

22.106 Neutron Interactions and Applications (Spring 2005)
Lecture 6-7 (2/17/05-2/24/05)

Further Discussions: Monte Carlo in Statistical Physics and Radiation Transport

There are two versions of MC – one is for *Statistical Physics* and the other for *Radiation Transport*. Each is used by a large and active community. Curiously the two communities have little to do with each. This is, however, NOT the attitude we want to promote in this class. We would like to understand the reasons why MC is useful for each type of problems, anticipating that the students are likely to encounter problems of both types in their future studies and research. We recognize also that in this department the students may have more reasons to be interested in *Radiation Transport* as the application of Monte Carlo. This is only natural since most of the research in the department have to do with particle transport rather than with statistical physics.

Even though statistical physics may not be so familiar to our students one should at least have rough ideas about this area of study. Statistical physics (also statistical mechanics) is that branch of science concerned with the description of physical matter, such as solids and liquids, in terms of the constituent particles. The systems of interest are composed of atoms which interact *strongly* with each other, forming phases of matter that we commonly classify as solid, liquid, and gas. Each state of matter has physical properties that we wish to understand more deeply. For example, we might ask (1) at what equilibrium conditions of density, temperature, and pressure does a simple material, say carbon, exist as a solid, and (2) under what conditions does the solid melt into a liquid? To answer questions of this type we need to study the stability of the various phases, expressed in relations known as equations of state (or phase diagram), as well as what happens when a particular phase transforms into another one. A basic objective in statistical physics is therefore to develop the fundamental understanding of how the various physical properties of matter are related to the underlying interactions between the constituent particles. In other words, if we knew the interactions between a pair of carbon atoms (potential energy as a function of their separation distance), can we predict

the properties bulk carbon which contains a large number of atoms? (Notice that this question is not unlike asking to predict the cumulative effects of many collisions given that the effect of a single collision is known.)

Moving Uphill in MC Sampling

Since we will not spend too much time on statistical physics, we want to emphasize that the Metropolis sampling procedure is at the heart of MC-Stat Phys simulation. Why is this? Stated simply, many problems in MC involve the search for the ground-state of the system, that set of atomic positions at which the system energy is a minimum. In this discussion it is understood that all physical systems prefer states that are low in potential energy over states high in the potential energy. If a system happens to find itself in a high energy state, it will do all it can to find a path to transform to a lower energy state. By this argument, the ground state of a system is the equilibrium state. When we speak of properties of a system, often we are interested first in the equilibrium properties, properties of the system at equilibrium or the ground state. But this is not always true. There are nonequilibrium properties that are also of interest, for example, the properties of a piece of material that has been exposed to radiation and is therefore no longer in the ground state.

When we speak of the potential energy of the system we can imagine that an undulating energy surface in the hyperspace of the particle positions. If the system is at a local minimum, then in order to reach an even lower energy-minimum somewhere else, it needs to surmount the surrounding barriers. Without going uphill the system cannot go downhill to reach that lower energy-minimum some distance away. This means that as the system moves around in the hyperspace, every now and then it has to be able to *move uphill* to surmount the local barriers. This then is the special feature of the Metropolis procedure, as represented by step 4.

Particle Interactions in Statistical Physics and Radiation Transport

While particle interactions are the underlying processes that determine the system behavior in both areas of studies, there is a distinction that should be spelled out at the outset. In statistical physics by particle interactions we mean the potential energy

function $U(\{\underline{R}_N\})$. If the potential were a quadratic function of the coordinates, then we have a system of oscillators, where the force between two oscillators is a linear function of their separation. (Recall that force is the derivative of the energy.) For this idealized system we can find exact solutions. For all other cases of interest the potential is a much more complicated function of the particle separations, for example, a well-known potential which we will discuss more in detail later, is of the form

$$U(\{\underline{R}_N\}) = \frac{1}{2} \sum_{i \neq j} V(r_{ij}) \quad (6-7.1)$$

with

$$V(r) = 4\sigma \left[\left(\frac{\varepsilon}{r} \right)^{12} - \left(\frac{\varepsilon}{r} \right)^6 \right] \quad (6-7.2)$$

In (6-7.1) we write the potential as a sum of pairwise (two-body) potential, with i and j being the particle indices, and r_{ij} being the separation distance between particles i and j , $r_{ij} = |\underline{r}_i - \underline{r}_j|$. This approximation is not always valid, but for many problems, including the description of phase transitions such as the melting of a solid and the boiling of a liquid, it is quite adequate. In (6-7.2) we show the two-body interaction to be repulsive at short separation and attractive at large separation. This is the basic behavior of all interatomic interactions as we will come back to discuss later. For now, it is sufficient to note that $V(r)$ is highly *nonlinear*. So in statistical physics we are generally interested in nonlinear particle interactions.

In radiation transport by interactions we mean the scattering or reaction between the radiation particle, say a neutron or a photon, and the nuclei and atoms in the medium. *What is neglected are the interactions between the radiation particles*, always justified by an estimate of the mean free path for neutron-neutron collision. Because the radiation particle density is very low, a typical mean free path for a neutron to collide with another neutron is so large compared to any physical system size that one is quite safe in ignoring

the interactions between the radiation particles. As a result, radiation transport is a linear problem in the sense that any equation describing the transport processes is linear in the radiation particle density (distribution function). This is the case for MCNP and for the neutron transport equation, the fundamental equation governing all reactor physics calculations – they are linear. The same statement should not be applied to the problem of gas dynamics where, like the statistical physics problems, the interactions between the gas atoms are nonlinear.

Sampling Distributions in Radiation Transport

Since in radiation transport the idea is to follow the radiation particle as it makes its way through the medium, we can apply the previous method of sampling distributions to sample the outcome of a collision. To determine how far a radiation particle should travel before the next collision, we construct the probability distribution for traversing a distance ℓ before the collision,

$$p(\ell) = \Sigma e^{-\Sigma \ell} \quad (6-7.3)$$

where $\Sigma = N\sigma$ is the macroscopic cross section, N the number density of the target nuclei and σ is the microscopic cross section. One can check that (6-7.3) is normalized over the range $(0, \infty)$. The corresponding cumulative distribution is

$$P(\ell) = \int_0^{\ell} p(t) dt = 1 - e^{-\Sigma \ell} \quad (6-7.4)$$

Setting this equal to a random number ξ we obtain a value for the mean free path,

$$\ell = -\frac{1}{\Sigma} \ln \xi \quad (6-7.5)$$

In writing this result we have taken $\ell n(1 - \xi) = \ell n\xi$ because if ξ is uniformly distributed, so is $1 - \xi$. Using (6-7.5) repeatedly one generates a set of mean free paths according to the distribution (6-7.3).

The same procedure can be applied to determine the polar and azimuthal angles of the outgoing particle after an interaction. Suppose the emission of the particle is spherically symmetric. One can write

$$p(\theta, \varphi) = p_1(\theta)p_2(\varphi) \quad (6-7.6)$$

After constructing the appropriate probability distributions for p_1 and p_2 , one obtains

$$\mu_i = 2\xi_i - 1, \quad \varphi_i = 2\pi\xi_i \quad (6-7.7)$$

where $\mu = \cos\theta$. In the case of energy transfer after an elastic scattering collision where the target nucleus is at rest and the scattering is isotropic in CMCS, we have a distribution that is given by $F(E \rightarrow E')$,

$$F(E \rightarrow E') = \begin{cases} \frac{1}{E(1-\alpha)} & \alpha E \leq E' \leq E \\ 0 & \text{otherwise} \end{cases} \quad (6-7.8)$$

One then finds

$$E'_i = E(1-\alpha)\xi_i + \alpha E \quad (6-7.9)$$

The details of these calculations are left as exercise for the reader.