References

Ch. 3 in D.E. Knuth, "The art of computer programming" vol. 2, Addison-Wesley, 1981
W.H. Press, et. al. Numerical Recipes in FORTRAN (also avail. in C), 2nd Ed. Cambridge
U. Press, 1992 (available electronically)

"Anyone who considers arithmetic methods of producing random numbers as, of course, in a state of sin"
John von Neumann (1951)

Uses of "Random" Numbers

- Simulation, Sampling, Numerical analysis, Recreation, decision making (e.g. assigning grades - is "3" random?)

Need a sequence of numbers that satisfy certain statistical properties

Mechanical: Dice, roulette etc still in use
Random Physical Processes: e.g. radioactive decay can be used to generate "truly random" numbers

Disadvantages: 1) Impossible to reproduce calculations
               2) Speed/ convenience

Numerical methods on computers: "pseudorandom"

Sequences that satisfy most statistical tests of randomness

Generating Uniform Random Numbers

Simple, effective method: Linear congruential

\[ x_{n+1} = (a \cdot x_n + c) \mod (m) \]

produces numbers between 0 and m-1
Example: \( m = 2^4 = 16 \) \( a = 13 \) \( c = 1 \)
\[\begin{array}{cccccccccccccccc}
1 & 2 & 3 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
\times n & 10 & 3 & 8 & 9 & 15 & 4 & 5 & 2 & 11 & 9 & 1 & 47 & 12 & 13 & 10 \\
\end{array}\]

Cycle = 16 always \( \leq m \)

Practical Example: "Minimal Standard" ran\( \Phi \)
\( a = 7^5 = 16807 \) \( m = 2^{31} - 1 = 2147483647 \) \( c = 0 \)
Period \( = 2^{31} - 2 \approx 2.1 \times 10^9 \)

Spectral test in \( n \) dimensions:
Generate \( n \) random numbers in sequence, place on corresponding "cell" in \( n \)-dimensional box:

\( x \)
\( y \uparrow \)

Fraction of empty cells should decrease as \( e^{-t} \) \( t \) is number of "passes" over the lattice

Simple "minimal standard" generator is said to "fill the spectral test for 2 dimensions for \# of samples > \( O(10^3) \), much less than the period" \( \rightarrow \) low order serial correlations are present[Num. Recipes Book]. More sophisticated algorithms:

\( \rightarrow \) "shuffle" output so that the random number is picked from a short table with e.g. 32 entries. This removes low-order correlations
Combine two different sequences so that the new sequence has a period equal to the least common multiple of the two periods:

\[ I_{j+1} = [\alpha_1 I_j \mod(m_1) + \alpha_2 I_j \mod(m_2)] \mod (m) \]

E.g. generator ran2 in Numerical recipes has period \( \approx 2.3 \times 10^{18} \), uses shuffling to remove low-order correlations.

From a uniformly distributed sequence, any other "random" function can be recovered.

**Application Issues**

Consider \( N_2 \), suppose we want to model it as a two-center Lennard-Jones system connected by a harmonic spring, with

\[ U_b = \frac{1}{2} k (r - r_0)^2 \quad k > 0 \]

**Problem:** Generate a "random" configuration in a cubic box of length \( L \times L \times L \), representative of the state of the system at a certain temperature \( T \).

- Placing the first atom is relatively straightforward.

- Placing the second atom is not as easy:

\[ x = L \times \text{ran8()} \quad y = L \times \text{ran8()} \quad z = L \times \text{ran8()} \]
In principle, one could place the second atom at a random position in the box, but the resulting configuration (almost always) will have a very high bond energy $U_b$. Still, to generate configurations representative of the state at temp. $T$, we can accept or reject the result with probability

$$\exp\left(-\frac{U_b}{kT}\right) \rightarrow \text{generate random number } \text{rand}()$$

compare to $\exp(-B_U)$, if $\text{rand} > \exp(-B_U)$, reject, if $\text{rand} \leq \exp(-B_U)$, accept.

More effective method: generate bond lengths with the correct probability distribution:

Find the maximum and minimum possible bond lengths $r_0 + \Delta r$, $r_0 - \Delta r$ by setting a "cutoff" probability

$$P = 10^{-10} = \exp\left(-\frac{kT(\Delta r)^2}{2kT}\right)$$

Generate bond lengths in the interval $r_0 - \Delta r$, $r_0 + \Delta r$ uniformly? No!

Probability of a certain bond length must be proportional to $r^2$! The available volume for placing a second atom is more at longer distances!

$\rightarrow$ Generate a number uniformly distributed in the interval $(r_0 - \Delta r)^3$ to $(r_0 + \Delta r)^3$

$\rightarrow$ Take cube root: $P = \text{rand}()$

$$\delta r = \sqrt[3]{(r_0 - \Delta r)^3(1 - P) + P \cdot (r_0 + \Delta r)^3 - r_0}$$
\( \rightarrow \) Compute \( \exp \left( -\frac{E(G)}{k_B T} \right) \), accept or reject configuration.

\( \rightarrow \) Generate new center position on surface of a sphere of radius \( r_0 + \delta r \):

[Similar to ranor, algorithm 42 in f+s]

\[
\text{ranSQ} = 2.
\]

\[
do \text{while} \quad \text{ranSQ} \geq 1 \\
\quad \text{ran1} = 1 - 2 * \text{ranF}(\cdot) \\
\quad \text{ran2} = 1 - 2 * \text{ranF}(\cdot) \\
\quad \text{ranSQ} = \text{ran1} * \text{ran1} + \text{ran2} * \text{ran2}
\end{do}

enddo

\[
\text{ranH} = 2 * \text{sqrt}(1 - \text{ranSQ})
\]

\[
x_2 = x_1 + \text{ran1} * \text{ranH} * (r_0 + \delta r)
\]

\[
y_2 = y_1 + \text{ran2} * \text{ranH} * (r_0 + \delta r)
\]

\[
z_2 = z_1 + (r_0 + \delta r) * (1 - 2 * \text{ranSQ})
\]

Any alternatives?
Generating the normal (Gaussian) Distribution

For zero mean and unit variance,

\[ p(x) = \frac{1}{\sqrt{2\pi}} \exp \left(-\frac{x^2}{2}\right) \]

(a) generate uniform random numbers \( z_1, z_2 \) in \((0,1)\)

(b) \( j_1 = (2z_1)^{\frac{1}{2}} \cos 2\pi z_2 \), \( j_2 = (2z_1)^{\frac{1}{2}} \sin 2\pi z_2 \)

\( j_1, j_2 \) are normally distributed

A small variation of this is Algorithm 44 in FFS

(from Numerical Recipes)

\( r=2 \)

\( \text{do while (r.ge.2.)} \)

\( \text{v1 = 2.*ran8()-1.} \)

\( \text{v2 = 2.*ran8()-1.} \)

\( r = \text{v1}^2 + \text{v2}^2 \)

\( \text{end do} \)

\( l = \text{v1} * \text{sqrt} (-2.* \text{log} (r)/r) \)