The Pulse Height Distribution Tally in MCBEND

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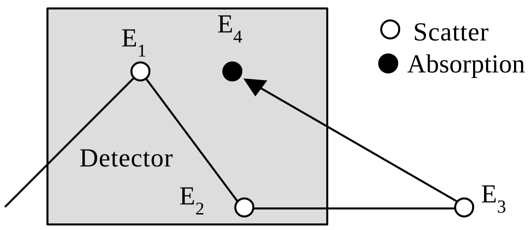
Certain detectors respond to the passage of a photon by recording the energy that it deposits. The net response is a spectrum of pulses with heights proportional to the frequency of events in distinct energy bands. Application of the Monte Carlo method to the analysis of such detectors is complicated: contributions to a pulse cannot be accumulated directly at each collision event since the tally bin is not known until the end of the history. In a simple, analogue calculation this problem can be resolved by accumulating the energy deposited in each spatial mesh until a history is completed then adding contributions to appropriate tally bins. In realistic calculations, using variance reduction methods, a complete particle history can include many branching events through particle splitting. Physical branching also occurs in events such as pair production or the explicit treatment of charged particles produced in gamma ray interactions. The net effect is that a complete particle history is a tree with many branches. Embodied in such a tree are contributions of different tally weight to a number of distinct pulses. This paper describes the methods used in the Monte Carlo code MCBEND to resolve these difficulties.

KEYWORDS: Pulse height distribution, Monte Carlo, Energy deposition, MCBEND

I. Introduction

Certain detectors respond to the passage of a photon by recording the energy that it deposits. The net response is a spectrum of pulses with heights proportional to the frequency of events in specific energy bands. The following sketch illustrates the passage of a single particle through a detector volume.



The particle deposits energies E_1, E_2, E_3 at scattering events and is finally absorbed with the deposition of E_4. The total energy deposited in the detector is $E_1 + E_2 + E_4$. This simple mechanism is relatively easy to simulate in a Monte Carlo calculation with one small complication: the contribution made by a given history cannot be assigned to an appropriate tally bin until the history is complete and the total energy deposition known. This contrasts with estimators for particle flux and activation rates which simply acquire contributions at each event in the random walk of a particle.

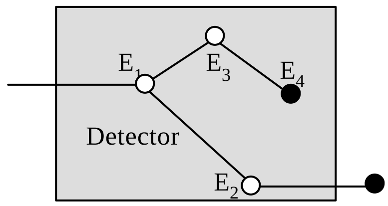
Practical Monte Carlo calculations are made significantly more complicated by the combination of the following effects:

- a particle history will divide if a collision event produces more than one secondary particle:
- the particle history may split into two or more independent components of reduced weight when variance reduction methods are introduced.

These processes lead to particle histories that are trees with many branches. The following sections describe how appropriately weighted contributions to different pulses are extracted from such particle histories in the Monte Carlo code MCBEND(1)

II. Multiple secondary particles.

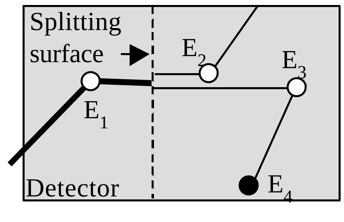
Events such as pair production lead to multiple secondary particles emerging from a collision. If charged particles are treated explicitly then some reactions produce a mixture of charged particles and photons. Schematically we have the following basic situation.



All energy depositions E_1 to E_4 contribute to the same pulse because they are all events in the life of a single particle. The total energy deposition is not known until both branches have been tracked to extinction.

III. Splitting through variance reduction.

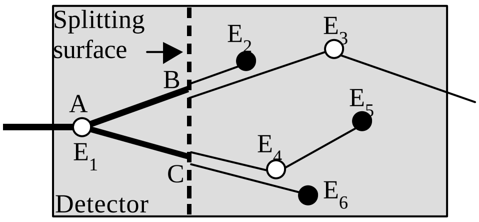
In MCBEND, a particle may split when it crosses a boundary into a region of higher importance. The split fragments travel together as a beam but follow independent sub-histories after successive collisions. An example of simple, binary splitting is sketched below.



After the splitting event, the particle history is effectively divided into two, independent sub-histories of reduced weight. One sub-history deposits a total energy in the detector given by: $E_1 + E_2$; the other deposits $E_1 + E_3 + E_4$. This form of division of the particle history differs in its logic from the physical branching of the previous section.

IV. Combined splitting and branching.

Combining the two forms of track division described above illustrates the complexity of scoring pulse heights in a realistic Monte Carlo calculation.



The division of the history at A is a genuine physical event; divisions at B and C are caused by variance reduction. One of the routes through AB and beyond must be combined with one of the routes through AC and beyond to form a complete pulse. E.g.

$E_1 + E_2 + E_4 + E_5$

The remaining pair of routes form another pulse. E.g.

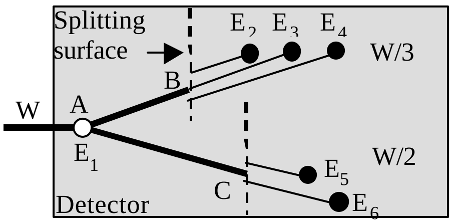
$E_1 + E_3 + E_6$

Each of these pulses has a reduced tally weight to compensate for the splitting. The following, alternative pairings are equally valid:

$E_1 + E_2 + E_6$ and $E_1 + E_3 + E_4 + E_5$

The choice between the two possibilities may be made randomly. This is a fair game: in an analogue calculation, either combination could occur with equal probability.

In this simple example, if the initial weight of the particle is W then each of the two pulses generated will have a weight 0.5W and there is no difficulty in matching the weights on either side of the division at A. The following extension to the method illustrates how a more general set of weighted tracks are combined.



The two scattered particles from the event at A cross different splitting surfaces. One branch divides into three fragments of weight W/3; one divides into two fragments of weight W/2. (Note that ternary splitting is used here only to illustrate the method; MCBEND always splits into powers of two.) The problem is to combine events on either side of this division to generate pulses of a particular weight.

Any path through the tree may be considered to have started at the source point and travelled to extinction at a constant weight. In the early part of the history, before any splitting, all routes are common and are effectively processed as a single fragment with a weight equal to the sum of all the distinct routes.

In the above sketch, the route through AC that finally deposits an energy of E_5 has a weight of W/2. It may alternatively be regarded as two identical routes: one of weight W/3 and one of weight W/6. The former can be combined with a route of similar weight from the other side of the branch at A. Thus we might generate a pulse of weight W/3 with total energy deposition $E_1 + E_5 + E_2$.

The route through AB that finally deposits an energy of E_3 (weight W/3) may be resolved into two identical routes of weight W/6. One of these may be combined with the residual deposition (weight W/6) from the other branch that deposited $E_1 + E_5$

By continuing this process, all the weight from one side of the branch at A can be matched with that in the other branch to form a set of pulses. A specific set of combinations might be:

$E_1 + E_5 + E_2$	Weight W/3
$E_1 + E_5 + E_3$	Weight W/6
$E_1 + E_6 + E_3$	Weight W/6
$E_1 + E_6 + E_4$	Weight W/3

Inspection shows that the correct, total weight is associated with each particular energy deposition. E.g. a weight W is associated with the deposition of E_1.

The selection of combinations from either side of the branching at A uses a randomising element to avoid, say, always combining the first collision on one side of the branch with the first on the other side. In an extremely long calculation, a given event tree might occur a number of times and all combinations will eventually be selected. In a calculation of practical length one may expect sets of 'similar' trees that will be resolved using different combinations.

Even the complexity of this last example falls far short of that occurring in the tree structures of practical calculations. A history may involve the crossing of many geometrical splitting surfaces, splitting will occur with energy changes and physical branching may occur more than once – particularly when charged particle production is included. MCBEND stores a record of the relevant events in a complete particle history and the energy depositions associated with each collision. When a history is complete it resolves the tree into a set of distinct pulses. The energy bin associated with each pulse is identified and the weight attributed to the pulse is added into appropriate tally registers.

V. Russian Roulette.

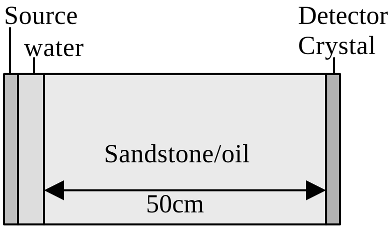
Complementary to the splitting process of most variance reduction methods is the playing of Russian roulette to decrease the population of particles entering unimportant regions of the problem space. Survivors have their weight increased. The mechanism for scoring pulse height distributions restricts the use of this technique under the following conditions.

> If a particle history has branched then Russian roulette is suppressed for the rest of the history to avoid an imbalance of the total weight on either side of the branch.

If a particle has deposited some energy in a detector then Russian roulette is suppressed for the rest of the history to avoid the tallying of incomplete pulses. Even if a particle has passed beyond a detector it could always return to deposit more energy; the history must not be terminated artificially.

VI. Example

The following example is a stylised representation of an oil well logging problem.



A 14.0MeV pulsed neutron source emits into a slab containing a mixture of sandstone and oil representing a rock formation. Gamma rays are produced by inelastic scatter and capture. The Monte Carlo model is required to evaluate the pulse height distribution in the detector crystal. Of particular interest are the pulse heights at energies corresponding to inelastic scatter in oxygen (6.1MeV) and carbon (4.5MeV). In practical cases these are analysed to deduce the properties of the rock strata into which a well logging tool is lowered. The gamma rays produced are sufficiently energetic for pair production events to be significant.

Three variations on the above case have been executed.

1 Analogue mode (no variance reduction) to provide reference results
2 With splitting and Russian roulette and a simple scoring of pulse height distributions. This resolves each path through the event tree into an individual pulse without combining the contributions on either side of a physical branching. It is only valid if there is no pair production and no treatment of charged particle production. For the chosen example, these results are expected to be incorrect and demonstrate the requirement for the treatment described earlier.
3 With splitting and Russian roulette using the detailed mechanism described above. These results are expected to be in agreement with (1) but more efficiently calculated.

VII. Example results.

Counts per second in the energy range 6.1-6.2 MeV corresponding to the Oxygen inelastic scatter energy.

Variation	CPS	S.D. %
1	8.42E4	6.15
2	2.94E4	3.77
3	8.43E4	0.91

Counts per second in the energy range 4.0-4.5 MeV corresponding to the Carbon inelastic scatter energy

Variation	CPS	S.D. %
1	4.04E4	9.6
2	1.70E4	5.90
3	4.59E4	1.37

These results illustrate agreement (within statistical limits) between values obtained in analogue mode (1) and using the defined algorithm (3). Both variations were executed for the same length of time; the introduction of variance reduction improves the efficiency by a factor of about 40.

The results for variation 2 are in error, as expected. Without a treatment to combine the contributions to a pulse from both progeny of a pair production event, many pulses are incompletely scored. Many of the incomplete contributions appear as an enhanced count in the energy bin containing the annihilation energy of 0.511 MeV as shown in the following table.

Counts per second in the energy range 0.5-0.6 MeV corresponding to the pair production/annihilation energy

Variation	CPS	S.D. %
1	0.68E6	2.74
2	1.33E6	0.63
3	0.67E6	0.72

VIII. Summary

The scoring of pulse height distribution tallies in a Monte Carlo calculation in conjunction with variance reduction methods is made difficult by the requirement to identify complete pulses from the event tree of a given sample history.

A method of achieving this task has been implemented in the Monte Carlo code MCBEND.

Results have been presented which demonstrate the validity of the proposed mechanism and show the gains in efficiency which can safely be achieved by using it in conjunction with variance reduction. The inadequacies of a simple treatment have also been demonstrated.

¾ References ¾

(1) Chucas, S. J. *et al.*, Preparing the Monte Carlo Code MCBEND for the 21st Century, *Proc 8th Int. Conf. On Radiation Shielding*, Arlington, Texas (1994)