7.10 Variational Methods

Consider a random number generator with a relatively short period and strong sequential correlation and show that this shuffling scheme improves the quality of the random number sequence.

At least some of the statistical tests given in Problem 7.35 should be done whenever serious calculations are contemplated. However, even if a random number generator passes all these tests, there can still be problems in rare cases. Typically, these problems arise when a small number of events have a large weight. In these cases a very small bias in the random number generator might lead to systematic errors, and two generators, which appear equally good as determined by various statistical tests, might give statistically different results in a specific application (see Project 15.34). For this reason it is important that the particular random number generator that was used be reported along with the actual results. Confidence in the results can also be increased by repeating the calculation with another random number generator.

Because all random number generators are based on a deterministic algorithm, it is always possible to construct a test generator for which a particular algorithm will fail. The success of a random number generator in passing various statistical tests is necessary, but it is not a sufficient condition for its use in all applications. In Project 15.34 we discuss an application of Monte Carlo methods to the Ising model for which some popular random number generators give incorrect results.

7.10 ■ VARIATIONAL METHODS

Many problems in physics can be formulated in terms of a variational principle. In the following, we consider examples of variational principles in geometrical optics and classical mechanics. We then discuss how Monte Carlo methods can be applied to these problems. A more sophisticated application of Monte Carlo methods to a variational problem in quantum mechanics is discussed in Chapter 16.

Our everyday experience of light leads naturally to the concept of light rays. This description of light propagation, called *geometrical* or *ray optics*, is applicable when the wavelength of light is small compared to the linear dimensions of any obstacles or openings. The path of a light ray can be formulated in terms of Fermat's principle of least time: A ray of light follows the path between two points (consistent with any constraints) that requires the least amount of time. Fermat's principle can be adopted as the basis of geometrical optics. For example, Fermat's principle implies that light travels from a point A to a point B in a straight line in a homogeneous medium. Because the speed of light is constant along any path within the medium, the path of shortest time is the path of shortest distance, that is, a straight line from A to B. What happens if we impose the constraint that the light must strike a mirror before reaching B?

The speed of light in a medium can be expressed in terms of c, the speed of light in a vacuum, and the index of refraction n of the medium:

$$v = \frac{c}{n}. (7.63)$$

Suppose that a light ray in a medium with index of refraction n_1 passes through a second medium with index of refraction n_2 . The two media are separated by a plane surface. We

now show how we can use Fermat's principle and a simple Monte Carlo method to find the path of the light. The analytical solution to this problem using Fermat's principle is found in many texts (cf. Feynman et al.).

Our strategy, as implemented in class Fermat, is to begin with a straight path and to make changes in the path at random. These changes are accepted only if they reduce the travel time of the light. Some of the features of Fermat and FermatApp include:

- 1. Light propagates from left to right through N regions. The index of refraction n[i] is uniform in each region [i]. The index i increases from left to right. We have chosen units such that the speed of light in a vacuum equals unity.
- 2. Because the light propagates in a straight line in each medium, the path of the light is given by the coordinates y[i] at each boundary.
- 3. The coordinates of the light source and the detector are at (0,y[0]) and (N,y[N]), respectively, where y[0] and y[N] are fixed.
- 4. The path is the connection of the set of points at the boundary of each region.
- 5. The path of the light is found by choosing the boundary i at random and generating a trial value of y[i] that differs from its previous value by a random number between -dy to dy. If the trial value of y[i] yields a shorter travel time, this value becomes the new value for y[i].
- 6. The path is redrawn whenever it is changed.

Listing 7.6 Fermat class.

```
package org.opensourcephysics.sip.ch07;
public class Fermat {
                   // y coordinate of light ray, index is x coordinate
   double v[]:
   // light speed of ray for medium starting at index value
   double v[]:
                   // number of media
   int N:
   // change in index of refraction from one region to the next
   double dn;
   double dy = 0.1: // maximum change in y position
   int steps;
   public void initialize() {
      y = new double[N+1];
      v = new double[N];
      double indexOfRefraction = 1.0;
      for(int i = 0:i \le N:i++) {
        y[i] = i; // initial path is a straight line
      for(int i = 0:i < N:i++) {
        v[i] = 1.0/indexOfRefraction;
        indexOfRefraction += dn;
      steps = 0:
   public void step() {
      int i = 1+(int) (Math.random()*(N-1));
      double yTrial = y[i]+2.0*dy*(Math.random()-0.5);
```