Monte Carlo modelling and applications to imaging

The Monte Carlo method is a method to obtain a result through repeated random sampling of the outcome of a system. One of the earliest applications, in 1946, of the technique provides a good example as to how it works. One of the physicists who was working on the problem of how to initiate fusion in the hydrogen bomb, Stanislaw Ulam, (http://en.wikipedia.org/wiki/Stanislaw_Ulam) had become intrigued by the card game 'Solitaire'. Sometimes this game can be completed, other times it cannot, depending on the order of the cards. As the cards are shuffled before play commences whether a game can be completed or not is essentially random. Ulam decided to work out the likelihood of shuffling cards such that a game can be completed. There are 52 cards and hundreds of possible moves in even the shortest game and hence calculating the odds was (and in fact still is) impossible. Knowing this Ulam decided to estimate the likelihood by merely playing 100 games and seeing how many games he could finish. Hence he arrived at an approximate answer[*] to a mathematically intractable problem.

Because you only run a limited number of times you cannot avoid sampling error: this is the square root of the number of times you run the test. So for example in the solitaire example if you found you completed 15 games out of 100 games you get a completable likelihood of 15%. However the error would be $100^{½}$ giving your result a standard error of +/-5%.

Monte Carlo 'by hand' is extremely time consuming and not possible or at least practical for most problems. However Ulam worked on the Manhattan project (the name given to the American research into creation of a nuclear bomb) which had recently acquired the first[**] general purpose computer called ENIAC. Due to the $n^{½}$ scaling on the error and thus the often large number of runs needed for accuracy; computers and the Monte Carlo method are ideally matched.

After discussions with other researchers including the mathematician and early computer pioneer von Neumann, they realised that they could estimate the range of neutrons in fissionable materials using a computational Monte Carlo technique. The random nature of a neutron's path and its interactions had previously presented a very serious problem to fission based research[***].

There does remain one problem in that computers by their deterministic nature cannot calculate truly random numbers. Hence computational use of random sampling methods such as Monte Carlo might seem impossible. However there are practical solutions which produce numbers that are sufficiently 'random' for most applications. Such solutions include using pre-recorded lists of truly random numbers, using techniques which generate long series of numbers before repeating or including readings from devices physically sampling external sources of entropy (e.g. radioactive decay).

Once this issue was solved the first use of Monte Carlo in radiation research was successfully completed. The very fast growth in available computer power and the fact that Monte Carlo is classed as an 'embarrassingly parallelizable' problem (results from separate calculations are independent and can be merely added) means that Monte Carlo is now a common technique in numerous fields, including in radiation research. Such a technique is especially suited to the task of radiation simulation due to the nature of the physical processes being simulated.

The observed interaction of a particle with another particle is stochastic. This means that the individual interactions of radiation (which can be considered as a beam of particles) with matter (another collection of particles) are also stochastic. As such the exact path of an individual particle of radiation through matter cannot be predicted. However the path of individual particles is of little practical consequence: what normally matters is the likelihood of transmission and thus the number of particles arriving. For example in designing lead shielding for a X-ray scanner control room the fact that 1 in 10 billion particles might get through the shielding is not really important.

The reason being we are surrounded at all times by a weak background radiation and so if the added radiation from the scanner leakage is much lower than this, its effect can be pretty much ignored. Hence the Monte Carlo method which essentially only provides likelihoods is still acceptable for almost all modelling of radiation interactions.

However by far the biggest limitation on the use of the Monte Carlo method is the fact that the number of runs needed for a sufficient certainty in the result might become impractical even with modern computing resources. Several Monte Carlo simulations of a mouse X-ray are shown below to demonstrate the effect of using too few runs.

A surface rendering of a virtual mouse included in the simulation is shown in Figure 1. This virtual mouse was created using the Moby package described in greater detail in this site: http://deckard.mc.duke.edu/xcatmobyrobyphantom.html

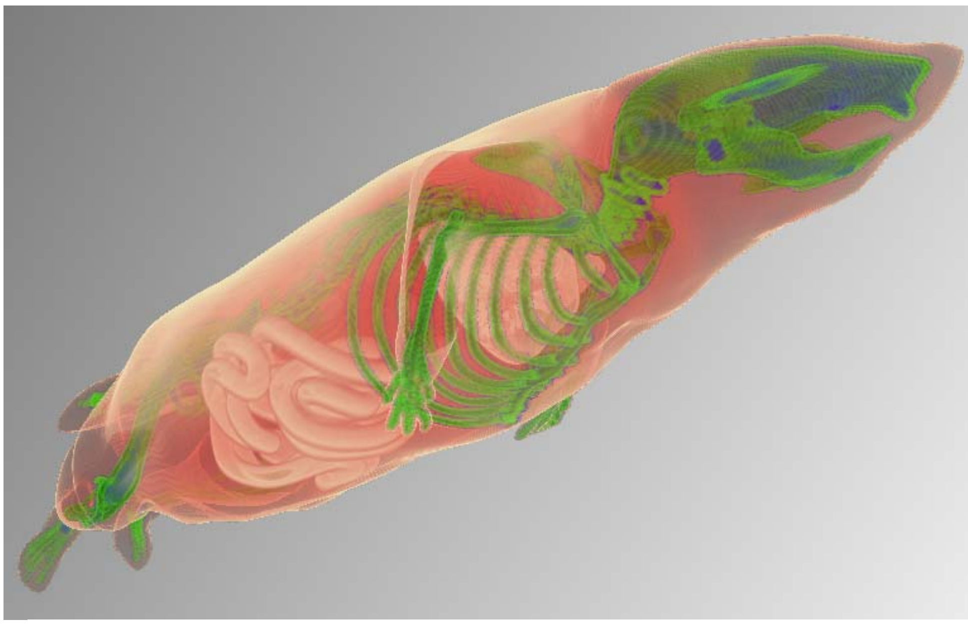
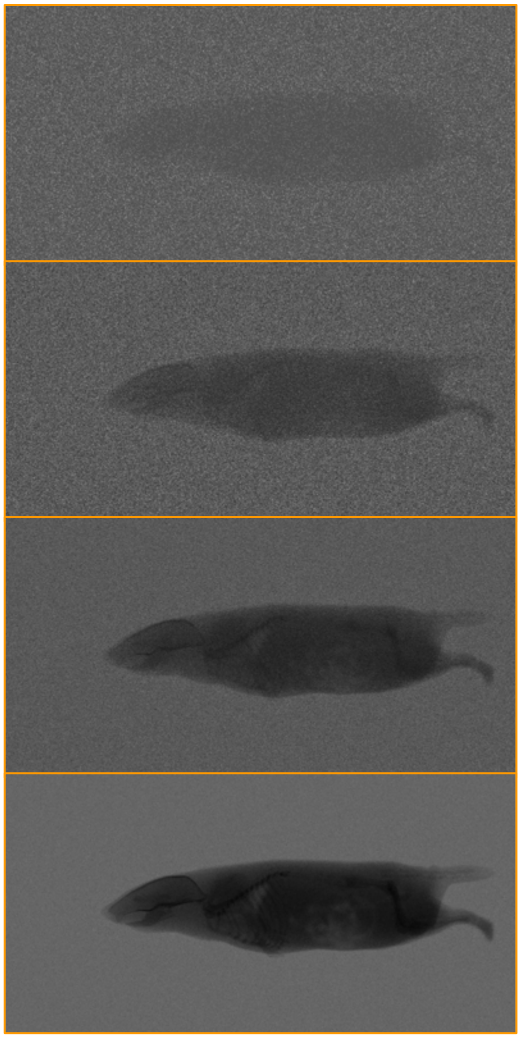


Figure 1: A virtual mouse model created using the Moby package

The Monte Carlo simulation modelled 150 keV X-ray photons emitted from a point source. The photons were modelled as ballistic particles following the Beer-Lambert law. An X-ray imaging plate was placed in line with the mouse, 1 m away from it and the illuminating point source was placed 1.6m forward of the mouse. The simulations were identical and only the number of runs or simulated particles changes. The brightness and contrast of the resultant images were adjusted, so as to make presentation easer.



Result after 10^6 photons: A possible mouse shape is clear but few other features are apparent. The image black level has been increased so as to make the background grey level comparable to the other three images below.

Result after 10^7 photons: the bone structure and rear feet are starting to appear but distinguishing anatomical regions is still almost impossible.

Result after 10^8 photons: The bones are becoming clear now. There are only small differences in X-ray attenuation between soft tissue thus the soft tissue interfaces are not clear.

Result after 10^9 photons: The bone structure is relatively clear now and certain soft tissues (such as the lungs and the intestines are obvious). This simulation took 10 hrs on a 2 GHz CPU.

Figure 2: Improvement of image contrast as total photon number is increased. In this instance, the photon number refers to the total illuminating the image, which was composed of 720000 pixels (1200 x 600 pixels). The dynamic range of the image after 10^9 photons is ~700:1, though in these examples, each image has been compressed down to 255:1

The $n^{½}$ scaling on the error means doubling the number of runs (taking twice as long or alternatively twice as much computer power) only improves the simulation by about 40%. Hence naively adding computational power to an underperforming Monte Carlo simulation is rarely the best option. There are however several other speed-up options available. The most powerful of which is variance reduction.

This as the name implies aims to reduce the spread in the tested distribution. This reduction is justified by the assumption that the untested particles would not contribute to the result in a significant way.

By way of an example consider a point X-ray source, a sample and an X-ray detector screen as shown in Figure 3.

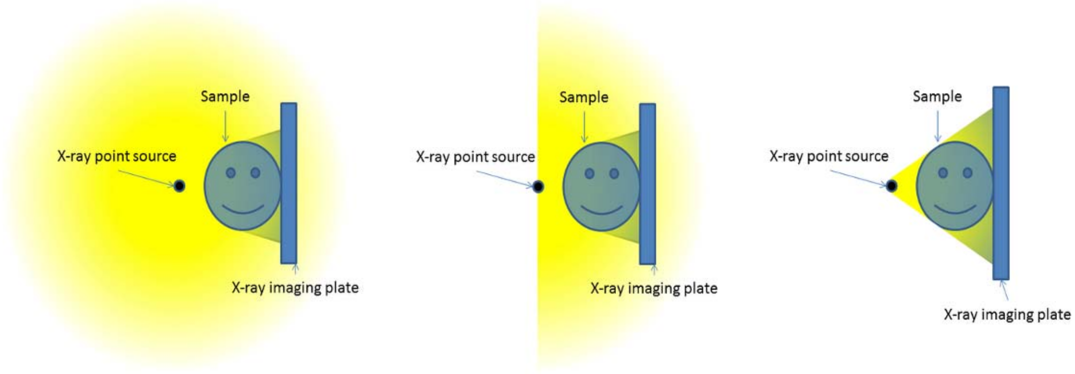


Figure 3: Speed reduction in Monte Carlo modelling; please see text for explanation.

A simple Monte Carlo simulation emits photons from the point source in a random direction, calculates if the emitted photon makes it through to the imaging plate and records a hit on the detector where the photon would impact.

The yellow glow represents the X-ray photons that are simulated. In all three cases the same numbers make it to the detector and so the final result would be the same. However by limiting the emission angle first to forward facing direction then to within the angle defined by the sample we reduce the number of required runs and thus time taken by a factor of 2 or ~10 respectively.

Variance reduction is in fact always used at some level be it by simulating a limited volume or by not including physical processes which are unlikely to influence the outcome. For example particle interactions can trigger release of other lower energy particles which may do the same in turn. Hence a reasonable energy cut-off is required to limit the number of tracked particles. Particles that drop below the energy cut-off are either simply stopped or removed with their final energy and location being recorded.

All variance reduction limits the realism of the simulation but does not necessary reduce accuracy or quality of results. In practice there exists always a three way trade-off between (a) time needed for simulation, (b) accuracy of the physical processes modelled and (c) computational power required.

There are many situations in which Monte Carlo techniques cannot be used, such as situations in which a particle's path is dependent on the paths of other particles. For example an intense beam of electrons tends to expand due to Coulomb repulsion or space charge between the composite electrons but this effect would not be seen in a pure Monte Carlo model no matter how many runs were performed. Furthermore, Monte Carlo should not be used in situations in which the environment is changed by the particle path. For example thin films in an intense particle beam. Naturally in these cases Monte Carlo style models may still be useful but only if they are extended or included along with other computational methods.

The art of making a good Monte Carlo model is in using previous knowledge to verify that the Monte Carlo technique is valid and to select the various cut-offs and other variance reduction techniques to make the required number of runs practical.

[*] The exact answer you get depends on what rules you use when playing the game. See http://www.roziturnbull.com/bill/Solitaire/solitaire.htm which provides much more detail,

[**] Whether this is the first or not is open to interpretation see "Electronic Brains: Stories from the Dawn of the Computer Age" Publisher: Joseph Henry Press (September 30, 2005) for more details on the history of early computers.

[***] Many people have argued that it was mistakes in Heisenberg's calculations on the neutron path in fissionable material that discouraged Nazi nuclear scientists from pursuing creation of their own nuclear weapon.

This note was prepared by A Kavanagh and B Vojnovic in October 2011

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