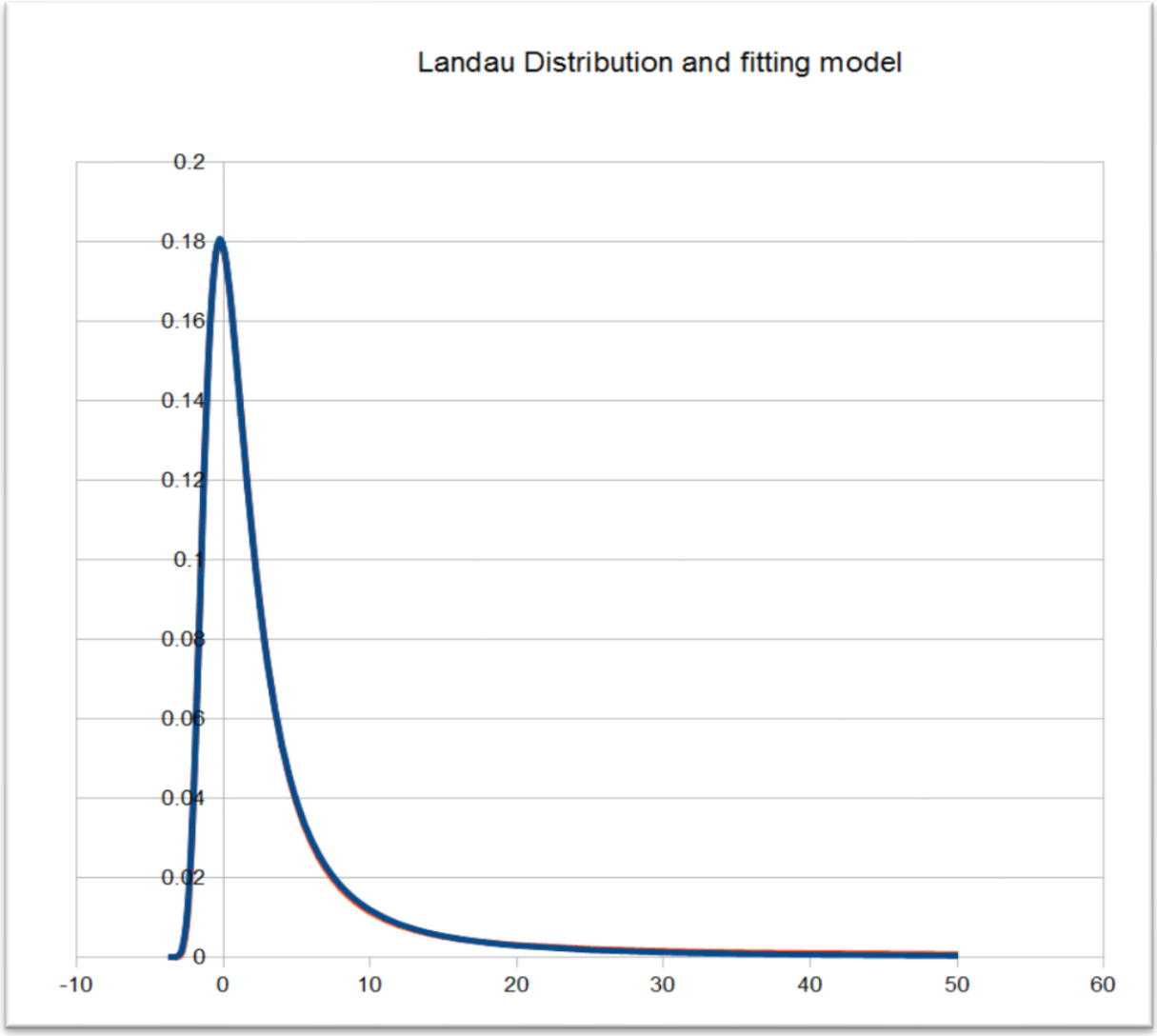

Fig. 2

Figure 2 shows that the correspondence between a rigorous evaluation of Landau's distribution and our fitting model is good for most simulations purposes.

Figure 3 shows the Vavilov distribution for electrons in Water. The initial energy is 10 MeV, Es is 0.2 Mev and K 0.128. The curve in blue is Vavilov, the red is our model. The optimum parameters were: N=0.98735, u = 0.4713, A = 0.04898, B = 0.32578, C=-0.282869.

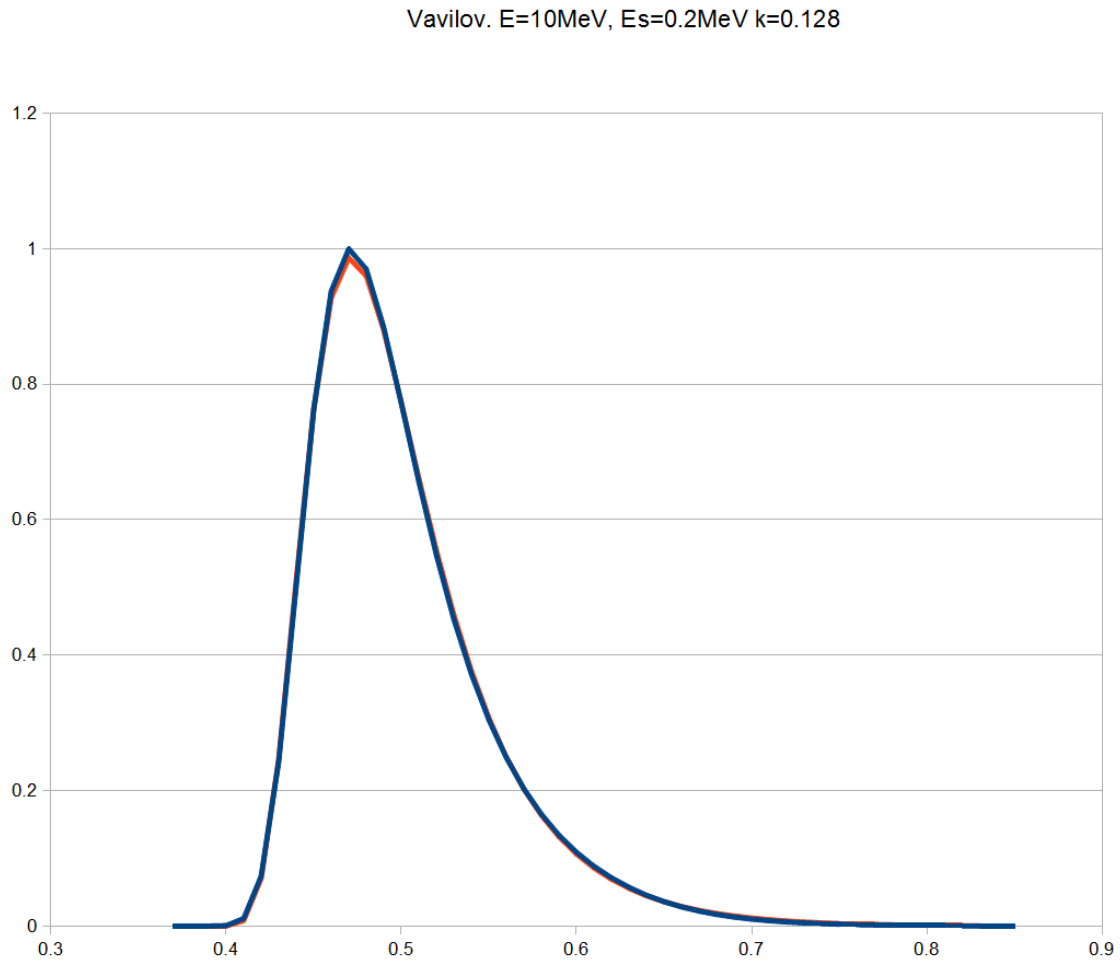

Fig. 3

Figure 4 shows Vavilov exact distribution overlapped with the implementation of Rotondi and Montagna [13] model. The implementation of Rotondi and Montagna was taken from CERNlib and translated into C99. The physical conditions are the same as those in figure 3. The blue trace is Vavilov and the red is Rotondi and Montagna. The model reproduces very well the Vavilov distribution at its central region. At the right tail (region of high energy loss) there is a step that almost ignores the possibility of energy losses with probabilities bellow 1%. As the documentation said, the error increases toward both tail, but in our experiments bigger errors were found on the high energy tail.

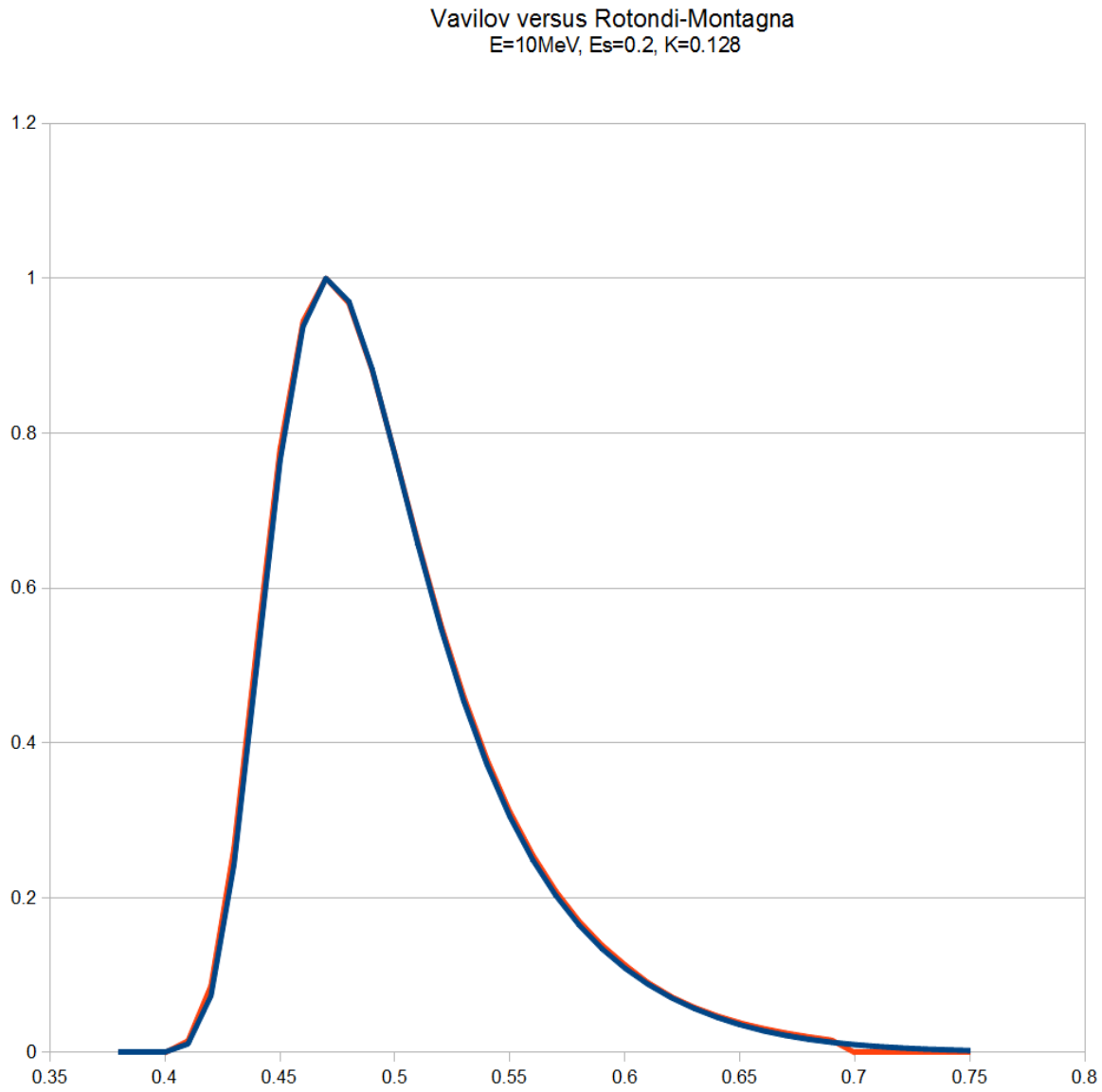

Fig. 4

Figure 5 shows the same test case from figure 3, but it compares Vavilov with Log-normal and our model. Vavilov curve is blue, Log-Normal is red and our model in yellow. This test case has the same conditions as one from Chibani work [7] using the log-normal distribution.

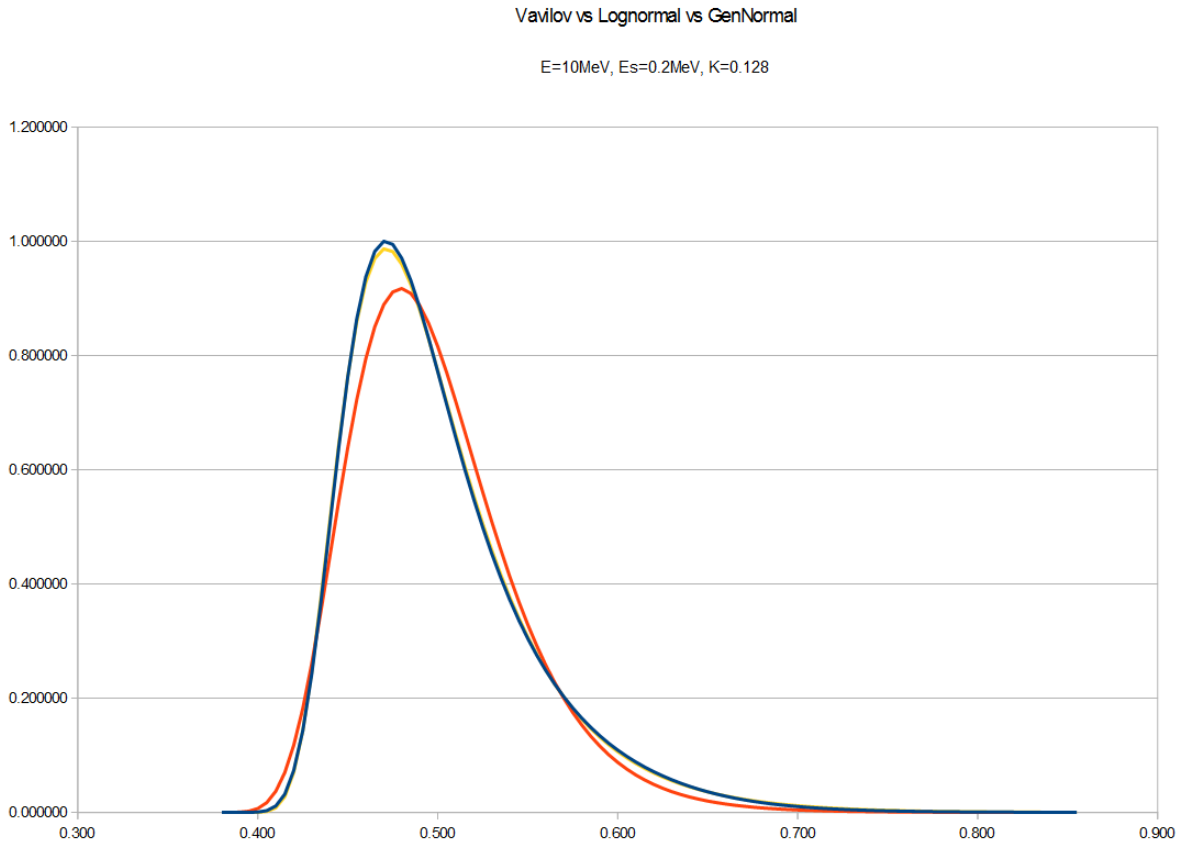

Fig. 5

Figure 6 shows the Vavilov distribution for electrons in Water. The initial energy is 10 MeV, Es is 0.1 Mev and K 0.266. This test case has the same conditions as one from Chibani work [7] using the log-normal distribution. The curve in blue is Vavilov, the red is our model, it is almost a perfect superposition. The optimum parameters were: N=99762, u = 0.48339, A = 0.043564, B = 0.250287, C=-0.415041.

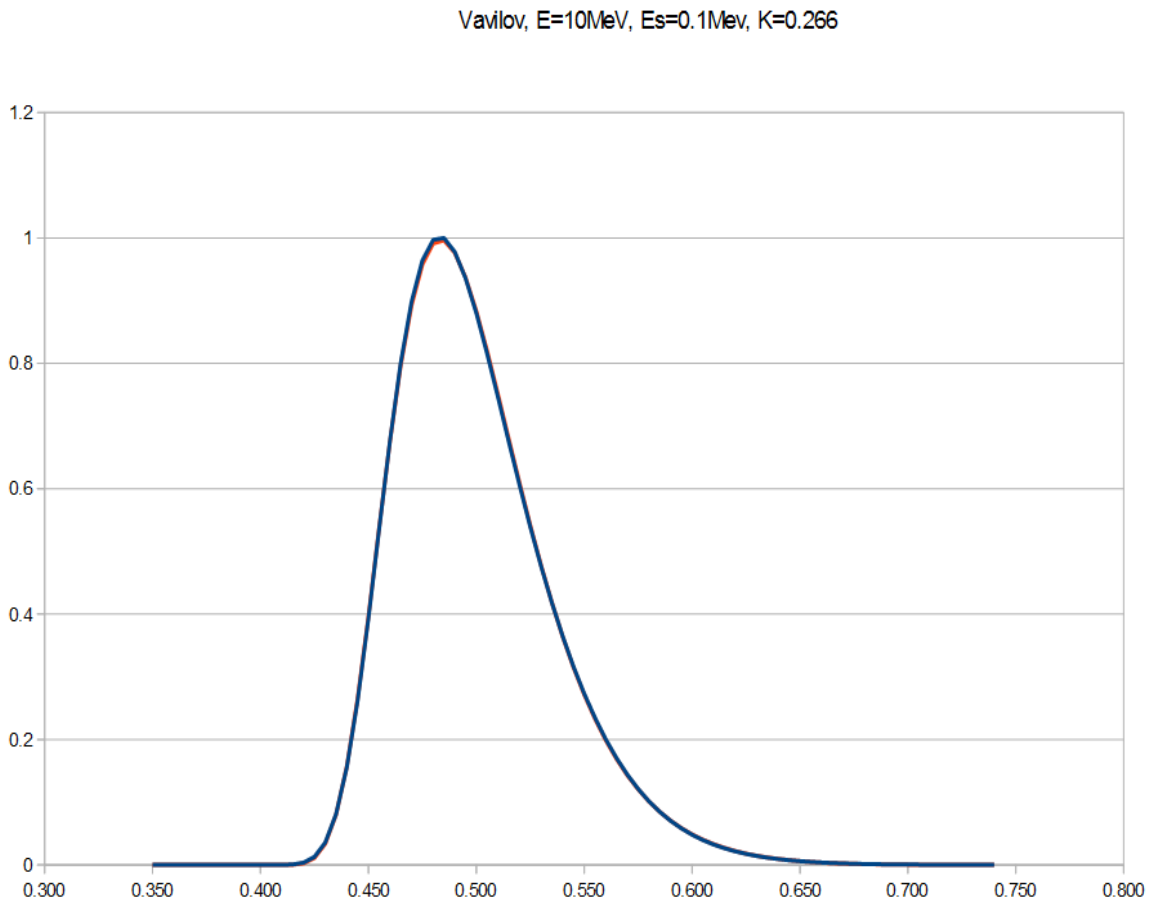

Fig 6

Figure 7 shows the fit of the model to experimental data for protons by Hancock et. al. [8]. Curve in blue follows the experimental data (range of error not shown) and the red curve is our model. We could not access the original data by Hancock et. al., the blue curve is the product of a digitalization from figure 2a at referenced paper [8].

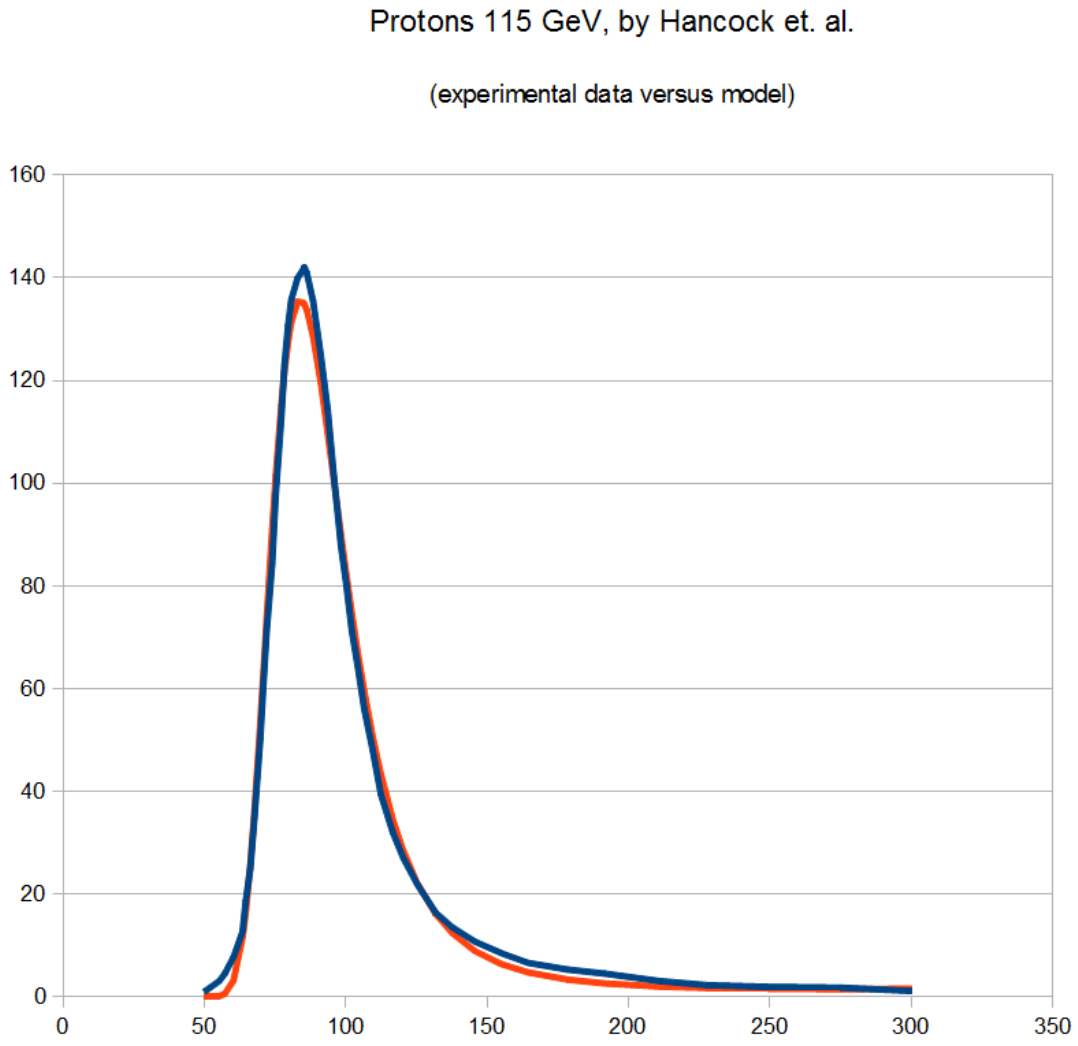

Fig. 7.

The idea proposed by Tabata et. al. [5], of using rational function approximation, was also tested. The original paper investigated only the use of rational fractions for Landau distributions, but we try the same method with some Vavilov cases. Figure 8 shows a Vavilov distribution for electrons in Water. The blue curve is the exact Vavilov distribution, the yellow curve is our model and the red curve is the rational function approximation. The rational function used had nine coefficients, four for the numerator and five for the polynomial denominator. It is necessary to split the range of energy loss, at less, into two subintervals; the position of the maximum of the distribution was the division of the domain. Therefore, this approximation needs 18 parameters for any case of the Vavilov distribution. As figure 8 shows, care must be taken with both ends of the range because oscillations of the distribution are common, even taking negative values. Our model (yellow) follows closely the exact Vavilov distribution, the only region with apparent differentiation between our model and Vavilov is close to the maximum.

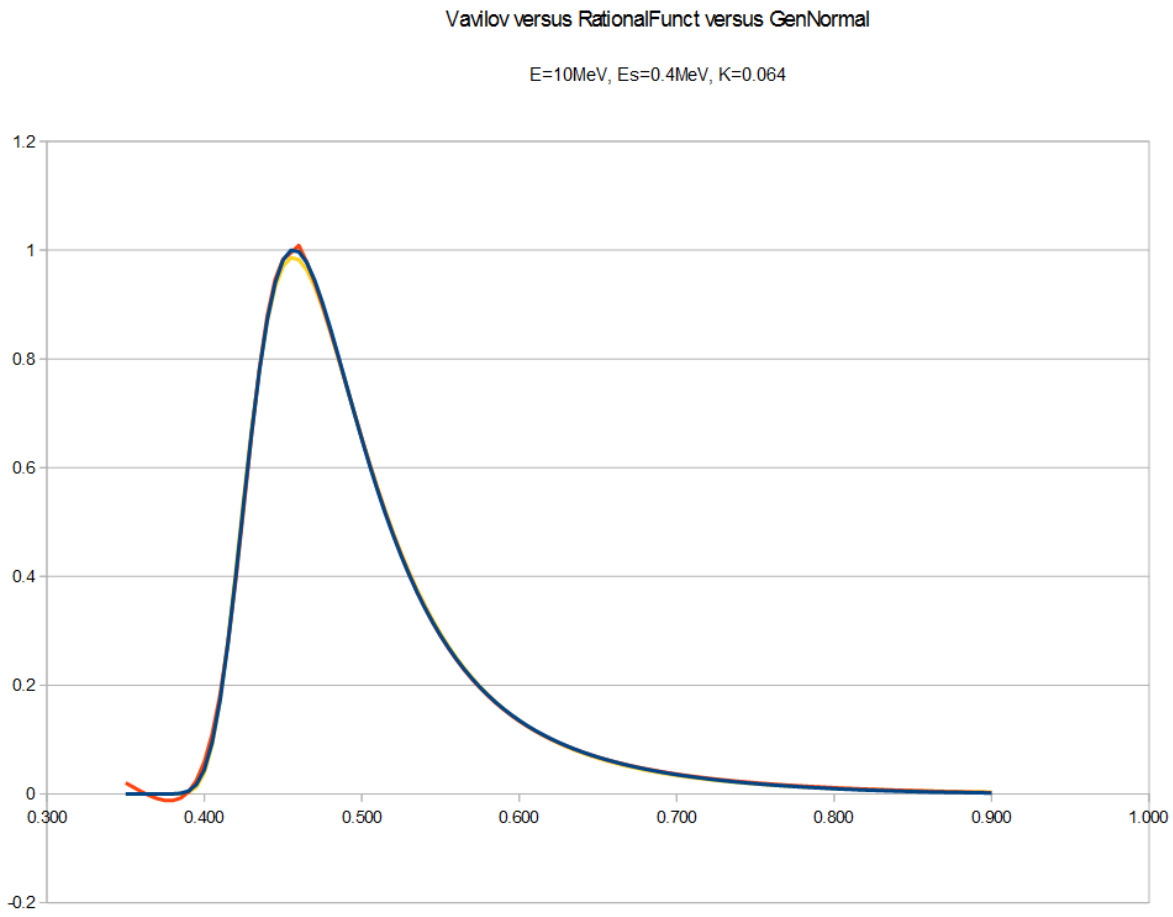

Fig. 8

The execution time needed to compute a Vavilov distribution was the main motivation of this and other works, so let us illustrate the issue with some results. All our numerical experiments used an Intel i7-4930K CPU at 3.40 GHz. The next table presents the results.

Function Model	Time to compute 1 point in distribution [s]
Landau exact (estimated better than 10^{-5})	2.983E-3
Vavilov exact (estimated better than 10^{-5})	1.696E-2
Log-Normal	5.911E-8
Rational function	2.157E-8
Our model (GenNormal)	2.092E-8
Rotondi/Montagna From CERNlib	2.105E-8

The implementation of all the models is in C99. The compiler used on the experiments was Intel C++ Composer XE 2013, SP1 [12].

Landau and Vavilov exact implementation had the Simpson's integration parallelized using OpenMP, but no other optimization technique was employed. Our Generalized Normal model, the Log-normal model and the rational functions did not gain with parallelization.

As the figures demonstrate, a direct implementation of either Landau or Vavilov are not feasible for most applications. A typical MC code with one million initial electron tracks in water may evaluate 100 million times the energy loss distribution. Assuming that the time for evaluation is equal to the number in the table it will take (it is more than that) 471 hours of CPU time only for Vavilov computation. The same task could take only 2 seconds using our model.

The Log-normal implementation takes 2.8 more CPU time than our generalized normal distribution. This should be the result of a logarithm not present in our model.

The rational function and our model shows equivalent execution time, but the need of 18 parameters and the risk of having oscillatory values at both ends renders the method as not recommended.

The Rotondi and Montagna method has equivalent execution time with our model, but our model has a much simpler functional form and is better for experimental data fitting.

As several of these models use transcendental functions, the resulting CPU times depends on the implementation of those transcendental functions in the compiler library. Some modern implementation of the exponential function, based in SSEx/AVX technologies, are very efficient, as it is the case with Intel compilers (C, C++ and FORTRAN).

Conclusion:

A functional form, simple and easy to evaluate, is presented to approximate the behavior of energy loss fluctuation of charged particles crossing slabs of matter. The model could be interpreted as a generalization of the original Gaussian distribution, a generalization that introduces and control skewness. We have experimented with several test cases, including theoretical distributions from Vavilov and Landau's model as well as measurements results published by other authors. Due to its simplicity the model is a good candidate for use as a regression function with experimental measurements of energy loss.

NOTE: Source code is available upon request from the author, Including Landau and Vavilov exact computations and the regression method to fit our model parameters.

References

1 - Landau, L. "On the energy loss of fast particles by ionization". *J. Phys. (USSR)* **8**: 201 (1944).

2 – Vavilov P.V. "Ionization losses of high-energy heavy particles". Soviet Physics JETP, vol 5, num 4 (1957).

3 - Börsch-Supan. J. Res. Natl Bur Standards 65B (1961)

4 - J.E. Moyal, Theory of ionization fluctuations, Phil. Mag. **46** 263 (1955).

5 – Tabata T., Ito R., Approximations to Landau's distribution functions for the ionization energy loss of fast electrons. Nucl. Instruments and Methods. 158, 521-523 (1979).

6 – Chibani O., New Algorithms for Vavilov distribution calculation and the corresponding energy loss sampling. IEEETransctions on Nuclear Science Vol 45, No.5 (1998).

7 – Chibani O., Energy-loss straggling algorithms for Monte Carlo electron transport. Med.Phys. 29. (2002).

8 – Robertson HT, Allison DB, "A Novel Generalized Normal Distribution for Human Longevity and other Negatively Skewed Data". PLoS ONE 7(5): e37025. doi:10.1371/journal.pone.0037025 (2012).

7 – Seltzer S.M., Berger M.J, "Energy-loss straggling of protons and mesons: Tabulation of the Vavilov distribution" book chapter in: "Studies in penetration of charged particles in matter", Nuclear Science Series, Report Number 39, Committee on Nuclear Sciences, (1964).

8 – Hancock S., James F., Movchet J., Rancoita P.G., VanRossum L., "Energy loss and energy straggling of protons and pions in the momentum range 0.7 to 115 GeV/c", Physical Review A, vol 28, num. 2, (1983).

9 – Temme N.M., “Exponential, Logarithmic, Sine, and Cosine Integrals”, chapter 6 in: “NIST Digital Library of Mathematical Functions”. version 1.0.9; http://dlmf.nist.gov/ (2014).

10 – Abramowitz M., Stegun I.A, “Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables”, chapter 5. Page 231. National Bureau of Standards, Tenth Printing, http://people.math.sfu.ca/~cbm/aands/page_231.htm . (1972).

11 - VanGinneken A., “Edgeworth series for collision energy loss and multiple scattering”, Nuclear Instruments and Methods in Physics Research Section B. vol 160, 4, (2000).

12 - Intel Parallel Studio, C++. https://software.intel.com/en-us/intel-parallel-studio-xe .

13 - A. Rotondi and P. Montagna, “Fast calculation of Vavilov distribution”, Nucl. Instr. and Meth. B47 (1990).