Goudsmit-Saunderson multiple scattering model: a new version

Mihály Novák
CERN PH-SFT
(simulation group)

28-09-2015

Outline

Outline

Outline

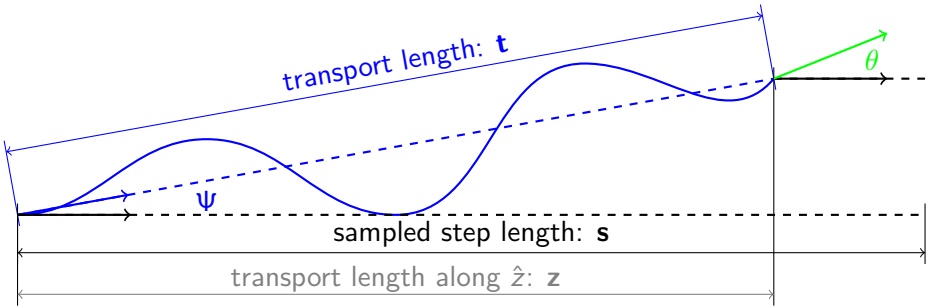
Outline

Outline

Contents

Why do we need multiple scattering model?

- event-by-event modelling of elastic scattering is feasible only if the mean number of interactions per track is below few hundred
- this limits the applicability of the detailed simulation model only for electrons with relatively low kinetic energies (up to $E_{kin} \sim 100$ keV) or thin targets
- fast ($E_{kin} > 100$ keV) electrons undergo a high number of elastic collisions in the course of its slowing down in tick targets
- detailed simulation becomes very inefficient, high energy particle transport simulation codes employ condensed history simulation model
- each particle track is simulated by allowing to make individual steps that are much higher than the average step length between two successive elastic interactions
- the net effects of these high number of elastic interactions such as angular deflection and spacial displacement is accounted at each individual condensed history step by using multiple scattering theories.
- the accuracy of modelling the cumulative effects of many elastic scattering in one step strongly depends on the capability of the employed multiple scattering theory to describe the angular distribution of electrons after travelling a given path length.



Multiple scattering model needs to provide:

- the angular deflection (θ) after travelling a given path length (s)
- path length correction (PLC), lateral correlation algorithm (LCA), longitudinal and lateral correlation algorithm (LLCA)
- where is the particle at the post step point and what is the direction of motion

Contents

Theoretical background in a nutshell

Geant4 Goudsmit-Saunderson model is the

- Kawrakow-Bielajew model for elastic scattering
  [I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336]
- based on the 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]
- based on the screened Rutherford DCS (differential cross section) for elastic scattering

Contents

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

Contents

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 $f_{B1}(\theta, \phi) = -\frac{2m}{4\pi\hbar^2} \int e^{i(\bar{k}_f - \bar{k}_i)\bar{r}'} V(\bar{r}') \mathrm{d}^3 r'$ 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]

Contents

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

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

[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.*

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

where

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

- 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 $F(s;\mu)^{2+}_{GS} \rightarrow$ pre-compute

Variable transformation is needed to obtain smooth distributions $\rightarrow$ 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)]

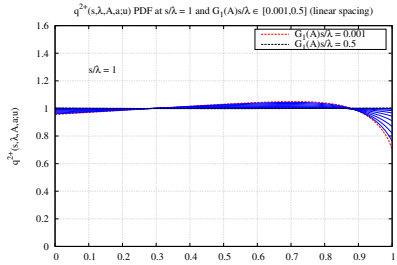
- in the case of using the Wentzel model one can take $u = f(a;\mu) = \frac{(a+1)(1-\mu)}{1-\mu+2a}$; the corresponding inverse transform $\mu = 1 - \frac{2au}{1-u+a}$ [note that $f(a;\mu)$ corresponds to the single scattering Wentzel CDF with a scaled $a = w^2A$ screening parameter, where the scaling 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).]

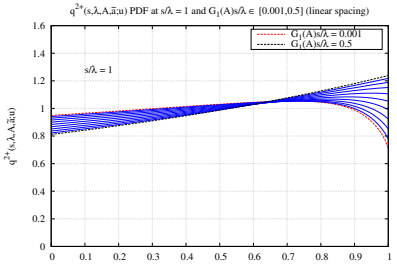
[I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336]

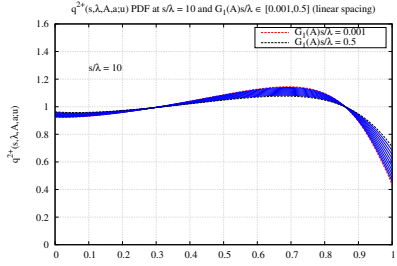
- the optimal parameter of the transformation can be determined by plugging the chosen transformation function $u = f(a;\mu) = \frac{(a+1)(1-\mu)}{1-\mu+2a}$ into the results of the optimization i.e.
  $0 = \int_{-1}^{+1} \left[F(s;\mu)^{2+}_{GS} \left(-\frac{[1-\mu+2a]^2}{2a(1+a)} \right) \right]^2 \left[-2\frac{1-\mu(1+2a)}{[1-\mu+2a]^3} \right] \mathrm{d}\mu$ 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

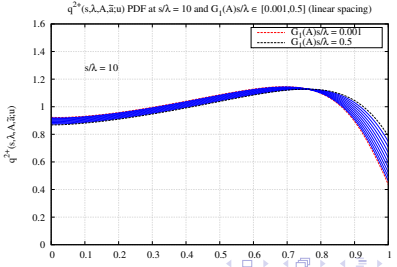
$$q^{2+}(s,\lambda,a,A;u) = \frac{2a(1-a)}{[1-u+a]^2} \sum_{\ell}^{\infty} (\ell+0.5) P_\ell \left[1 - \frac{2au}{1-u+a}\right] \gamma_\ell(s,\lambda,A)$$

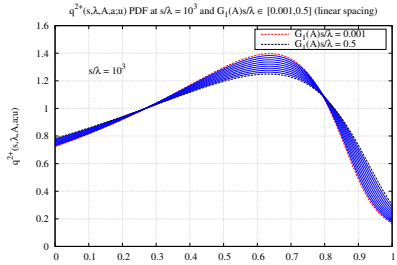
[I.Kawrakow,A.F.Bielajew, NIMB 134(1998)325-336, I Kawrakow et al., NRCC Report PIRS-701]

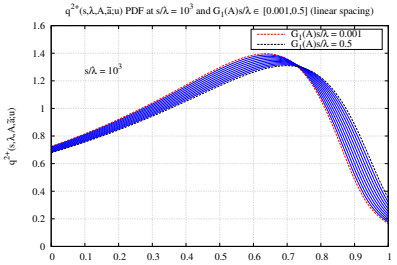

$q^{2*}(s,\lambda,A,a;u)$ PDF at $s/\lambda = 1$ and $G_1(A)s/\lambda \in [0.001,0.5]$ (linear spacing)
$G_1(A)s/\lambda = 0.001$
$G_1(A)s/\lambda = 0.5$
$s/\lambda = 1$
$q^{2*}(s,\lambda,A,a;u)$
u

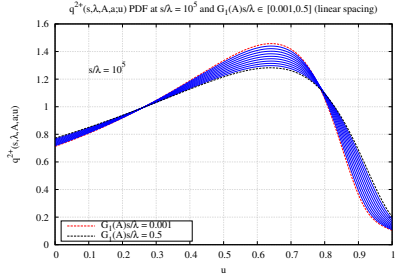

$q^{2*}(s,\lambda,A,\bar{a};u)$ PDF at $s/\lambda = 1$ and $G_1(A)s/\lambda \in [0.001,0.5]$ (linear spacing)
$G_1(A)s/\lambda = 0.001$
$G_1(A)s/\lambda = 0.5$
$s/\lambda = 1$
$q^{2*}(s,\lambda,A,\bar{a};u)$
u

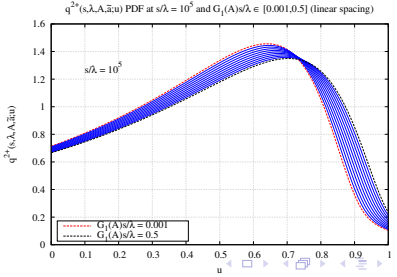

$q^{2*}(s,\lambda,A,a;u)$ PDF at $s/\lambda = 10$ and $G_1(A)s/\lambda \in [0.001,0.5]$ (linear spacing)
$G_1(A)s/\lambda = 0.001$
$G_1(A)s/\lambda = 0.5$
$s/\lambda = 10$
$q^{2*}(s,\lambda,A,a;u)$
u


$q^{2*}(s,\lambda,A,\bar{a};u)$ PDF at $s/\lambda = 10$ and $G_1(A)s/\lambda \in [0.001,0.5]$ (linear spacing)
$G_1(A)s/\lambda = 0.001$
$G_1(A)s/\lambda = 0.5$
$s/\lambda = 10$
$q^{2*}(s,\lambda,A,\bar{a};u)$
u


q^2*(s,λ,A,a;u) PDF at s/λ = 10^3 and G1(A)s/λ ∈ [0.001,0.5] (linear spacing)
G1(A)s/λ = 0.001
G1(A)s/λ = 0.5
s/λ = 10^3
q^2*(s,λ,A,a;u)
u


q^2*(s,λ,A,ã;u) PDF at s/λ = 10^3 and G1(A)s/λ ∈ [0.001,0.5] (linear spacing)
G1(A)s/λ = 0.001
G1(A)s/λ = 0.5
s/λ = 10^3
q^2*(s,λ,A,ã;u)
u


q^2*(s,λ,A,a;u) PDF at s/λ = 10^5 and G1(A)s/λ ∈ [0.001,0.5] (linear spacing)
G1(A)s/λ = 0.001
G1(A)s/λ = 0.5
s/λ = 10^5
q^2*(s,λ,A,a;u)
u


q^2*(s,λ,A,ã;u) PDF at s/λ = 10^5 and G1(A)s/λ ∈ [0.001,0.5] (linear spacing)
G1(A)s/λ = 0.001
G1(A)s/λ = 0.5
s/λ = 10^5
q^2*(s,λ,A,ã;u)
u

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
  - next slide: compare the old and new angular distributions/sampling

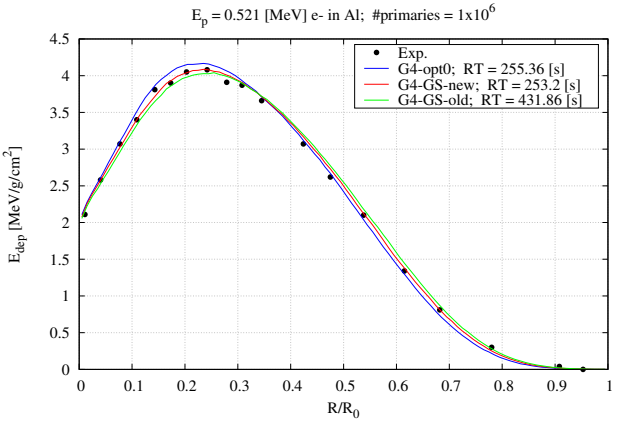


Figure: Geant4 ../examples/extended/electromagnetic/TestEm11 (Sandia): energy deposit of 512 [keV] electrons in Al.

experimental data: G.J.Lockwood et al. Sandia report SAND79-0414.UC-34a, February 1987

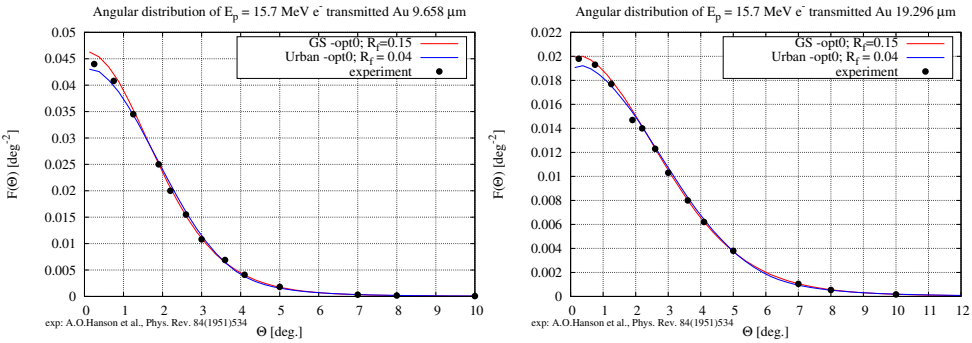


Figure: Geant4 ../examples/extended/electromagnetic/TestEm5

Contents

2-different path-length correction (displacement) options:

- the simple PRESTA(Parameter Reduced Electron-Step Transport Algorithm) algorithm : the transport distance in the initial direction of motion is set to its mean value $\langle z \rangle = \lambda_1[1 - \exp(-t/\lambda_1)]$)
- LLCA (Lateral and Longitudinal Correlation Algorithm): most accurate EGSnrc like transport algorithm (computationally more expensive, but it can give back the longitudinal and radial distributions obtained by using single scattering algorithm)

PRESTA: A.F.Bielajew et al., NIMB 18(1986)165-181; LLCA: I.Kawrakow et al.,NIMB 142(1998)253-280

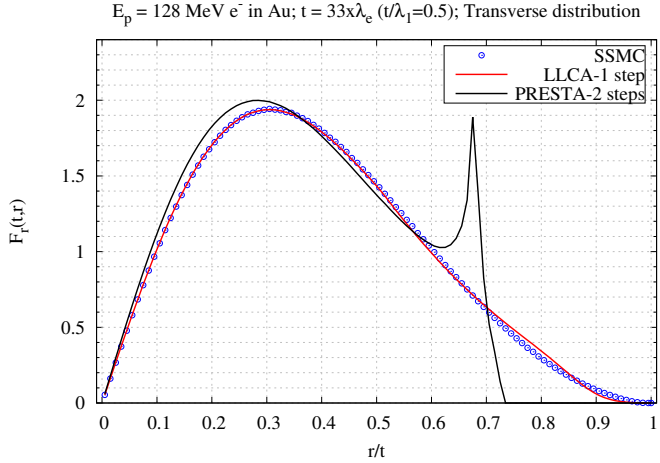


Figure: Transverse distribution

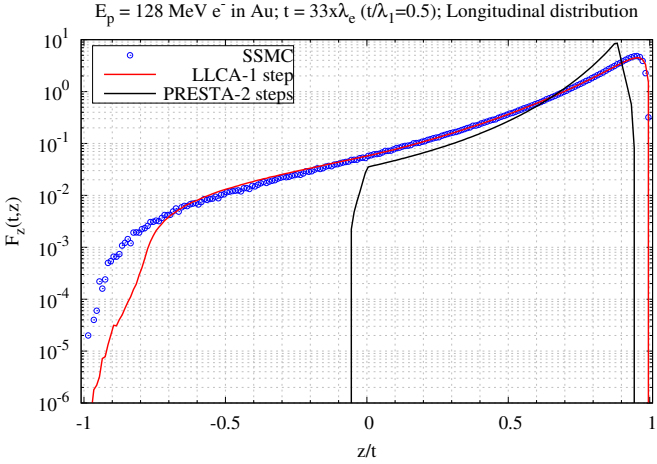


Figure: Longitudinal distribution

3-different step limitations in multiple scattering

- `fUseSafety` ⇒ error free stepping : ensures that everything(regarding MSC) can be done in the step-limit phase. It is possible only if we know the `true-step length` before transportation → we need to make sure, that transportation won't hit any boundaries.
  - `skin-depth`, defined in terms of (few)elastic mean free path is used
  - whenever `safety` (or the current-minimum step) is smaller that `skin-depth` we switch to single scattering mode
  - if the particle is out of `skin-depth` it is ensured that the `true-step length` is not longer than `safety`
  - boundaries can be reached only in single scattering mode (i.e. no MSC)
  - we know in the step limit phase(before transportation) what will be the `true-step length` everything can be done in the step-limit phase
  - everything can be done in the step-limit phase (if we are doing an MSC step):
    - sampling of angular deflection that corresponds to the given `true-step length` (using the most accurate EGSnrc like energy loss correction)
    - sampling of final position (by using the most accurate EGSnrc like displacement sapling and computation)
    - `true-step length` is always known and corresponding `geometrical length` is given by the displacement computation (including accurate energy loss correction). Since transportation cannot hit boundary we do not need any other `true-geometric-true` path length conversion
  - **range-factor** can be set to any value (0.2 by default) since we limit the true step length to the first-transport mean free path (theoretical limit of any condensed history techniques that (in 2-step sampling) corresponds to $\langle\cos(\theta)\rangle = \exp(-t/\lambda_1) \rightarrow t_{max} = 0.5\lambda_1 \Rightarrow 0.9191[\text{rad}] = 52.66^o$)

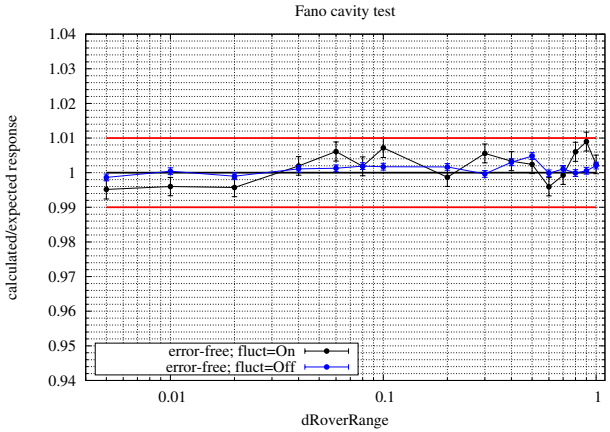


Figure: Geant4 ../examples/extended/medical/fanoCavity

more details: E.Poon et al., Phys.Med.Biol.50(2005)681-694

- `fUseDistanceToBoundary` $\Rightarrow$ corresponds to Urban's `fUseDistanceToBoundary` i.e. `opt3` without having any minimum path length limit (GS model works for any short true-path lengths); range-factor = 0.2
- `fUseSafetyPlus` $\Rightarrow$ corresponds to Urban's `fUseSafety` i.e. `opt0` without having any minimum path length limit (GS model works for any short true-path lengths); range-factor = 0.15

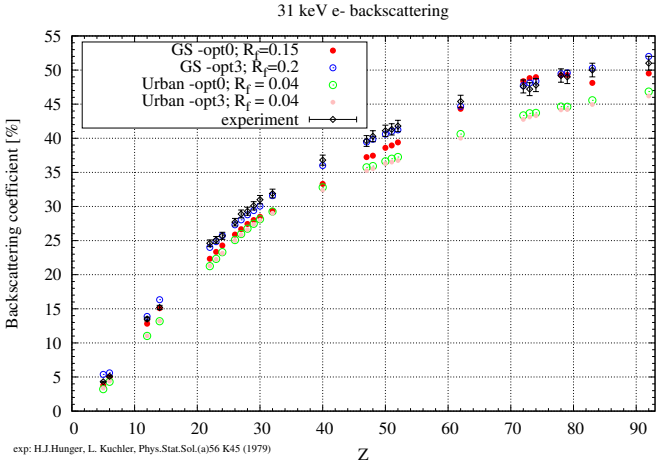
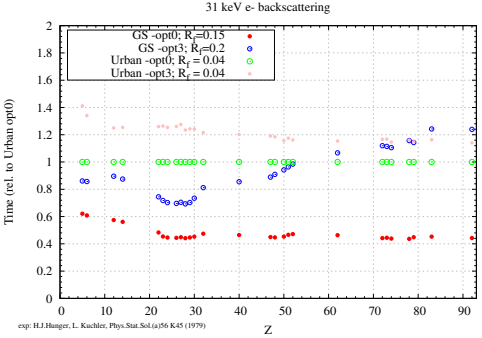
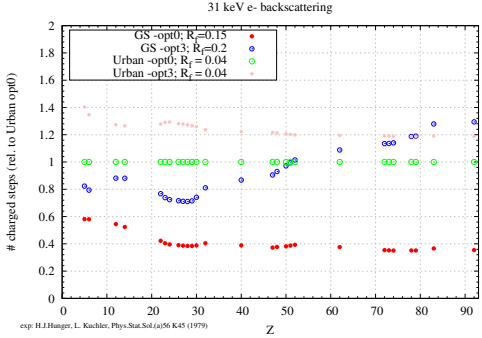


Figure: Geant4 ../examples/extended/electromagnetic/TestEm5


31 keV e- backscattering
GS -opt0; R_f=0.15
GS -opt3; R_f=0.2
Urban -opt0; R_f = 0.04
Urban -opt3; R_f = 0.04
Time (rel. to Urban opt0)
Z
exp: H.J.Hunger, L. Kuchler, Phys.Stat.Sol.(a)56 K45 (1979)


31 keV e- backscattering
GS -opt0; R_f=0.15
GS -opt3; R_f=0.2
Urban -opt0; R_f = 0.04
Urban -opt3; R_f = 0.04
charged steps (rel. to Urban opt0)
Z
exp: H.J.Hunger, L. Kuchler, Phys.Stat.Sol.(a)56 K45 (1979)

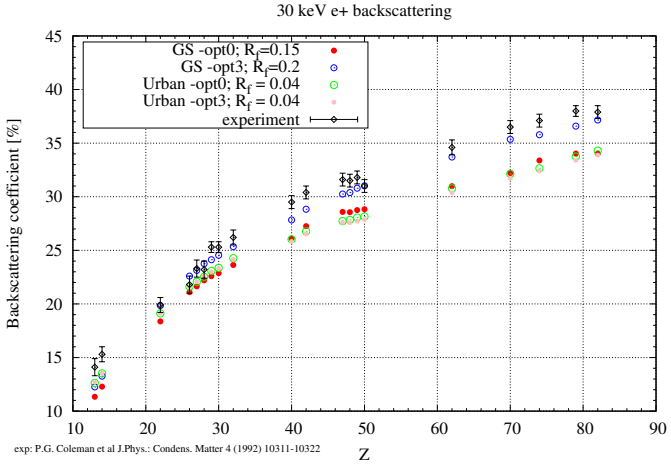
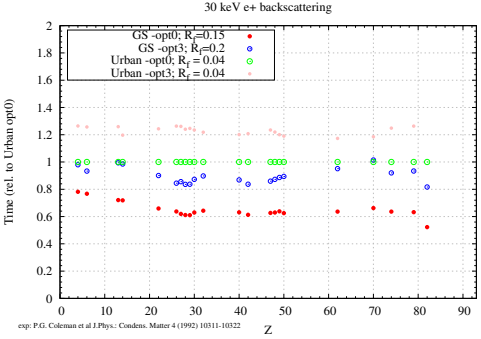
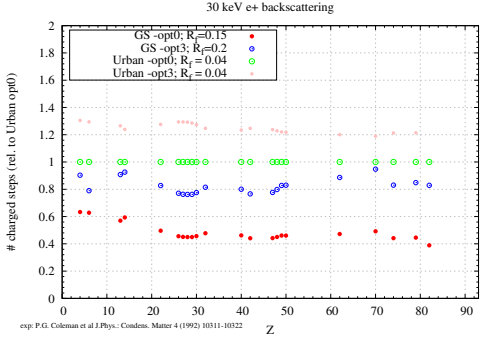


Figure: Geant4 ../examples/extended/electromagnetic/TestEm5

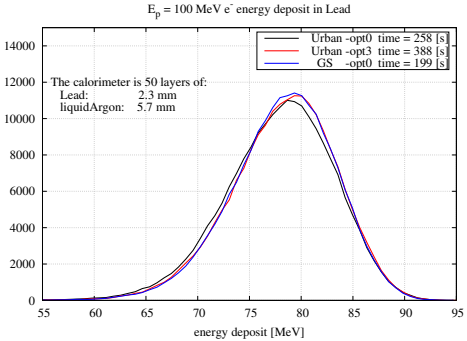

30 keV e+ backscattering
GS -opt0; R_f=0.15
GS -opt3; R_f=0.2
Urban -opt0; R_f = 0.04
Urban -opt3; R_f = 0.04
Time (rel. to Urban opt0)
Z
exp: P.G. Coleman et al J.Phys.: Condens. Matter 4 (1992) 10311-10322

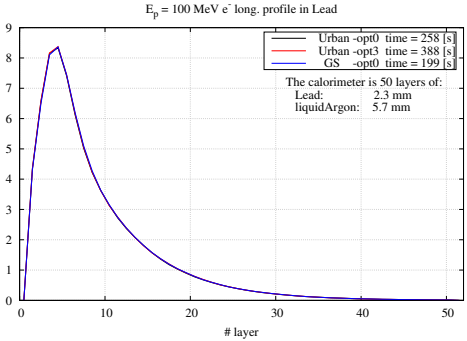

30 keV e+ backscattering
GS -opt0; R_f=0.15
GS -opt3; R_f=0.2
Urban -opt0; R_f = 0.04
Urban -opt3; R_f = 0.04
charged steps (rel. to Urban opt0)
Z
exp: P.G. Coleman et al J.Phys.: Condens. Matter 4 (1992) 10311-10322

Contents

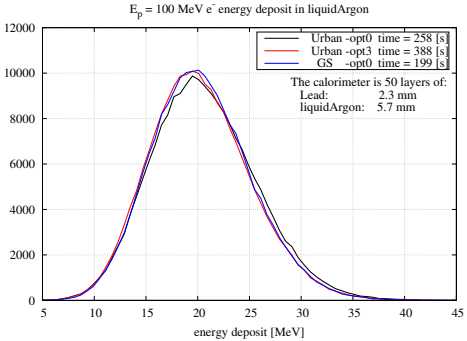
Contents

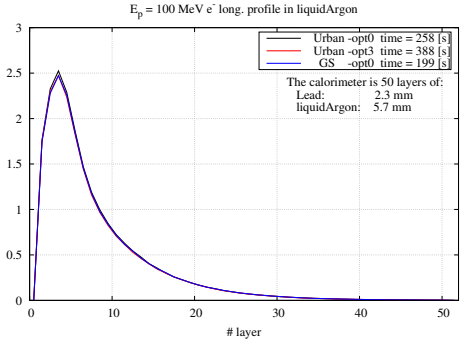
Simplified calorimeter (TestEm3)



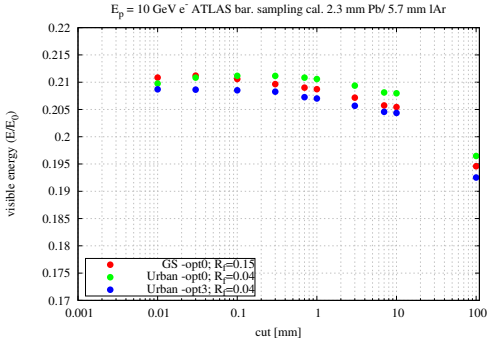


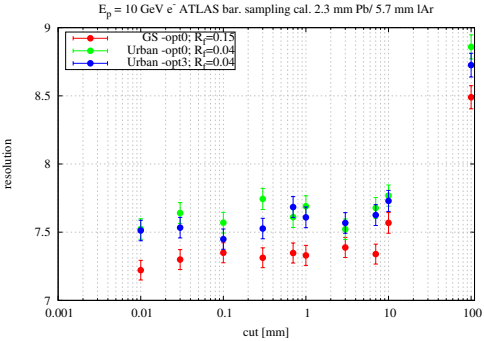
Simplified calorimeter (TestEm3)

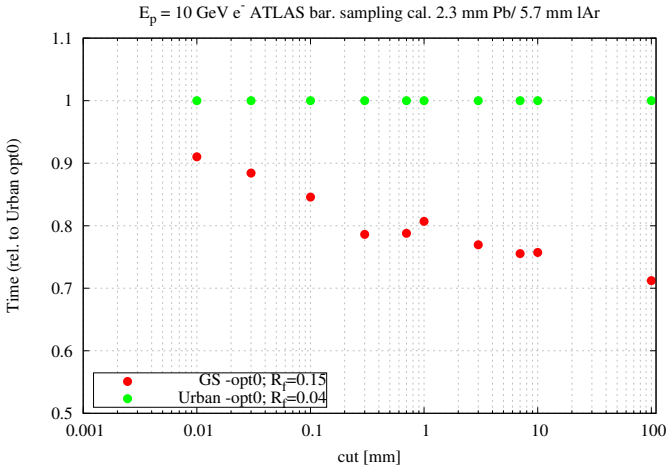




Contents


E_p = 10 GeV e^- ATLAS bar. sampling cal. 2.3 mm Pb/ 5.7 mm lAr
visible energy (E/E_p)
cut [mm]
GS -opt0; R_f=0.15
Urban -opt0; R_f=0.04
Urban -opt3; R_f=0.04


E_p = 10 GeV e^- ATLAS bar. sampling cal. 2.3 mm Pb/ 5.7 mm lAr
resolution
cut [mm]
GS -opt0; R_f=0.15
Urban -opt0; R_f=0.04
Urban -opt3; R_f=0.04


E_p = 10 GeV e^- ATLAS bar. sampling cal. 2.3 mm Pb/ 5.7 mm lAr
Time (rel. to Urban opt0)
cut [mm]
GS -opt0; R_f=0.15
Urban -opt0; R_f=0.04
1.1
1
0.9
0.8
0.7
0.6
0.5
0.001
0.01
0.1
1
10
100

cut [mm]	Urban-opt0	GS-opt0	Urban-opt3
100	2.11e+03	2.11e+03	2.11e+03
10	3.72e+03	3.73e+03	3.73e+03
7	3.92e+03	3.93e+03	3.92e+03
3	4.60e+03	4.60e+03	4.60e+03
1	5.08e+03	5.09e+03	5.09e+03
0.7	5.21e+03	5.22e+03	5.22e+03
0.3	5.86e+03	5.87e+03	1.02e+04
0.1	7.14e+03	7.15e+03	1.16e+04
0.03	8.67e+03	8.68e+03	1.38e+04
0.01	1.01e+04	1.01e+04	1.69e+04

Table: number of gammas

cut [mm]	Urban-opt0	GS-opt0	Urban-opt3
100	3.76e+03	3.76e+03	3.76e+03
10	6.91e+03	6.92e+03	6.92e+03
7	7.17e+03	7.18e+03	7.18e+03
3	7.98e+03	8.01e+03	8.01e+03
1	8.70e+03	8.72e+03	8.72e+03
0.7	8.96e+03	8.98e+03	8.98e+03
0.3	1.01e+04	1.01e+04	1.47e+04
0.1	1.26e+04	1.26e+04	1.73e+04
0.03	1.71e+04	1.71e+04	2.25e+04
0.01	2.71e+04	2.71e+04	3.42e+04

Table: number of electrons

cut [mm]	Urban-opt0	GS-opt0	Urban-opt3
100	27241	15510	51862
10	35789	21898	64588
7	36505	22457	65431
3	38760	24270	68165
1	41341	26216	71677
0.7	42182	26867	72870
0.3	45024	29348	81452
0.1	50420	34467	87487
0.03	59302	43295	95970
0.01	78181	62549	114558

Table: number of charged steps

cut [mm]	Urban-opt0	GS-opt0	Urban-opt3
100	20709	20940	20869
10	34169	34695	34501
7	34655	35203	34979
3	35766	36402	36160
1	36436	37076	36824
0.7	36592	37258	37003
0.3	37383	38130	43745
0.1	38756	39590	45304
0.03	40291	41165	47547
0.01	41692	42571	50793

Table: number of neutral steps

Contents

Work is still in progress! The new Goudsmit-Saunderson model:

- very promising, purely theory-based model for multiple scattering
- physics performance is at least as good as Urban model but it shows even better results in many cases
- significant run-time improvements compared to Urban model
- it seems that after 20 years we have a candidate to replace Urban model for low energy ($E < 0.1 - 1$ GeV) $e^{\mp}$ multiple scattering

Thank you for your attention!

Contents

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 $xi_\ell = \mathcal{P}(u_\ell)$

Contents

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

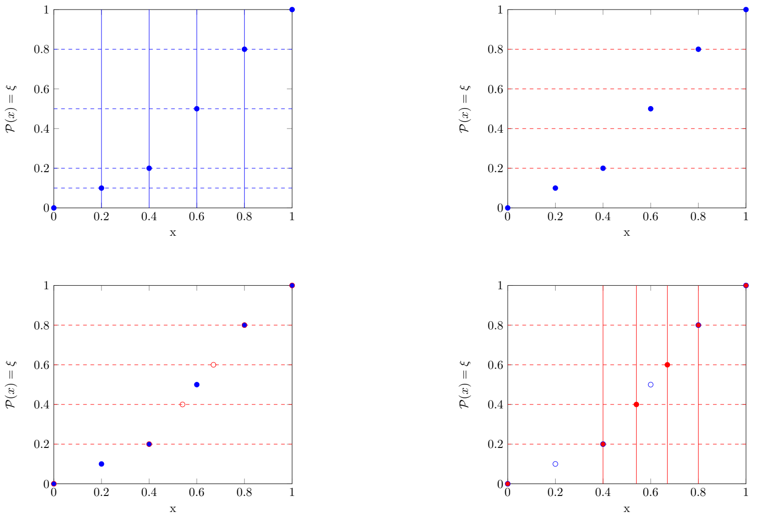
Contents

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]

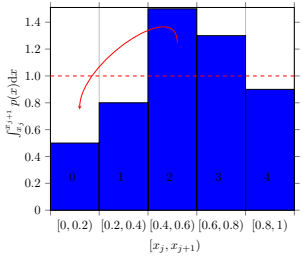
Sampling of bins in case of pre-computed PDF

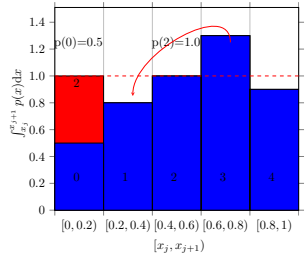


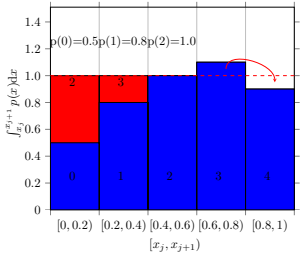
Identification of grid points: when we need to sample from a pre-computed $p(x)$ PDF table with the corresponding $\mathcal{P}(x)$ CDF we need to solve the inverse equation $\mathcal{P}^{-1}(\xi) = x$ where $\xi \in \mathcal{U}(0,1)$.

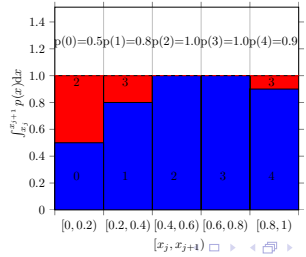
- the first step is to find k such that $\mathcal{P}(x_k) = \xi_k \leq \xi < \mathcal{P}(x_{k+1}) = \xi_{k+1}$
- this step can be done quickly if the inverse CDF $\mathcal{P}^{-1}(\xi)$ is known at equally probably intervals
- it means that $\mathrm{Dom}[\mathcal{P}^{-1}] = [0,1]$ is divided up to equal 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)
  - 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]


$\int_{x_j}^{x_{j+1}} p(x)dx$
0
1
2
3
4
[0, 0.2)
[0.2, 0.4)
[0.4, 0.6)
[0.6, 0.8)
[0.8, 1)
$[x_j, x_{j+1})$


p(0)=0.5
p(2)=1.0
$\int_{x_j}^{x_{j+1}} p(x)dx$
2
0
1
2
3
4
[0, 0.2)
[0.2, 0.4)
[0.4, 0.6)
[0.6, 0.8)
[0.8, 1)
$[x_j, x_{j+1})$


p(0)=0.5p(1)=0.8p(2)=1.0
$\int_{x_j}^{x_{j+1}} p(x)dx$
2
3
0
1
2
3
4
[0, 0.2)
[0.2, 0.4)
[0.4, 0.6)
[0.6, 0.8)
[0.8, 1)
$[x_j, x_{j+1})$


p(0)=0.5p(1)=0.8p(2)=1.0p(3)=1.0p(4)=0.9
$\int_{x_j}^{x_{j+1}} p(x)dx$
2
3
3
0
1
2
3
4
[0, 0.2)
[0.2, 0.4)
[0.4, 0.6)
[0.6, 0.8)
[0.8, 1)
$[x_j, x_{j+1})$

- 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)

Contents

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
- 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 $\mathcal{P}^{-1}(\xi_j) = x_j$, $\mathcal{P}^{-1}(\xi_{j+1}) = x_{j+1}$
- 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
    $\left.\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}\right|_{\xi=\xi_j} = \frac{1}{p(x_j)}$
    $\left.\frac{\mathrm{d}\tilde{\mathcal{P}}^{-1}(\xi)}{\mathrm{d}\xi}\right|_{\xi=\xi_{j+1}} = \frac{1}{p(x_{j+1})}$
  - 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]