The Geometrical Sensitivity option in MCBEND

E Shuttleworth

The ANSWERS Software Service, AEA Technology plc, Winfrith Technology Centre, Dorchester , Dorset DT2 8ZE, United Kingdom

1. Introduction: the differential sensitivity algorithm.

A scored result, R, in a Monte Carlo calculation may be represented in the form:

$$R = Q\prod_i P_i \tag{1}$$

Where P_i are the probabilities associated with a each event, i, in the random walk of a particle and Q is a scaling constant. If the result is sensitive to some parameter, s, then:

$$\frac{dR}{ds} = Q\sum_j \left(\frac{dP_j}{ds} \prod_{i \neq j} P_i \right) = Q\prod_i P_i \left(\sum_i \frac{1}{P_i} \frac{dP_i}{ds} \right) = R\sum_i \frac{1}{P_i} \frac{dP_i}{ds} \tag{2}$$

The summation of the terms (1/P.dP/ds) is effectively a weight factor that is accumulated during the calculation. It is applied to the scored result to give its differential with respect to parameter s.

In the Monte Carlo code MCBEND[1], geometry models use the differences and intersections of simple solid bodies to define volumes of space occupied by a uniform material. The geometrical sensitivity option allows the perturbation 'ds' to represent a differential displacement of a body along one of its local co-ordinate axes or a change to one of its dimensions – e.g. the radius of a cylinder.

The differential sensitivity method has advantages over making finite perturbations and observing the changes in results. If the overhead for evaluating sensitivity terms is less than a factor two then it is more efficient than executing two calculations. If small, finite changes are made to the model then the precise difference in the results will be masked by the Monte Carlo statistical noise. If larger changes are made they may be physically unrealistic.

2. The probability of reaching a boundary

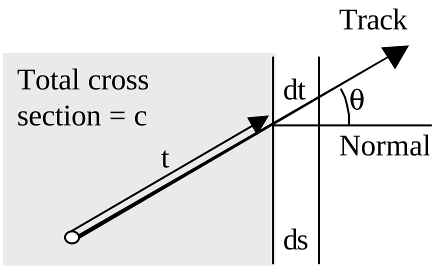
From any arbitrary point on a particle track approaching a boundary, the probability of reaching that boundary without a collision is simply:

$P = e^{-ct}$ t = the geometrical distance to the boundary
c = the total cross section of the material before the boundary.

$$\frac{dP}{dt} = -ce^{-ct} \text{ and } \frac{1}{\mathrm{P}} \frac{dP}{dt} = -c \tag{3}$$

The term may be related to a geometrical displacement of a parameter, s:

$$\frac{1}{\mathrm{P}}\frac{dP}{ds} = \frac{1}{\mathrm{P}}\frac{dP}{dt}\frac{dt}{ds} = -c\frac{dt}{ds} \tag{4}$$



The differential dt/ds is purely geometrical. The example in the sketch illustrates a case where the specified geometrical perturbation is the displacement of a plane surface along its normal. The term dt/ds is then the secant of the angle (θ) at which the particle track crosses the surface. For first order sensitivities, the same result applies to curved surfaces - e.g. the crossing of a cylindrical boundary with ds representing a change in its radius.

The crossing of a perturbed boundary is a well defined event in the history of a particle; the above term may be evaluated and accumulated in a sensitivity weight register with little additional effort.

3. The probability of colliding before a boundary

From any arbitrary point on a particle track approaching a boundary, the probability of colliding before reaching that boundary is given by:

$$P = 1 - e^{-ct}$$

$$\frac{dP}{dt} = ce^{-ct} \text{ and } \frac{1}{\mathrm{P}}\frac{dP}{dt} = \frac{ce^{-ct}}{1-e^{-ct}} = \frac{c}{e^{+ct}-1} \tag{5}$$

However, it is not appropriate to apply this weight term to every collision event. Pre-boundary collisions could occur several mean-free-paths before a boundary and it would be illogical to weight them for a perturbation that has not been reached or even approached.

The sensitivity term for the crossing of a perturbed boundary (equation 4) is negative for a displacement along the particle track: fewer particles reach the boundary as a result of the displacement. The number of pre-boundary collisions increases (equation 5) but the increase should be confined to collisions within the differential limit of the boundary. In a practical Monte Carlo calculation the probability of such events is vanishingly small.

One solution attempted during development of the sensitivity algorithm was to confine the application of sensitivity weights to collisions that occurred *close* to a boundary: say within 0.1mfp. This leads to the following weight term to apply to collisions that occurred within Δt of a boundary:

$$\frac{1}{\mathrm{P}}\frac{dP}{dt} = \frac{c}{e^{+c\Delta t}-1} \approx 9.5 \text{ for } c\Delta t = 0.1 \tag{6}$$

Thus we would be applying a relatively high weight to a relatively small number of events.

This solution met with limited success: if the chosen interval was reduced then the approximation became more valid but the statistical noise on the sensitivity results increased; if the interval was increased then the statistics improved but the approximation became greater. The method was found to be entirely inadequate for second order sensitivity calculations.

A practical solution was found by re-examining the basic form of the sensitivity calculations (equation 2). Consider a less formal representation involving only three probabilities:

$$R = QP_1P_2P_3$$
$$\frac{dR}{ds} = QP_1P_2P_3\left(\frac{1}{P_1}\frac{dP_1}{ds} + \frac{1}{P_2}\frac{dP_2}{ds} + \frac{1}{P_3}\frac{dP_3}{ds}\right) \qquad (7)$$

Suppose one of the probabilities is extremely small (e.g. $P_2 = \varepsilon$) but its differential is not. The equation reduces to:

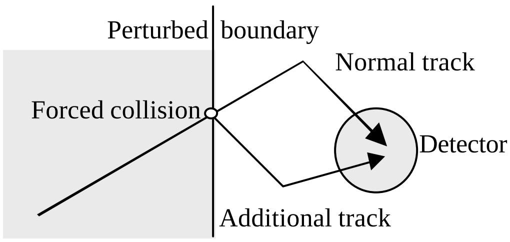
$$\frac{dR}{ds} = Q\left(P_2P_3\frac{dP_1}{ds} + P_1P_3\frac{dP_2}{ds} + P_1P_2\frac{dP_3}{ds}\right)$$
$$= Q\left(\varepsilon P_3\frac{dP_1}{ds} + P_1P_3\frac{dP_2}{ds} + P_1\varepsilon\frac{dP_3}{ds}\right)$$
$$= QP_1P_3\frac{dP_2}{ds} \quad \text{as } \varepsilon \to 0 \qquad (8)$$

A collision within the differential limit of the perturbed boundary is such an event. Its probability and differential are:

$$P = 1 - e^{-c\delta t} \ \ (\to c\delta t = \varepsilon); \qquad \frac{dP}{dt} = ce^{-c\delta t} \ (\to c) \qquad (9)$$

Such an event may be forced to happen in a Monte Carlo calculation when a particle track crosses a perturbed boundary. The progeny of the collision are assigned an extremely low weight so that the contribution they make to any detectors which they enter is negligible. The chosen weight is arbitrary - say 10^{-6} - and may be equated to ε in the above analysis.

$$R = QP_1\varepsilon P_3 \qquad = \text{negligible}$$
$$\frac{dR}{ds} = QP_1\varepsilon P_3\left(\frac{c}{\varepsilon}\right) \qquad = \text{finite} \qquad (10)$$



By this method, we have represented a very rare event and given it a very large sensitivity weight. However, we have made the event frequent (by forcing it) so the statistical noise does not become unacceptable. An example of such an event is sketched on the right.

There is clearly a computational overhead here: additional tracks from the forced collisions must be traced. The severity depends on how late in the particle history the perturbed boundary is crossed; if it is near the detector then the extra tracks are relatively short. In MCBEND, provision is made for restricting the frequency of forced collisions with a compensating weight enhancement for those that do occur.

4. Post-boundary events.

The above analysis has been confined to events in the material preceding a perturbed boundary. Contributions to the sensitivity weight are also generated by the fact that the path length of the particle in the material beyond the boundary is reduced when the boundary is displaced along the track. If c' is the total cross section of the material beyond a boundary then the sensitivity weight for a particle track that crosses it is increased by c' dt/ds. A forced collision must be generated immediately after the boundary with a sensitivity weight $(-c'/\varepsilon)$ dt/ds. Quite correctly, these terms cancel those of the pre-boundary events when the material on either side of the boundary is the same.

5. Types of perturbation.

The simplest form of perturbation is one in which a single surface is moved. Applications include the following examples.

Assessing the sensitivity of reactor pressure vessel damage to its inner radius. A large pressure vessel may change its radius significantly due to thermal expansion. There may be some uncertainty over the difference between the design radius and the 'as-built' dimension.

The biological dose beyond a shield wall will depend upon its thickness. During a cycle of design calculations, the outer boundary of the shield may be declared as a perturbed boundary to provide an estimate of the gradient of the dose vs thickness curve. This can reduce the number of survey calculations required and allow rapid convergence on the thickness required to attain a given dose level.

A more complex application is one in which a component of the geometrical model may be displaced – particularly if it contains a source.

In a well logging calculation the source and detector are contained within a tool that is lowered down a bore hole. The measurements obtained will be sensitive to the position of the tool relative to the bore hole centre. The geometrical sensitivity option allows this to be quantified.

In this mode, the source point and the particle tracks undergo the same differential displacement as the tool. Boundary crossings within the tool and at its surface are not deemed to be perturbed relative to the track. Differential sensitivity terms are derived when the displaced track crosses the fixed surfaces of the bore hole and its environment.

6. Second order sensitivities.

In many applications, the variation of the result with a geometrical change is non-linear. The curvature of the variation may be assessed by evaluating the second differential terms. A simple approach here is to take the mean gradient of the first order sensitivities between two points and use it as an estimate of the second order differential.

Alternatively, the method of evaluating the first order sensitivities may be extended to second order. The following terms can be derived for the probability of a particle reaching a perturbed boundary.

$$\frac{d^2P}{ds^2} = \frac{d^2P}{dt^2}\left(\frac{dt}{ds}\right)^2 + \frac{dP}{dt}\frac{d^2t}{ds^2} \quad \rightarrow \quad \frac{1}{P}\frac{d^2P}{ds^2} = c^2\left(\frac{dt}{ds}\right)^2 - c\frac{d^2t}{ds^2} \qquad (11)$$

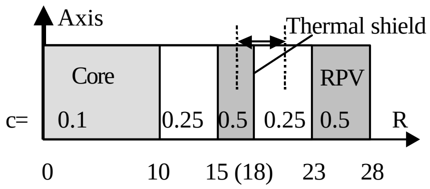
Terms such as the above are generated when the second differential of the result, R, is taken with respect to a geometrical parameter s. For plane surfaces, the geometrical term d^2t/ds^2 is zero; for curved surfaces it is dependent on the shape of the surface and its curvature.

Detailed analysis of the provision to be made for forced boundary collisions shows that *two* collisions must be forced to obtain the second order sensitivity contributions. A number of combinations are required for distributing these two collisions about a perturbed boundary.

The complexity of this process, and the extra computing effort required to track the plethora of extra particles associated with second order sensitivities renders the method unattractive compared with the relative simplicity of the first order evaluation. A prototype implementation has been attempted in MCBEND with limited success. The statistical uncertainties on the second order sensitivities were very poor compared with those obtained for first order.

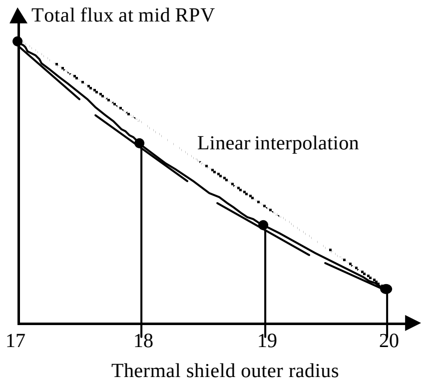
7. Example application.

The following example illustrates the type of calculation that may be executed. The materials are formed from a fictitious nuclide that has the property of scattering isotropically with the loss of half the incident energy. The calculation records the fluxes in groups representing 0 – 4 scattering events together with a response function that is the sum over all groups.



The geometry is a cylindrical system representing a notional reactor system.

The outer radius of the thermal shield (nominally 18.0units) is defined as a perturbed boundary. Calculations were executed for specific variations: 17.0, 18.0, 19.0, 20.0.



The sketch left plots the results of calculations with explicit variations of the thermal shield radius. Superimposed are the gradients at each point provided by the geometrical sensitivity results. Had the variations been confined to the two end points (R=17 and R=20) then, in the absence of geometrical sensitivity results, a linear interpolation would not give correct intermediate values. The gradients at these points could be used to provide a reasonable estimate of the variation between them rather than requiring three or four executions.

In this example, a geometrical sensitivity estimation extended the execution time by about 25%. The uncertainty on dR/ds was of the order 4%.

8. Summary

The method of estimating differential sensitivities in Monte Carlo calculations has been extended to perturbations of the geometry model. The problem of representing differential changes in collision rates near perturbed boundaries has been resolved by forcing extra collisions at these boundaries. The extension to second order has been outlined. Some potential applications of the technique have been listed. An example application illustrates its usefulness.

Reference

(1) Smith N R *et al.,* The Current Status and Future Plans for the Monte Carlo Codes MONK and MCBEND, *Proceedings of MC2000,* Lisbon (2000)