Review of Geant4 Goudsmit-Saunderson model

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Outline

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1. Motivation, about, not about
2. Theoretical background in a nutshell
   - Goudsmit-Saunderson(GS) theory
   - Combination of GS-theory with screened Rutherford DCS
   - Kawrakow-Bielajew theory

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2. Theoretical background in a nutshell
   - Goudsmit-Saunderson(GS) theory
   - Combination of GS-theory with screened Rutherford DCS
   - Kawrakow-Bielajew theory
3. Few words on sampling
   - Sampling from parametrized PDF
   - Sampling of bins in case of pre-computed PDF
   - Interpolation of the inverse CDF

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Motivation:

- looking for candidate model for multiple elastic scattering of low energy ($< 100[MeV]$) electrons/positrons that can be used for optimization/vectorization within the `Geant-V` project [1]
- Kawrakow-Bielajew model is investigated as the first candidate
- one version of this model is currently available in `Geant4`
- a different version is under implementation in `Geant4` only for testing purposes

What's this presentation about?

- the new version of the model
- the model involves sampling from pre-computed distributions stored in table over a 2D parameter grid
- some advanced sampling techniques are used in the new version that are not frequently used in `Geant4` however accurate, fast sampling can be achieved by using them
- these techniques will be discussed as well

What it's not about?

- this is not a code review !!!
- the currently available `Geant4` version of the model won't be discussed or jugged
- the presentation will mainly focus on modelling of angular sampling and other parts like energy loss correction, computation of Lewis's moments are not discussed [but taken into account in the new version in a self consistent way]

Additional remark: detailed discussion of the theory itself would take more than 20 minutes so we will run through that very quickly and will focus on more practical issues. [However, information on the "theory" slides for more detailed study is available]

[1] http://geant.cern.ch/content/about-geant5

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Geant4 Goudsmit-Saunderson model is the

- Kawrakow-Bielajew model for elastic scattering
  [I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336]
- based on Goudsmit-Saunderson theory of multiple elastic scattering
  [S.Goudsmit,J.L.Saunderson, PR 57(1940)24-29]
- hybrid model for (no, single) and multiple elastic scattering of e^-/e^+
  [A.F.Bielajew, NIMB 111(1996)195-208]
- the screened Rutherford DCS is used for elastic scattering

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Goudsmit-Saunderson angular distribution after travelling a path s:

$$F(s;\theta)_{GS} = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \exp(-s/\lambda_\ell) P_\ell(\cos(\theta))$$

- $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$-elastic DCS; $\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega$-elastic cross section; $\lambda^{-1} = \mathcal{N}\sigma$-elastic mean free path
- $f_1(\theta) = \frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ is single elastic scattering distribution (note that $2\pi f_1(\theta) = 2\pi\frac{1}{\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = p(\cos(\theta))$)
- $f_1(\theta)$ is expressed in terms of orthogonal polynomials (Legendre series) $f_1(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} F_\ell P_\ell(\cos(\theta))$
- $F_\ell = 2\pi \int_{-1}^{1} f_1(\theta) P_\ell(\cos(\theta))\mathrm{d}(\cos(\theta)) = \langle P_\ell(\cos(\theta))\rangle$
- G_ℓ are the ℓ-th transport coefficients $G_\ell \equiv 1 - F_\ell = 1 - \langle P_\ell(\cos(\theta))\rangle$
- $\lambda_\ell^{-1} \equiv \frac{G_\ell}{\lambda} = \frac{1-F_\ell}{\lambda} = \frac{1-\langle P_\ell(\cos(\theta))\rangle}{\lambda}$
- then $F(s;\theta) = \sum_{n=0}^{\infty} f_n(\theta)\mathcal{W}_n(s)$
- $f_n(\theta)$ the angular distribution after n elastic interactions $f_n(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi}(F_\ell)^n P_\ell(\cos(\theta))$
- $\mathcal{W}_n(s) = \exp(-s/\lambda)\frac{(s/\lambda)^n}{n!}$ is the probability of having exactly n elastic interaction along a path s (i.e. Poisson)

[S.Goudsmit,J.L.Saunderson, PR 57(1940)24-29; J.M.Fernández-Varea,R.Mayol,J.Baró,F.Salvat NIMB 73(1993)447-473]

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Using a simple exponentially screened Coulomb potential as the scattering potential in the computation of the scattering amplitudes under the first Born approximation(Wentzel model):

- $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f|^2$ where $f \equiv f(\theta,\phi)$ is the scattering amplitude
- which $f_{B1}(\theta,\phi) = -\frac{2m}{4\pi\hbar^2}\int e^{i(\bar{k}_f-\bar{k}_i)\bar{r}'}V(\bar{r}')\mathrm{d}^3r'$ in the first Born approximation [where: $\bar{k}_i$, $\bar{k}_f$ and $V(\bar{r}')$ are the wave vectors of the incident plane, the outgoing(scattered) spherical spherical wave and the scattering potential respectively. Note that: (i) in case of elastic scattering $k_i = k_f \equiv k$; (ii) $\hbar\bar{q} = \hbar(\bar{k}_f - \bar{k}_i)$ is the momentum transfer and $q^2 = |\bar{k}_f - \bar{k}_i|^2 = 2k^2(1-\cos(\theta)) = 2k^2(2\sin^2(\theta/2))$ where $\theta \equiv \angle(\bar{k}_i,\bar{k}_f)$ is the scattering angle]
- assuming $V(\bar{r}) \equiv V(r)$ i.e. spherically symmetric scattering potential, substituting $\bar{q} = \bar{k}_f - \bar{k}_i$ and choosing the coordinate system for the integration such that $\bar{q} = q\hat{\bar{z}}$
  $f_{B1}(\theta) = -\frac{2m}{q\hbar^2}\int_0^\infty \sin(qr')r'V(r')\mathrm{d}r'$
- then using a simple exponentially screened Coulomb potential as the scattering potential i.e.
  $V(r) = \frac{ZZ'e^2}{r}e^{-r/R}$ [Z target atomic number, $Z'e$ projectile charge, R screening radius] we can get
  $f_{B1}(\theta) = -\frac{2m}{\hbar^2}ZZ'e^2\left[\frac{1}{2k^2[1-\cos(\theta)+R^{-2}/(2k^2)]}\right]$
- which gives $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2\frac{1}{(1-\cos(\theta)+R^{-2}/(2k^2))^2}$
- one can introduce $A \equiv \frac{1}{4}\left(\frac{\hbar}{p}\right)^2 R^{-2}$ screening parameter [note that $1/(2k^2R^2) = 2A$] that gives the DCS for elastic scattering $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2\frac{1}{(1-\cos(\theta)+2A)^2}$ and the corresponding

So DCS for elastic scattering within the Wentzel model is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2}$$

- $\sigma^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{\pi}{A(1+A)}$
- $f_1^{(W)}(\theta) = \frac{1}{\pi}\frac{A(1+A)}{(1-\cos(\theta)+2A)^2}$
- $G_\ell^{(W)}(A) = 1 - F_\ell = 1 - \ell[Q_{\ell-1}(1+2A) - (1+2A)Q_\ell(1+2A)]$ [$Q_\ell(x)$ are Legendre functions of the second kind]
- $G_{\ell=1}^{(W)}(A) = 2A\left[\ln\left(\frac{1+A}{A}\right)(A+1) - 1\right]$
- note that $\frac{1}{\lambda_1} = \frac{G_{\ell=1}^{(W)}(A)}{\lambda}$ gives the possibility set the screening parameter A such that the corresponding DCS $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)}$ will give back λ_1 [therefore e.g. $\langle\cos(\theta)\rangle = \exp(-s/\lambda_1)$ will be correct]

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First derive Bielajew's hybrid form of the GS distribution i.e. separate the no, single and at least two elastic scattering contributions:

- $$\mathcal{W}_{n=0}(s) = \exp(-s/\lambda); \;\; \mathcal{W}_{n=1}(s) = \exp(-s/\lambda)(s/\lambda); \;\; \mathcal{W}_{n\geq 2}(s) = 1 - \exp(-s/\lambda) - \exp(-s/\lambda)(s/\lambda)$$

- the GS series becomes [note that it is a p.d.f. of θ i.e. $\int_\Omega F(s;\theta)\mathrm{d}\Omega = 1$]

$$F(s;\theta)_{GS} = \sum_{n=0}^{\infty} f_n(\theta)\mathcal{W}_n(s) = f_{n=0}(\theta)\mathcal{W}_{n=0} + f_{n=1}(\theta)\mathcal{W}_{n=1} + \sum_{n=2}^{\infty} f_n(\theta)\mathcal{W}_n(s) = \mathrm{e}^{-s/\lambda}\frac{\delta(1-\cos(\theta))}{2\pi}$$

$$+ (s/\lambda)\mathrm{e}^{-s/\lambda} f_{n=1}(\theta) + \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} P_\ell(\cos(\theta)) \left\{ \mathrm{e}^{-(s/\lambda)G_\ell} - \mathrm{e}^{-(s/\lambda)} \left[1 + (s/\lambda)(1-G_\ell)\right] \right\}$$

- make the transformation $\theta \rightarrow \mu \equiv \cos(\theta)$ [which is the p.d.f. of μ i.e. $\int_{-1}^{+1} F(s;\mu)\mathrm{d}\mu = 1$]

$$F(s;\mu)_{GS} = 2\pi F(s;\theta\rightarrow\mu)_{GS} = \mathrm{e}^{-s/\lambda}\delta(1-\mu) + (s/\lambda)\mathrm{e}^{-s/\lambda} 2\pi f_{n=1}(\mu) +$$

$$\sum_{\ell=0}^{\infty} (\ell+0.5) P_\ell(\mu) \left\{ \mathrm{e}^{-(s/\lambda)G_\ell} - \mathrm{e}^{-(s/\lambda)} \left[1 + (s/\lambda)(1-G_\ell)\right] \right\}$$

[A.F.Bielajew, NIMB 111(1996)195-208; I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336;]

- in order to get all 3 terms in the form of *probability x p.d.f.*

$$F(s;\mu)_{GS} = \mathrm{e}^{-s/\lambda}\delta(1-\mu) + (s/\lambda)\mathrm{e}^{-s/\lambda}2\pi f_{n=1}(\mu) + (1-\mathrm{e}^{-s/\lambda}-(s/\lambda)\mathrm{e}^{-s/\lambda})F(s;\mu)_{GS}^{2+}$$

where

$$F(s;\mu)_{GS}^{2+} \equiv \sum_{\ell=0}^{\infty}(\ell+0.5)P_\ell(\mu)\frac{\mathrm{e}^{-(s/\lambda)G_\ell}-\mathrm{e}^{-(s/\lambda)}\left[1+(s/\lambda)(1-G_\ell)\right]}{1-\mathrm{e}^{-s/\lambda}-(s/\lambda)\mathrm{e}^{-s/\lambda}}$$

  - no-scattering case: trivial
  - single scattering case: using the Wentzel model, the PDF for single scattering $p(A;\mu) = 2\pi f_{n=1}(\mu) = \frac{2A(1+A)}{(1-\mu+2A)^2}$ the corresponding CDF $\mathcal{P}(A;\mu) = \frac{(A+1)(1-\mu)}{1-\mu+2A}$ and the sampling $\mu = \mathcal{P}^{-1}(A;\xi) = 1-\frac{2A\xi}{1-\xi+A}$ where $\xi \in \mathcal{U}(0,1)$
  - multiple scattering case: need to sample from $F(s;\mu)_{GS}^{2+} \rightarrow$ pre-compute

Variable transformation is needed to obtain smooth distributions → reduce memory footprint and improve sampling

- suppose that we apply the transformation $u = f(a_1, ..., a_n; \mu)$ [where $u \in [0,1]$ the transformed variable f is the transformation function with $a_1, \ldots, a_n$ parameters that control the shape of the result of the transform]
- let $q^{2+}(u)$ PDF of u be the transformed $F(s;\mu)^{2+}_{GS}$ PDF of μ that needs to satisfy the requirement $q^{2+}(s;u)\mathrm{d}u = F(s;\mu)^{2+}_{GS}\mathrm{d}\mu$ [i.e.the probability of having u falling into the $\mathrm{d}u$ interval around u according to the transformed PDF $q^{2+}(u)$ is equal to the probability of having μ falling into the $\mathrm{d}u$ interval around μ according to the original PDF $F(s;\mu)^{2+}_{GS}$]
- which means that $q^{2+}(s;u) = F(s;\mu)^{2+}_{GS}\frac{\mathrm{d}\mu}{\mathrm{d}u}$ where $\frac{\mathrm{d}\mu}{\mathrm{d}u} = \left(\frac{\mathrm{d}u}{\mathrm{d}\mu}\right)^{-1} = \left(\frac{\partial f(a_1,\ldots,a_n;\mu)}{\partial\mu}\right)^{-1}$
- the parameters a_i $i = 1, ..., n$ of the transformation can be determined through the optimization

$$0 = \frac{\partial}{\partial a_i}\left[\int_0^1 \left[q^{2+}(s;u) - 1\right]^2 \mathrm{d}u\right] = \int_{-1}^{+1}\left[F(s;\mu)^{2+}_{GS}\left(\frac{\partial f(a_1,...,a_n;\mu)}{\partial\mu}\right)^{-1}\right]^2\left[\frac{\partial^2 f(a_1,...,a_n;\mu)}{\partial\mu\partial a_i}\right]\mathrm{d}\mu$$

[we want the transformed $q^{2+}(s;u)$ PDF to be as close as possible to the uniform distribution (in least-square sense)]

- in the case of using the Wentzel model one can take $u = f(a;\mu) = \frac{(a+1)(1-\mu)}{1-\mu+2a}$; the corresponding inverse transform $\mu = 1 - \frac{2au}{1-u+a}$ [note that $f(a;\mu)$ corresponds to the single scattering Wentzel CDF with a scaled $a = w^2A$ screening parameter, where the scaling factor w is arbitrary at the moment; the motivation behind this: if $\mathcal{P}(\mu)$ would be the exact CDF that corresponds to the original PDF $F(s;\mu)^{2+}_{GS}$ and one would use $f(\mu) \equiv \mathcal{P}(\mu)$, the transformed distribution would be the uniform distribution(in order to see this, just plug $f(\mu) \equiv \mathcal{P}(\mu)$ into the third item on this page).]

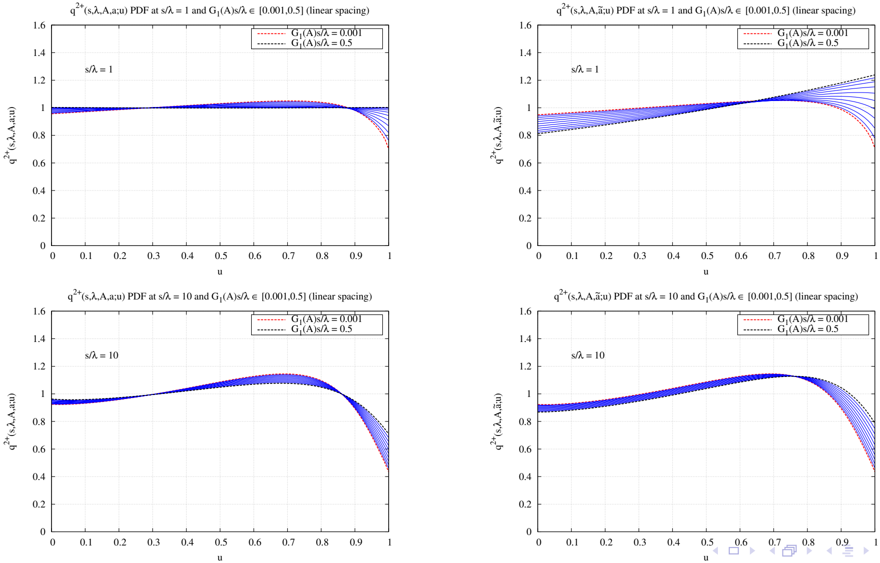
[I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336]

Kawrakow-Bielajew theory

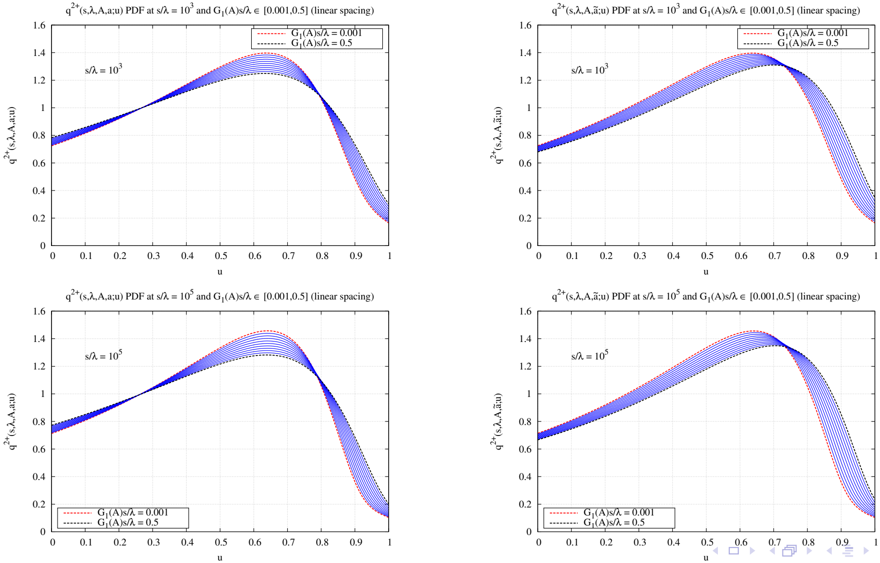
- the optimal parameter of the transformation can be determined by plugging the chosen transformation function $u = f(a;\mu) = \frac{(a+1)(1-\mu)}{1-\mu+2a}$ into the results of the optimization i.e. $0 = \int_{-1}^{+1} \left[F(s;\mu)_{GS}^{2+} \left(-\frac{[1-\mu+2a]^2}{2a(1+a)} \right) \right]^2 \left[-2\frac{1-\mu(1+2a)}{[1-\mu+2a]^3} \right] \mathrm{d}\mu$ that leads to the optimal solution
$$a = \frac{\alpha}{4\beta} + \sqrt{\left(\frac{\alpha}{4\beta}\right)^2 + \frac{\alpha}{4\beta}}$$
where
$\alpha = \sum_{\ell=0}^{\infty} \gamma_\ell(s,\lambda,A) \left\{ \left(1.5\ell + \frac{0.065}{\ell+1.5} + \frac{0.065}{\ell-0.5} + 0.75\right) \gamma_\ell(s,\lambda,A) - 2(\ell+1)\gamma_{\ell+1}(s,\lambda,A) + \frac{(\ell+1)(\ell+2)}{(2\ell+3)} \gamma_{\ell+2}(s,\lambda,A) \right\}$
$\beta = \sum_{\ell=0}^{\infty} (\ell+1)\gamma_\ell(s,\lambda,A)\gamma_{\ell+1}(s,\lambda,A)$ and $\gamma_i(s,\lambda,A) = \frac{\mathrm{e}^{-(s/\lambda)G_i(A)} - \mathrm{e}^{-(s/\lambda)}[1+(s/\lambda)(1-G_i(A))]}{1-\mathrm{e}^{-s/\lambda}-(s/\lambda)\mathrm{e}^{-s/\lambda}}$
- it would be too expensive to compute these optimal values of a at runtime (at the back transform) so one can use a polynomial fit to the optimal $w^2 \approx \tilde{w}^2$ then $a \approx \tilde{a} = \tilde{w}^2 A$ can be obtained (both at pre-computation and at run time for the back transform). Kawrakow obtained
$$\frac{\tilde{w}^2}{0.5(s/\lambda)+2} = \begin{cases} 1.347 + t(0.209364 - t(0.45525 - t(0.50142 - t0.081234))) & \text{if } s/\lambda < 10 \\ -2.77164 + t(2.94874 - t(0.1535754 - t0.00552888)) & \text{otherwise} \end{cases}$$
where $t = \ln(s/\lambda)$.
- the transformed distribution $q^{2+}(s,\lambda,a,A;u) = \frac{2a(1-a)}{[1-u+a]^2} \sum_{\ell}^{\infty} (\ell+0.5) P_\ell \left[1 - \frac{2au}{1-u+a}\right] \gamma_\ell(s,\lambda,A)$

[I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336, I Kawrakow et al., NRCC Report PIRS-701]

Kawrakow-Bielajew theory



Kawrakow-Bielajew theory



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We have the $q^{2+}(s/\lambda, G_1 s/\lambda; u)$ PDFs pre-computed over a pre-defined 2D grid of $\{(s/\lambda)_i\}$ and $\{(G_1 s/\lambda)_j\}$ sets of parameter values carefully chosen such that linear interpolation in $\log(s/\lambda)$ and $G_1 s/\lambda$ will yield accurate results. If the actual parameter values are $(s/\lambda)_i \leq s/\lambda < (s/\lambda)_{i+1}$, $(G_1 s/\lambda)_j \leq G_1 s/\lambda < (G_1 s/\lambda)_{j+1}$ and suppose that the final sampling from the PDF gives u i.e. $\mathcal{P}^{-1}(\xi) = u \; \xi \in \mathcal{U}(0,1) \; u_k \leq u < u_{k+1}$

- interpolation in the parameters
- identification of grid points $u_k \leq u < u_{k+1}$ such that $\mathcal{P}(u_k) \leq \xi < \mathcal{P}(u_{k+1})$
- interpolation of the inverse CDF to obtain $\mathcal{P}^{-1}(\xi) = u$ i.e. interpolation in the $\mathcal{P}^{-1}(\xi_k) = u_k \leq \mathcal{P}^{-1}(\xi) = u < \mathcal{P}^{-1}(\xi_{k+1}) = u_{k+1}$ interval where $xi_\ell = \mathcal{P}(u_\ell)$

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Interpolation in the parameters: suppose that (i) we have $p(A;x)$ PDF of the stochastic variable x pre-computed over an A grid with $\{a_i\}$ pre-defined values of the parameter; (ii) the $\{a_i\}$ grid is dense enough for linear interpolation in A

- for a given $a_i \leq a < a_{i+1}$ value of the parameter, first we should interpolate the the PDF between the $a_i \leq a < a_{i+1}$ parameter grid points to get $p(a;x)$, then we should sample from the interpolated PDF $p(a;x)$
- however, since the $\{a_i\}$ grid is dense enough for linear interpolation of the PDF in A, we can use interpolation by weights(or statistical interpolation) in the form $p(a;x) = \frac{a_{i+1}-a}{a_{i+1}-a_i}p(a_i;x) + \frac{a-a_i}{a_{i+1}-a_i}p(a_{i+1};x)$
- which results in a form of composition(i.e. in general $p(x) = \sum_k P_k(p_k(x))p_k(x))$ since the probability of taking the PDF $p(a_i;x)$ is $P(p(a_i;x)) = \frac{a_{i+1}-a}{a_{i+1}-a_i}$ and the $1 - P(p(a_i;x))$ is the probability of taking the PDF $p(a_{i+1};x)$
    - first we make the selection between the $p(a_i;x)$ and $p(a_{i+1};x)$ PDFs
    - we take $p(a_i;x)$ if $\xi < \frac{a_{i+1}-a}{a_{i+1}-a_i}$, $\xi \in \mathcal{U}(0,1)$ and $p(a_{i+1};x)$ otherwise
    - then we need to sample from the selected, already pre-calculated and stored PDFs
- note, that we can use this method since the $q^{2+}(s/\lambda, G_1 s/\lambda; u)$ PDFs are smooths and the pre-defined parameter grids are dense enough that linear interpolation in $\log(s/\lambda)$ and $G_1 s/\lambda$ will yield accurate results
- the proper pre-computed q^{2+} PDF can be selected by using two uniform random sample

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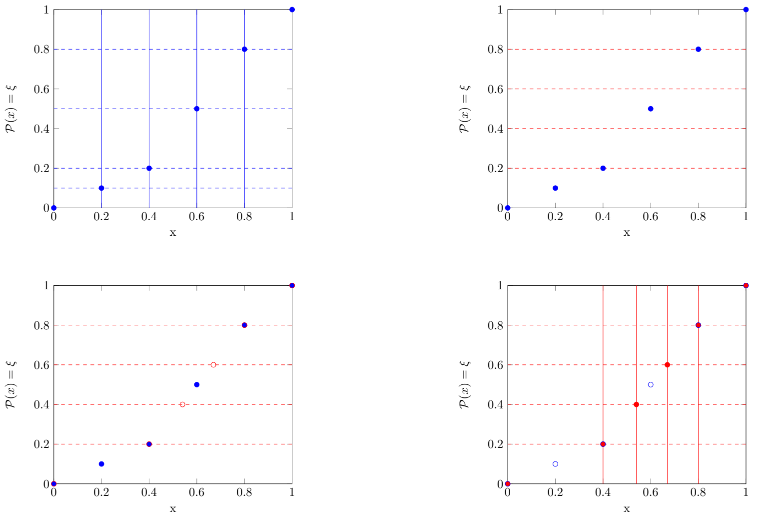
Identification of grid points: when we need to sample from a pre-computed $p(x)$ PDF table with the corresponding $\mathcal{P}(x)$ CDF we need to solve the inverse equation $\mathcal{P}^{-1}(\xi) = x$ where $\xi \in \mathcal{U}(0,1)$.

- the first step is to find k such that $\mathcal{P}(x_k) = \xi_k \leq \xi < \mathcal{P}(x_{k+1}) = \xi_{k+1}$
- this step can be done quickly if the inverse CDF $\mathcal{P}^{-1}(\xi)$ is known at equally probably intervals
- it means that $\mathrm{Dom}[\mathcal{P}^{-1}] = [0,1]$ is divided up to equal bins $\{\xi_k\}_{k=0}^N$, $\xi_{k+1} - \xi_k = \mathrm{const.} = 1/N \; \forall k \in 0,...,N-1$ and the corresponding $\mathcal{P}^{-1}(\xi_k) = x_k$ values are known
- however, usually it is the domain of the PDF that we divide up $\{x_j\}_{j=0}^M$, $x_0 = x_{min}$, $x_M = x_{max}$ and we compute the PDF $p(x_j)$ at the grid points
- in this case we have two possibilities to achieve equally probably intervals:
    - adjust the size of the individual bins of the $\{x_j\}_{j=0}^M$ grid such that $\int_{x_j}^{x_{j+1}} p(x)\mathrm{d}x = \mathrm{const} \; \forall j = 0,...,M-1$. The easiest way to achieve this is: *(i)* define the grid $\{\xi_k\}_{k=0}^N$, $\xi_{k+1} - \xi_k = \mathrm{const.} = 1/N \; \forall k \in 0,...,N-1$; *(ii)* then determine the $\mathcal{P}^{-1}(\xi_k)$ inverse CDF values by interpolation using the know $\mathcal{P}^{-1}(\xi_j = x_j)$ values. HOWEVER, special care needs to be taken when one interpolates the (inverse) CDF!!! (see later)

[A.J.Walker,Electronics Letters 10(8)(1974)127-128]

Sampling of bins in case of pre-computed PDF



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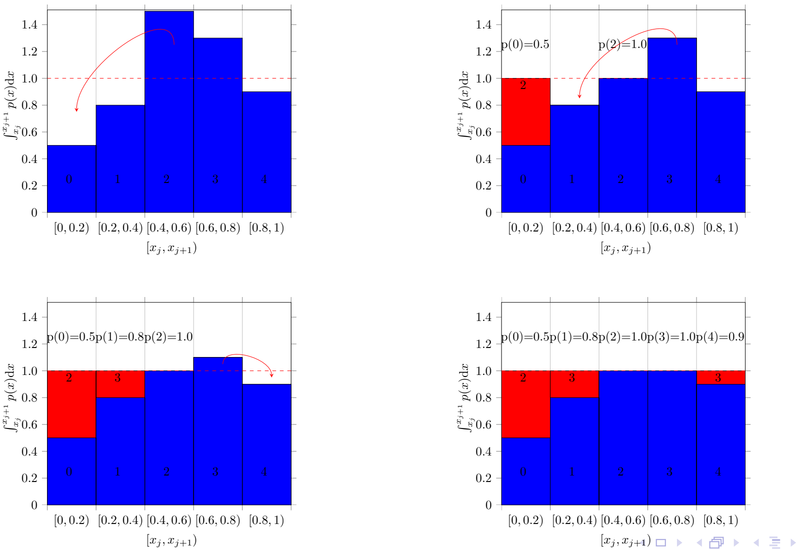
  - keep the equal size of the individual bins of the $\{x_j\}_{j=0}^{M}$ grid and reshuffle the $p(x_j)$ PDF values such that $\int_{x_j}^{x_{j+1}} p(x)\mathrm{d}x = \mathrm{const} = \mathrm{mean} \; \forall j = 0,...,M-1$ by mixing "probabilities" from different bins i.e. barrow/lend probabilities and record it in a table (Walker's alias sampling)

[A.J.Walker,Electronics Letters 10(8)(1974)127-128]

Sampling of bins in case of pre-computed PDF



Sampling of bins in case of pre-computed PDF

- results in equally probably CDF bins
- if we store:
    - the probability of the lower bars $p(j) \rightarrow [0.5, 0.8, 1.0, 1.0, 0.9]$
    - and the original bin locations of the moved pieces $\rightarrow [2, 3, -, -, 3]$
    - in theory the sampling can be done with 2 independent random numbers ξ_1, ξ_2
    - the first will give one of the equally probably bins j
    - then if $\xi_2 < p(j)$ we will take the bin $j \rightarrow x_j$ and the corresponding alias bin otherwise
    - however the same sampling can be straightforwardly done even with only one random number
- drawbacks compared to the "simply" equally probably CDF:
    - the monotonic property of the CDF is "lost" i.e. $\xi_a < \xi_b \not\rightarrow x_a < x_b$ since probabilities are mixed from different bins (cannot used for sampling in a restricted interval)
    - additional random number is needed to perform the interpolation (within the sampled bin)

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Interpolation of the inverse CDF

interpolation of the inverse CDF: after the determination of bin j such that $\mathcal{P}(\xi_j) \leq \xi < \mathcal{P}(\xi_{j+1})$ one needs to solve $\mathcal{P}^{-1}(\xi) = x$ i.e. interpolation within $\mathcal{P}^{-1}(\xi_j) = x_j \leq \mathcal{P}^{-1}(\xi) = x < \mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$

- using liner interpolation is usually not appropriate because it is equivalent to approximate the PDF between x_j and x_{j+1} ($\mathcal{P}^{-1}(\xi_j) = x_j, \mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$) with a constant
- the applied interpolation should satisfy $\frac{\mathrm{d}\mathcal{P}^{-1}(\xi)}{\mathrm{d}\xi} = \left(\frac{\mathrm{d}\mathcal{P}(x)}{\mathrm{d}x}\right)^{-1} = \frac{1}{p(x)}$ and $\mathcal{P}^{-1}(\xi_j) = x_j$, $\mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$
- one can approximate the CDF within the bin by using second order Taylor approximation:
  - $\mathcal{P}(x) \approx \tilde{\mathcal{P}}(x) = \mathcal{P}(x_j) + \mathcal{P}'(x_j)[x - x_j] + 0.5\mathcal{P}''(x_j)[x - x_j]^2 = \mathcal{P}(x_j) + p(x_j)[x - x_j] + 0.5p'(x_j)[x - x_j]^2 \approx \mathcal{P}(x_j) + p(x_j)[x - x_j] + 0.5\frac{p(x_{j+1}) - p(x_j)}{x_{j+1} - x_j}[x - x_j]^2$
  - that results in $x = \mathcal{P}^{-1}(\xi) \approx \tilde{\mathcal{P}}^{-1}(\xi) = x_j - \left[p(x_j) - \sqrt{p^2(x_j) + 2c[\xi - \xi_j]}\right]/c$; $c = \frac{p(x_{j+1}) - p(x_j)}{x_{j+1} - x_j}$
  - $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi} = \frac{1}{\sqrt{2c(\xi - \xi_j) + p^2(x_j)}}$
    - $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}_{|\xi=\xi_j} = \frac{1}{p(x_j)}$ and $\tilde{\mathcal{P}}^{-1}(\xi_j) = x_j$
    - $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}_{|\xi=\xi_{j+1}} = \frac{1}{p(x_{j+1})}$ and $\tilde{\mathcal{P}}^{-1}(\xi_{j+1}) = x_{j+1}$ only if $p(x)$ is linear between x_j, x_{j+1}
  - then the sampled value $x \approx \tilde{x} = \tilde{\mathcal{P}}^{-1}(\xi) = x_j - \left[p(x_j) - \sqrt{p^2(x_j) + 2c[\xi - \xi_j]}\right]/c$, where $c = \frac{p(x_{j+1}) - p(x_j)}{x_{j+1} - x_j}$

interpolation of the inverse CDF: after the determination of bin j such that $\mathcal{P}(\xi_j) \leq \xi < \mathcal{P}(\xi_{j+1})$ one needs to solve $\mathcal{P}^{-1}(\xi) = x$ i.e. interpolation within $\mathcal{P}^{-1}(\xi_j) = x_j \leq \mathcal{P}^{-1}(\xi) = x < \mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$

- using liner interpolation is usually not appropriate because it is equivalent to approximate the PDF between x_j and x_{j+1} ($\mathcal{P}^{-1}(\xi_j) = x_j, \mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$) with a constant
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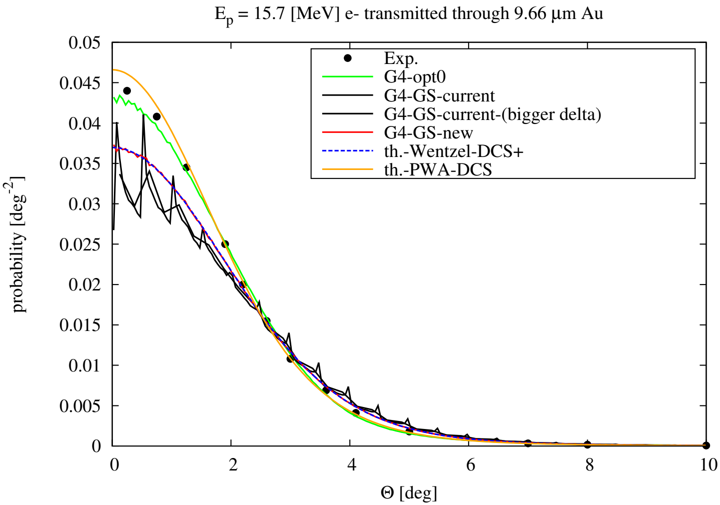
- a better solution is to use rational function approximation in the form of
  - $x = \mathcal{P}^{-1}(\xi) \approx \tilde{\mathcal{P}}^{-1}(\xi) = x_j + \frac{(1+a_j+b_j)\alpha}{1+a_j\alpha+b_j\alpha^2}[x_{j+1} - x_j]$, where $\alpha = \frac{\xi-\xi_j}{\xi_{j+1}-\xi_j}$
  - $\tilde{\mathcal{P}}^{-1}(\xi_j) = x_j$ and $\tilde{\mathcal{P}}^{-1}(\xi_{j+1}) = x_{j+1}$ independently form the values a_j, b_j
  - $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi} = \frac{(1+a_j+b_j)(1-b_j\alpha^2)}{[1+a_j\alpha+b_j\alpha^2]^2}\frac{x_{j+1}-x_j}{\xi_{j+1}-\xi_j}$ and the parameters a_j, b_j can be determined from the requirements
    $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}_{|\xi=\xi_j} = \frac{1}{p(x_j)}$
    $\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}_{|\xi=\xi_{j+1}} = \frac{1}{p(x_{j+1})}$
  - that yields $b_j = 1 - \left[\frac{\xi_{j+1}-\xi_j}{x_{j+1}-x_j}\right]^2 \frac{1}{p(x_j)p(x_{j+1})}$ and $a_j = \frac{\xi_{j+1}-\xi_j}{x_{j+1}-x_j}\frac{1}{p(x_j)} - 1 - b_j$
  - then the sampled value $x \approx \tilde{x} = \tilde{\mathcal{P}}^{-1}(\xi) = x_j + \frac{(1+a_j+b_j)\alpha}{1+a_j\alpha+b_j\alpha^2}[x_{j+1} - x_j]$, with $\alpha = \frac{\xi-\xi_j}{\xi_{j+1}-\xi_j}$

[F.Salvat,J.M.Fernández-Varea,J.Sempau,PENELOPE-2011,NEA/NSC/DOC(2011)5]

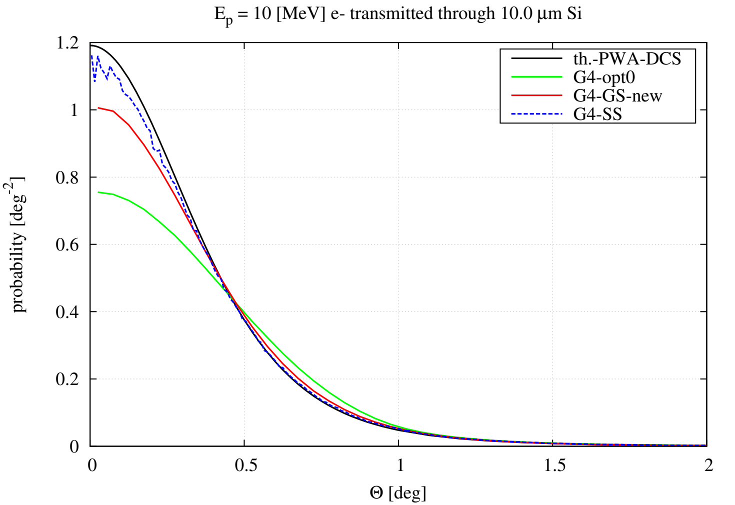
The new version of Kawrakow-Bielajew Goudsmit-Saunderson model:

- $q^{2+}(s/\lambda, G_1 s/\lambda; u)$ PDFs are pre-computed over a 2D s/λ, $G_1 s/\lambda$ grid using an $\ell_{\max} = 10^4$ limit in the GS series
- the previously discussed variable transformation is used to achieve smooth PDFs
- statistical interpolation in $\log(s/\lambda)$ and $G_1 s/\lambda$ is used that gives accurate results (no loop, no search, no conditions, 2 random numbers)
- pre-computed data are stored over the 2D parameter grid in form of inverse CDFs with equally probably bins achieved by using rational interpolation :
  - bin identification i.e. find k such that $\xi_k \leq \xi < \xi_{k+1}$ can be done in one step(no loop, no search, no conditions)
  - then rational interpolation is used to solve $\mathcal{P}^{-1}(\xi) = x$, $\xi_k \leq \xi < \xi_{k+1}$(proper derivatives, no loop, no search, no conditions)
  - only 1 random number is needed to preform the sampling
- results in:
  - accurate, robust sampling
  - significant speed-up: `TestEm5` with the new version is about 10% faster than the current version (reached or even faster than `opt0`)

Contents



exp.: [A.O.Hanson et al., Phys.Rev.84(1951)634]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Θ [deg]
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G4-GS-new
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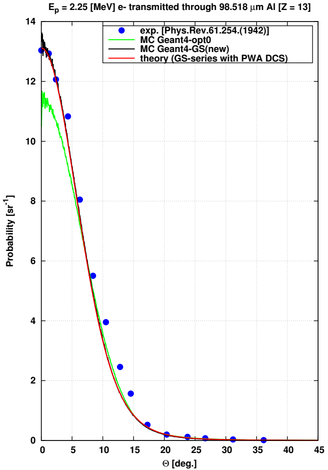
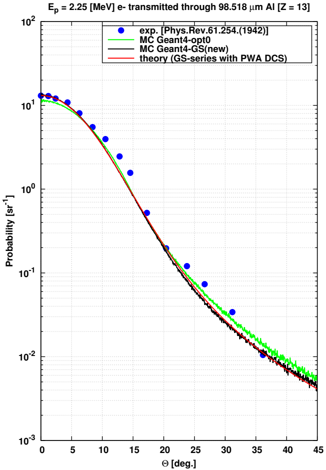
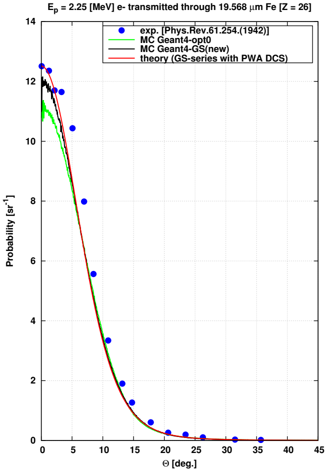
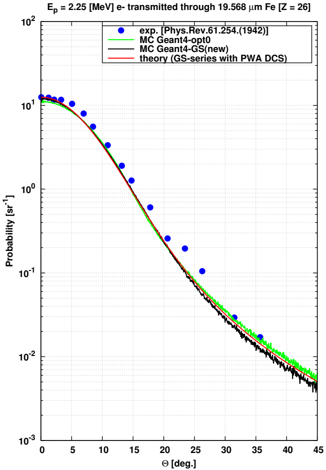
0.5
1
1.5
2





exp.: [L.Kulchitsky, Phys.Rev.61(1941)254]; normalized to theory at $\theta = 0$





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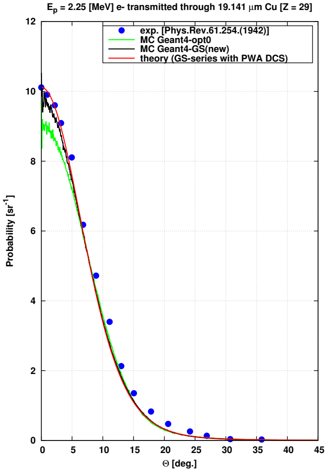

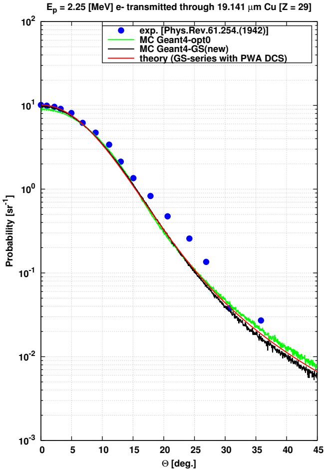

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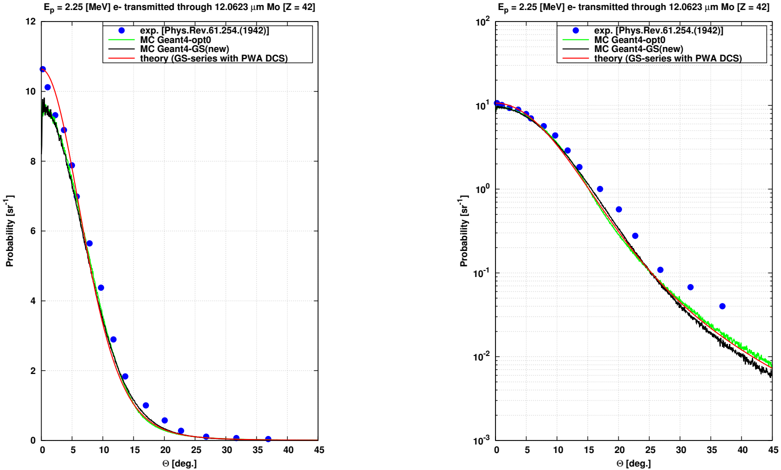

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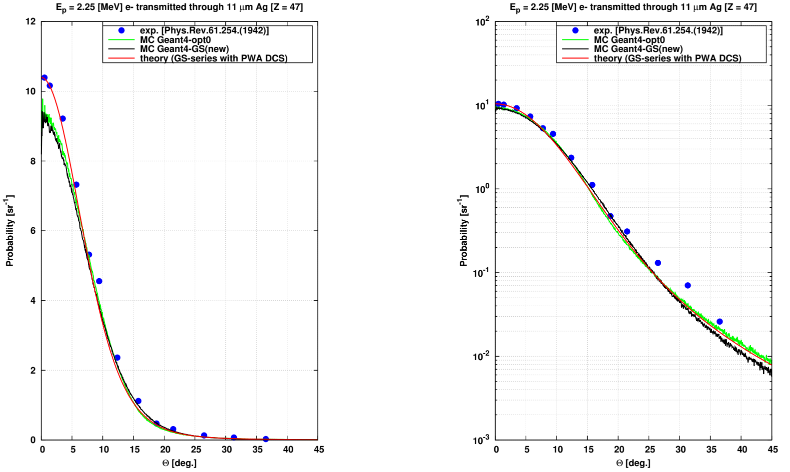

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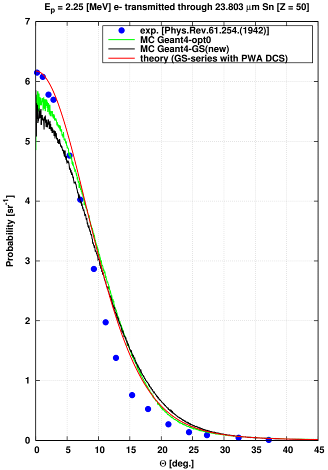

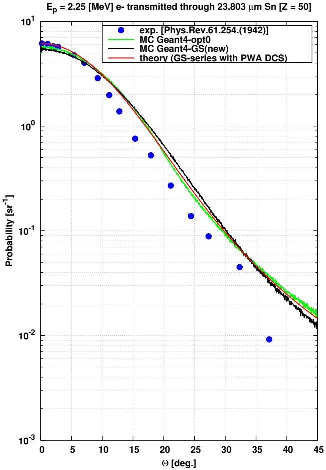

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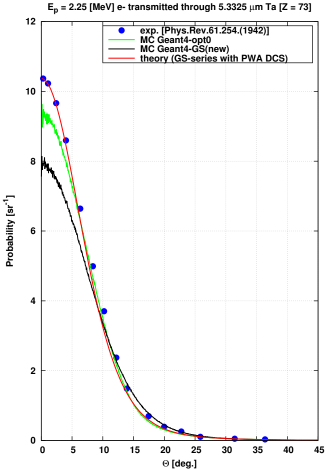

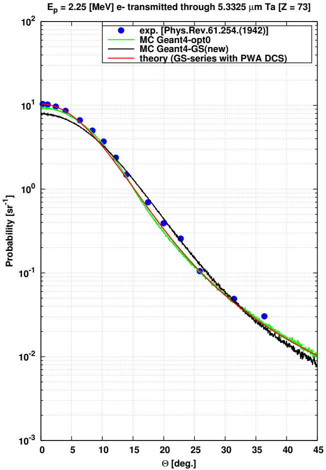

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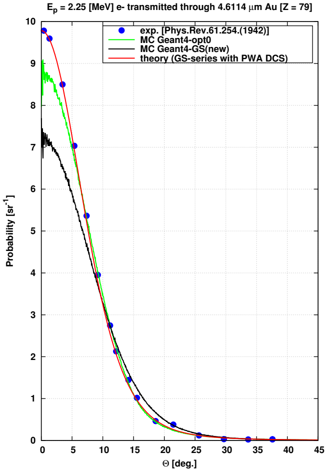

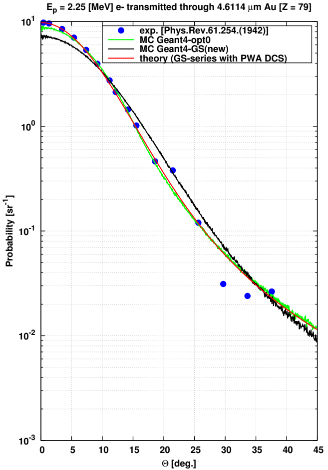

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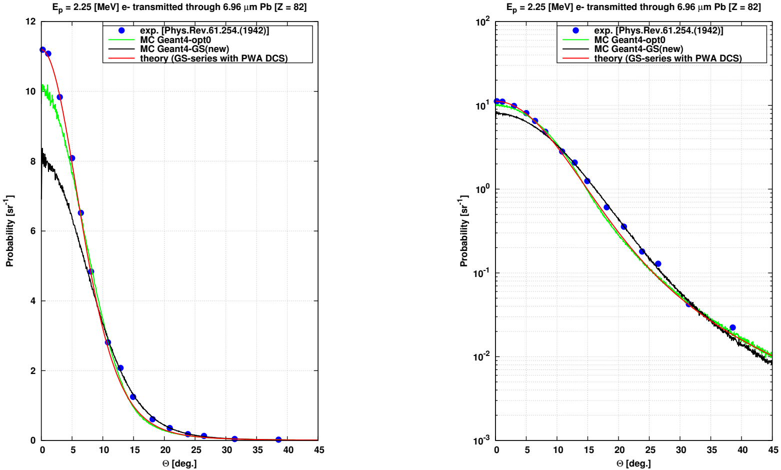
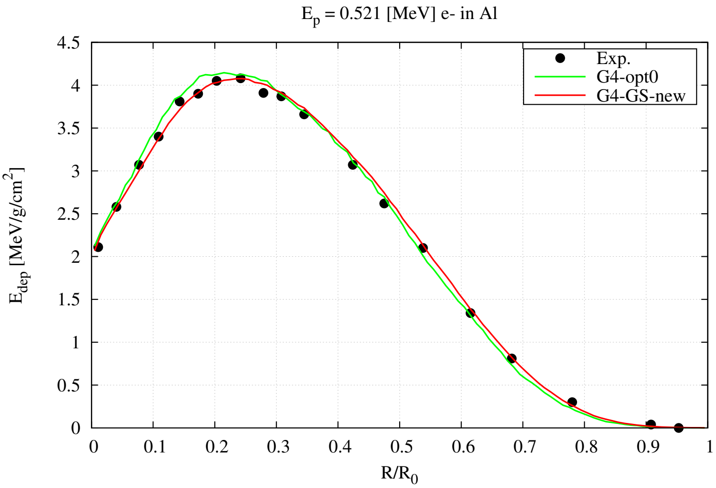


exp.: [L.Kulchitsky, Phys.Rev.61(1941)254]; normalized to theory at $\theta = 0$



exp.: [G.J.Lockwood et al., Sandia report SAND79-0414.UC-34a, February 1987; O.Kadri et al., NIMB 258(2007)381]

Contents

- the model in the form of the new implementation can be used as a relatively fast option with the advantages (compared to `opt0`):
  - the model is free from tuning parameters
  - with limitations that can be well understood ($\rightarrow$ no more surprise)
- the source of limitations is the simple form of the DCS for elastic scattering
- note, that it is this simple analytical form that makes possible to obtain a material independent, pre-computed table of angular distributions
- any correction would lead material dependency
- instead of introducing corrections based on more accurate numerical PWA-DCS for elastic scattering one should investigate the possibly of using a separate model that based on these PWA-DCS

Thank you for your attention!