Treatment of the Multiple Coulomb Scattering (MCS)
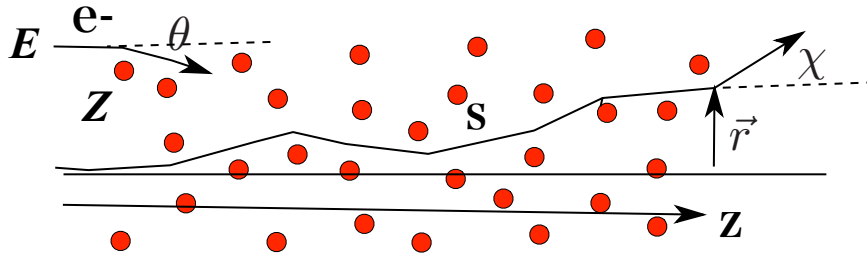
KK

Nov. 2014

1   Introduction

- Detailed simulation.
  If we know a differential cross-section (DCS)

$$\frac{d\sigma}{d\Omega} = f(E, Z, \theta) \tag{1}$$

  of the Coulomb scattering by a charge Z atom (upper left in the Figure), the cumulative scattering angle χ and displacement $\vec{r}$ of a charged particle (e- or e+) at z (net path length s) can be obtained by a M.C easily; we may sample each Coulomb scattering and path length for the scattering randomly.
  However, if s becomes order of 1 cm in a usual medium, the number of atoms becomes order of 10^8; this means the the same order of random sampling must be performed and the detailed simulation has no practical use.
- Condensed simulation
  The next idea is to get a distribution function, $F(E, Z, z, \vec{r}, \chi)$, based on DCS; if it is possible, we can sample $\vec{r}$ and χ for a given z without knowing details along the path (multiple Coulomb scattering: MCS).
  The method using only F is called condensed simulation.
  There are following problems:

- It's not possible to solve the equation expressing F (diffusion equation).
- Fermi expressed $F(\vec{r}, \chi)$ by a Gaussian distribution (the central limiting theorem would imply it's not so bad). It contains $\vec{r}, \chi$ correlation.
  It is not obvious how to determine the average and dispersion. Normally, those given in PDB are used (In Epics, Moliere=0 corresponds to this. With AlateCor=1 or 2, $\vec{r}$ correlated with χ is sampled. If AlateCor=0, only angle is sampled.
- Goudsmit & Sandaerson obtained formal solution of $F(\chi)$ without assuming DCS. But for a given realistic DCS, computation is difficult.
- Lewis advanced more. His F contains some dependence on the spacial factor ($\vec{r}$), but there remained difficulty in realistic calculations.
- Moliere $\Rightarrow$ Bethe. Moliere, after complex calculations and sophisticated approximations, obtained $F(\chi)$ for a fairly realistic DCS. Bethe gave a physical interpretation to that for easy understanding. He also improved so that the solution can be used for larger scattering angles.
  Epics uses the Bethe version of Moliere's theory with Moliere=1 or 2 (2 is more rigorous); since no $\vec{r}, \chi$ correlation is given, we require s be small in the simulation (but for very small s the theory cannot be used). If AlateCor=2 is specified, the correlation of $\vec{r}$ and χ is forced using Gaussian case.

- Mixed simulation.
  The mixed simulation saves defects in detailed and condensed simulations.
  It uses the following mathematical results.
  - Even if F is not known, averages like $< \cos \chi >$, $< \cos^2 \chi >$, $< z >$, $< r^2 >$, $< z \cos \chi >$ etc are expressed by using the transport mean free path.
  - The $l - th$ transport mean free path, $\lambda_{el,l}$, is defined via the $l - th$ transport cross-section,

$$\sigma_{el,l} = \int (1 - P_l(\cos(\theta)) \frac{d\sigma}{d\Omega} d\Omega \tag{2}$$

  as

$$N \lambda_{el,l} \sigma_{el,l} = 1 \tag{3}$$

  where. N is target number density (e.g, /g). $P_l(x)$ is the $l-$th Legendre polynomial; $P_1(x) = x, P_2(x) = (3x^2 - 1)/2$.
  For example,

$$< \cos(\chi) > = \exp(-s/\lambda_{el,1}) \tag{4}$$

$$< \cos^2(\chi) > = (1 + 2 \exp(-s/\lambda_{el,2}))/3 \tag{5}$$

$$< z > = \lambda_{el,l}(1 - \exp(-s/\lambda_{el,1})) \tag{6}$$

In a similar fashion, $< r^2 >, < z \cos(\chi) >$ etc can be expressed using $\lambda_{el,1}, \lambda_{el,2}$. To get its numerical values, DCS values are of course needed. If $s \ll \lambda_{el,1}$, we get $\chi^2/2 \sim s/\lambda_{el,1}$, i.e, MCS angles are small.

Brief introduction to the mixed simulation method: Small angle multiple scattering occur many times and can be well expressed by the condensed mode. Large angle scattering, though rather rare, leads to fluctuation, so it is sampled directly using DCS.

In stead of using scattering angle θ directly, we use $\mu = (1 - \cos(\theta))/2$ ($\mu = 0 \sim 1$) hereafter. The critical angle, μ_c, above which we regard the scattering angle large, is normally made to be smaller for larger energy. We use DCS at $\mu > \mu_c$ so if we put $\mu_c = 0$, complete detailed mode is realized. For $\mu < \mu_c$, a modified MCS function F^s is used so that it correspond to F for $\mu < \mu_c$.

However, even F is not easily obtained, how can we get F^s ? The key is that $< \cos(\chi) >$ etc for $\mu < \mu_c$ can be expressed also by Eq.4 etc. We may limit the integration region of Eq.2 to $0 \sim \mu_c$.

It is surprising that even if we don't know the explicit form of F, F^s, we may use a simple F, F^s and adjust $< \cos(\chi) >$, $< \cos^2(\chi) >$ so that they coincide with those derived from the correct DCS, then the resultant MCS angle distribution becomes quite adequate. The simple function could be as simple as combination of uniform distributions.

Treating MCS in this fashion has been developed by Salvat et al (Spanish group), Kawrakow et al (Canadian group), and Urban (Hungary)

DCS was calculated from the early quantum electrodynamics age but difficulty arises at "high energy" over MeV. Reliability at > 100 MeV region was only realized in 1990's, and long term effort by Salvat et al was converged in the CPC program library in 2005 as ELSEPA[*1]

2   Implementation

We make a DCS database using ELSEPA. The angular-lateral correlation in small angle MCS in the mixed mode, is taken into account by the hinge method developed by Fernandez and Salvat et al. For the largangle scattering, we use DCS directly. This hinge method is implemented in PENELOPE software (2011)[*2].

We calle this method El_hin model since it is the hinge method based on ELSEPA.

[*1] However, development is still ongoing.

[*2] PENELOPE was developed by Salvat et al and used mainly in the EU area, for investigating electron behavior in electron microscope, thin semi-conductor, film-badge etc. The manual can be obtained easily but the PENELOPE itself is not open to non-EU people.

On the other hand, we may put $\mu_c = 1$, i.e, we regard all angle small and use F^s always instead of F. (condensed mode simulation). As F, we need not use comlex functions such as Moliere's or Goudsmit & Sanderson's, but very simple ones which give the same averge and square average of angles as the correct DCS. Surprisingly, this gives not much different result as El_hin or Moliere's. This is named as El_con model.

ELSEPA can be used up to 1 GeV DCS so we use the same model as old ones above 1 GeV. As we show later, MCS above 1 GeV is almost negligible, model dependence may be neglected.

To leave the flexibility of choosing MCS model below 1 GeV, the old existing model is specified by Mol. Then, parameter Moliere is referred to fix details.

The MCS model may be specified in param file, as in the interaction model like: [*3]

```
 MCSmodel='"M1" E1 "M2" E2 "M3" E3 "M4" E4 "M5" E5 "M6"'
```

is the longest specification format, where Mi is one of El_hin, El_con, and Mol, Ei is electron kinetic energy (GeV); below Ei, model Mi is to be used. For example,

```
 MCSmodel='"El_hin" 10e-3, "El_con", 100e-3, "Mol"'
 MCSmodel='"Mol"'
 MCSmodel='"El_hin"'
 MCSmodel='"Mol" 1e-3, "El_hin", 100e-3, "Mol"'
```

The first and last one must be a model name. [*4].
The **default** is MCSmodel='"Mol"'.

[*3] "Moliere' parameter should be given in epicsfile as in past

[*4] There is no ELSEPA data base below 100 eV. Normally, the minimum energy in Epics by AutoEmin is 10 to 100 keV–though, near boundary sometimes electrons below 10 keV may be followed. There is no electron below 100 eV. As to positron, it can annihilate to generate 511 keV photons, so it is tracked down to 0 energy. But normally, annihilation takes place before the energy becomes so small. At any rate, details of such low energy e+/e- treatment is not important, and we use Moliere (=0, 1, 2) if such low energy e+/e- is encountered.
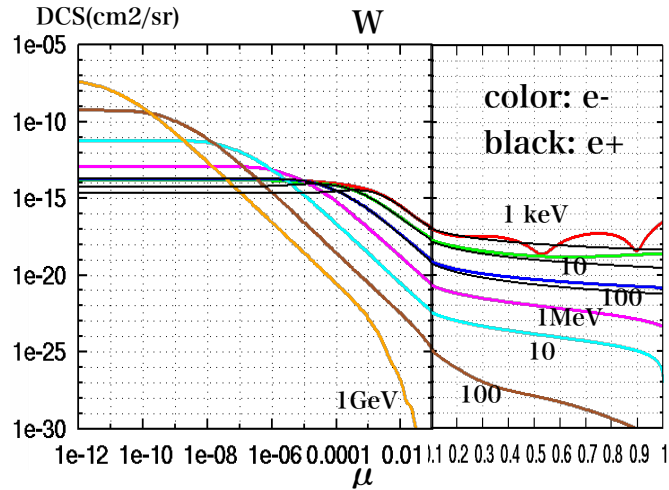
3 Example of basic data

図 1　DCS in W. Note that the x axis changes from log to ordinary scale at $\mu = 0.1$. There is some difference between e+ and e- at low energies (black lines for 1,10, 100 keV e+). At 1GeV, $\mu > 0.0001(\sim 1^\circ)$ is very rare.
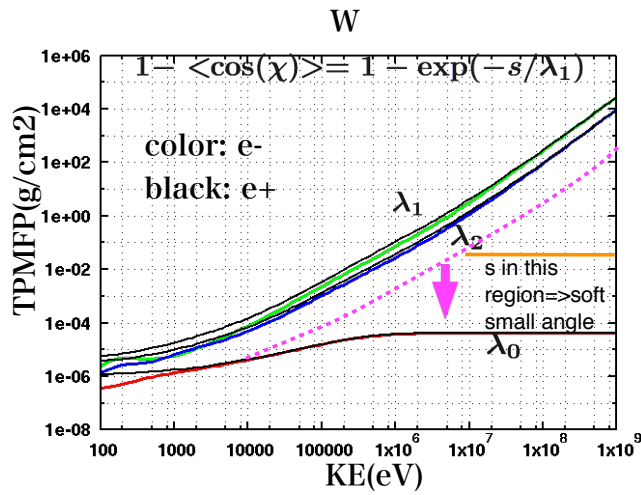

図 2　Example of transport mfp If the path lenngth, s, is short and $s/\lambda_1 \ll 1$, it is the soft region where scattering angle is small (say, the region below the dotted line). At high enegies, one may restrict the region narrower for safety like the orange line.

.

4 Simple tests

Making a detector consisting of 6 layers of (3.5mm(1r.l) thick W and $100\mu m$ thick nuclear emulsion) and a 1 GeV electron is vertically injected.

The lateral distribution of energy deposit in emulsion is obtained for 10^6 events[*5].

– MCS of >1GeV e+/e- is insensitive to the lateral spread: To see that, we inject 10 GeV e- and set $E_{min} = 1$ GeV.
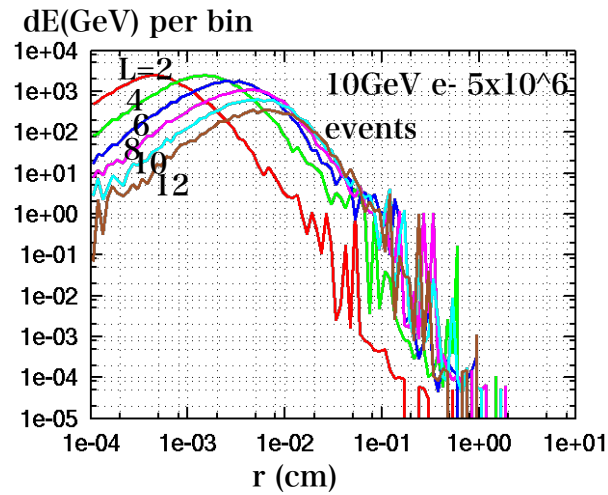

図 3　In view of the log scale vertical axis, 1 GeV electrons' contribution to the the lateral spread more than 0.1cm is very small.

– The lateral spread of partilces are mostly due to MCS: this can be seen by switching MCS on/off for 1 GeV showers as in Fig.4.

[*5] The sum of energy deposit (GeV) for all events in $r \sim r + \Delta r$; The vertical axis is not in density and hence the value in log and ordinary scale cases differ due to different Δr.
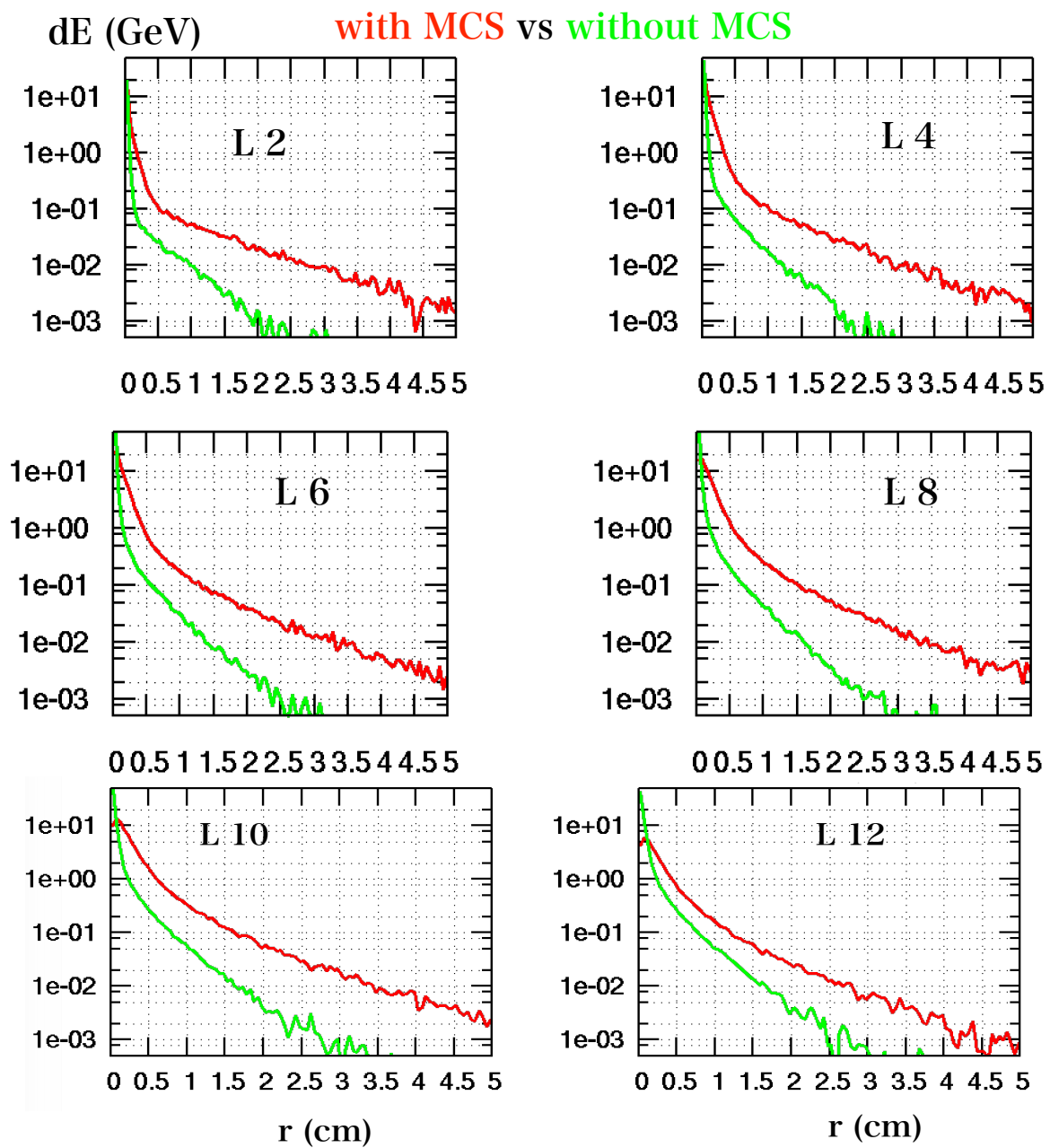
図 4　Lateral spread is due to mostly by MCS

– Comparison of MCSmodel='"El_hin"' and MCSmodel='"Mol"' (Moliere=2, AlateCor=0 or 1)

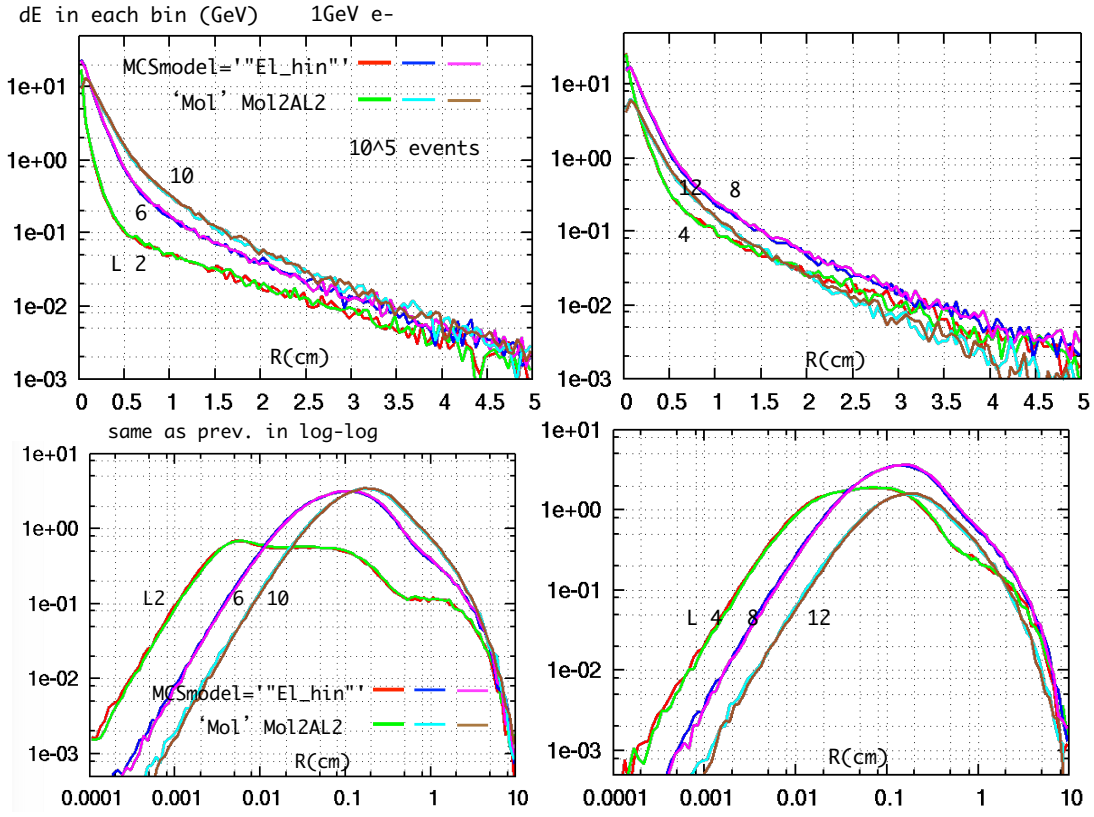図5　In the entire region, agreement of the both results is very good. It is surprising that completely different scheme gives such results. However, we must be careful that the both methods do not necessarily give the same results depending on the detector configuration.
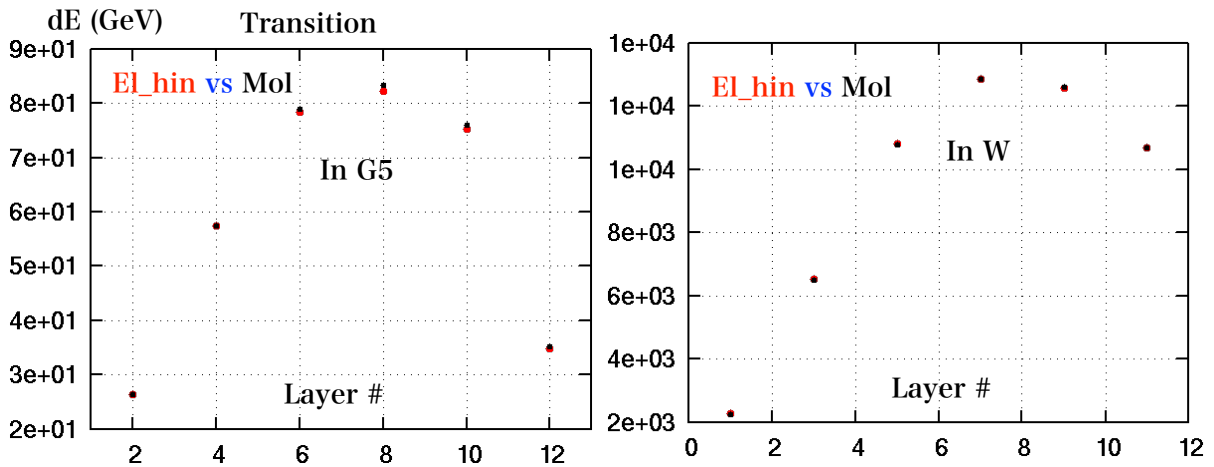

図6　Transition．　In the thin emulsion, El_hin seems to give smaller values a bit.

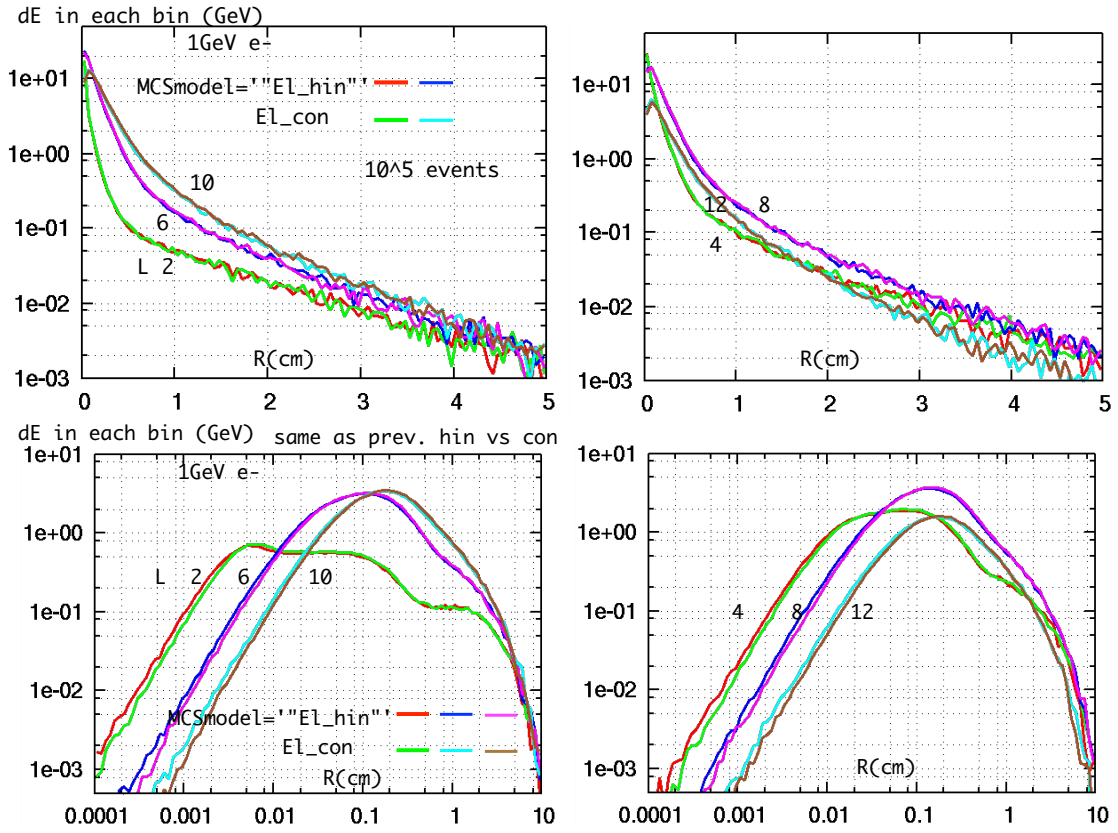– Comparison of MCSmodel='"El_hin"' and MCSmodel='"El_con"'.

図 7 Agreement is not bad but there seems some systematic smaller spread for El_hin in a small lateral region. It is also surprising that El_con using simple F for which only average and dispersion are adjusted to coincide with the accurate DCS case gives almost the same result as complex El_hin.
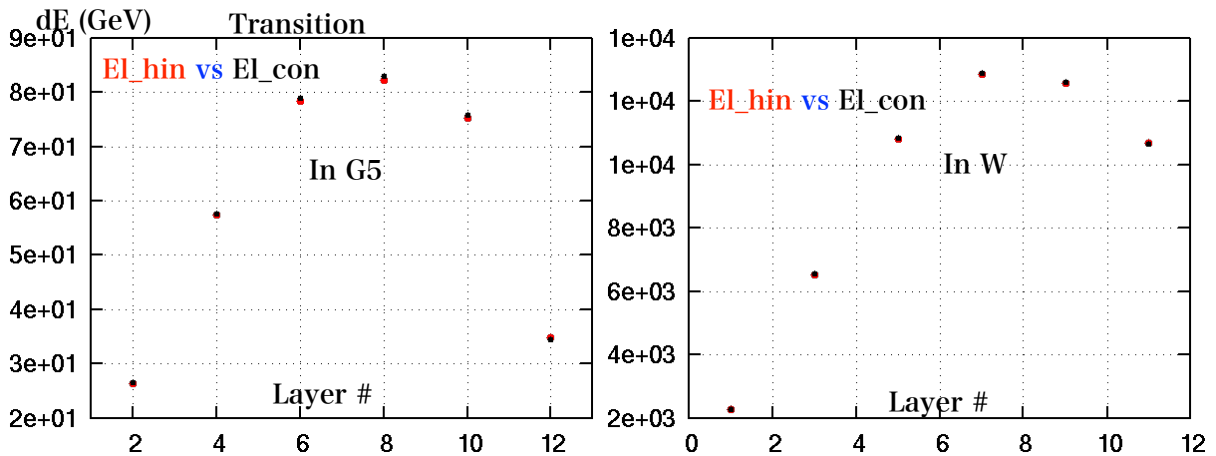

図 8 Transition. Similar tendency is seen as in the case of El_hin vs Mol. This seems due to difference between the condensed method and hinge method. The latter has better logic for crossing the boundary.

9

u

– Comparison of `MCSmodel='"El_hin"'` and `MCSmodel='"Mol"'` (Moliere=0, AlateCor=1 or 2; Gaussian with $\vec{r}$ and χ correlation).
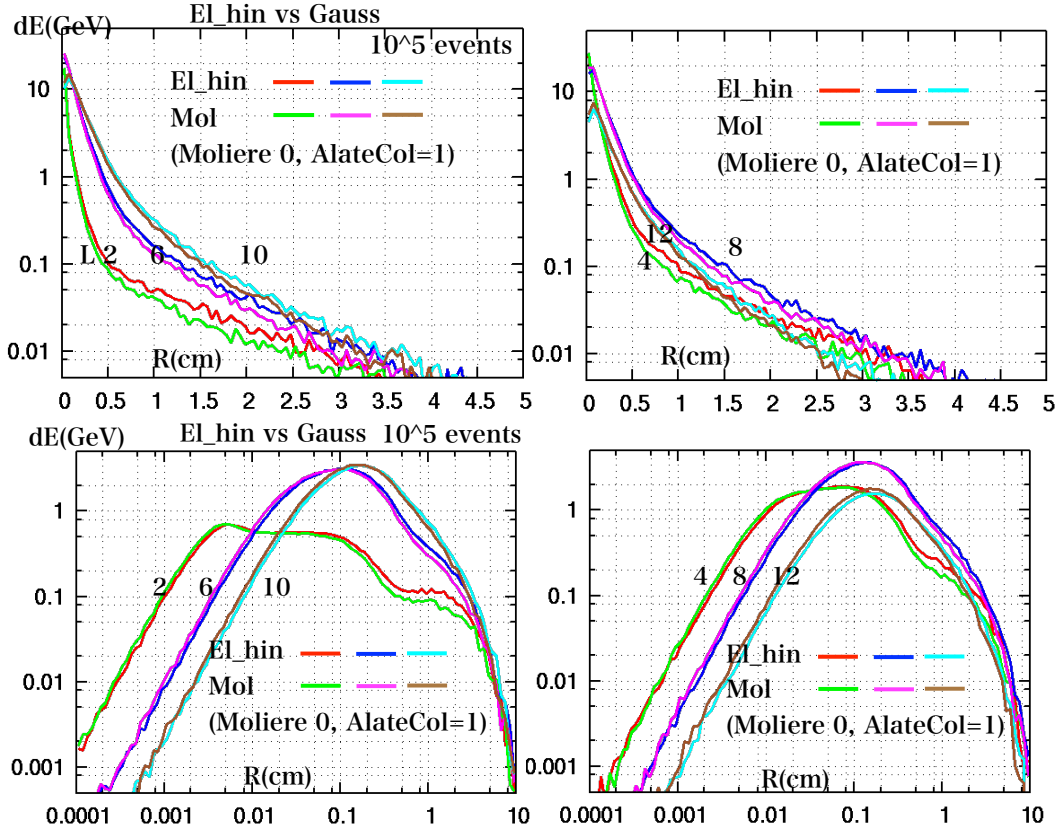

図 9 Obviously the Gaussian case give smaller lateral spread. If we neglect angular-lateral correlation (AlateCor=0) in the Gaussian case, a bit smaller spread is obtained
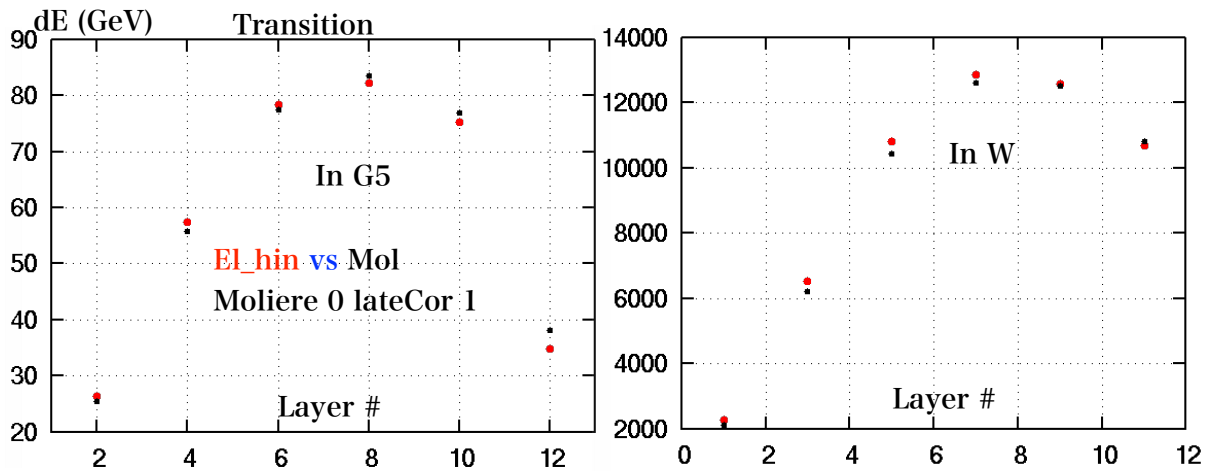

図 10 Transition. Diffrerence is seen in both thick and thin layers.

10

- Computation time. The `El_hin` model approaches to the detailed mode as energy goes lower and need $3 \sim 4$ time more time than other models.
- Comparisons here are very simple. It would be better to compare rigorous `El_hin` with Moliere=2 case in actual detector configuration.
  For default Moliere setting, Moliere=2 and ALateCor=0 (or 1) is recommended. For Moliere=2, ALateCor=0 and ALatCor=1 have the same effect (neglect angular-lateral correlation) and for Moliere=0(Gauss), correlation is taken into account. For Moliere=1 or 2, ALateCor$\leq$=1 seems better; agreement with `El_hin` is bit better. The difference between Moliere=1 and 2 is very small (1 is bit faster; but there is a report that 2 gives bit better coincidence with experimental data at microscopic scale distance).
- Data and program place:
  The DCS data table is in Cosmos/Data/Elsepa; they are classified by atomic charge Z and e+ and e-. ($\sim$ 316MB).
  The sampling table for Epics application is in Epics/Data/MCS with the same name as the media file name. (For Cosmos, osmos/Data/MCS/Air).
  The MCS model to be used controled in *Cosmos/Module/cHowMCS.f90*
  Programs reaading DCS and TPXS or doing sampling for random processes are in *Cosmos/Particle/Event/Elemag/MixedMCS*.
  Actural scattering is manged in `Epics/prog/{epeg.f,epdeflection.f}` and `Epics/prog/Elemag/epmulScat.f`
  by using above routines.
  If a new medium is introduced (and If El_hin or El_con is to be used for that medium) a corresponding data table must be created in Epics/Data/MCS For that, the user may go to Epics/Util/Elemag/MixedMCS/ and use ./ForManyMeida.sh
  It may also be used to make a new table with non-existing parameters. The parameters are defined in paramdata file.

Reference

For the mixed simulation and hinge method:

J.M. Femindez-Varea, R. Mayo1, J. Bar and F. Salvat, Nuclear Instruments and Methods in Physics Research B73 (1993) 447-473.

For the DCS:

Francesc Salvat, Aleksander Jablonski and Cedric J. Powell, Computer Physics Communications 165 (2005) 157190