

5.2 INITIALIZATION

With a form chosen for the model potential, we can turn to the use of the model in a molecular dynamics simulation. For the chosen model, a simulation generates a portion of the phase-space trajectory, and as shown in Figure 5.6, trajectory generation involves initialization, equilibration, and production. In this section we consider initialization, which we divide into two parts: decisions concerning preliminaries and initialization of the atoms. The preliminaries include a system of units in which the calculation will be carried out, the finite-difference algorithm to be used, and assignment of values to parameters that remain constant during a run. The preliminaries are discussed in Section 5.2.1. Initialization of the atoms means assignment of initial positions, initial velocities, and (perhaps) initial values for higher derivatives of the positions. These assignments are discussed in Section 5.2.2.

5.2.1 Preliminaries

System of Units. Simulation programs are conventionally written so that all quantities are unitless. As units of distance and energy we use the potential parameters σ and ϵ , respectively, and as the unit of mass, that of one atom.

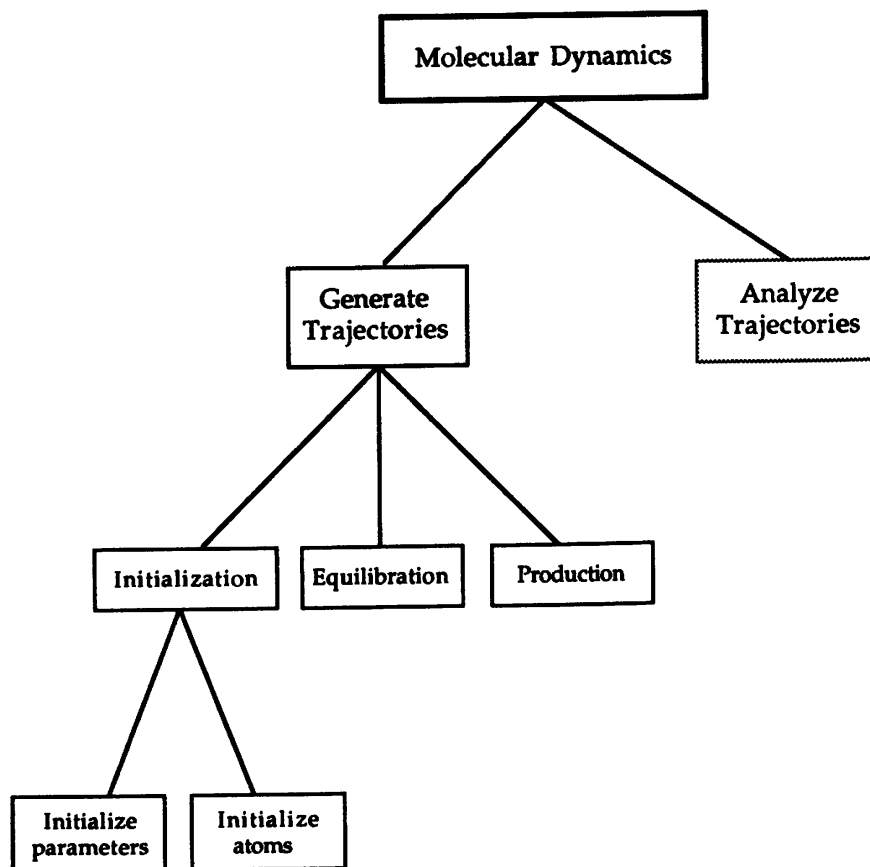


FIGURE 5.6 Trajectory generation divides into initialization, equilibration, and production.

TABLE 5.2 System of Units^a Used in Soft-Sphere Molecular Dynamics Programs*Fundamental Quantities*

Mass	$m = \text{mass of one atom}$
Length	σ
Energy	ε
Time	$\sigma\sqrt{m/\varepsilon}$

Derived Quantities

Adiabatic compressibility	$\kappa_s^* = \kappa_s \varepsilon / \sigma^3$
Configurational internal energy	$U_c^* = U_c / N\varepsilon = \langle \mathcal{U}^* \rangle = \langle \mathcal{U} / N\varepsilon \rangle$
Density	$\rho^* = N\sigma^3 / V$
Force	$F^* = F\sigma / \varepsilon$
Heat capacity	$C_v^* = C_v / Nk$
Radial position	$r^* = r / \sigma$
Pressure	$P^* = P\sigma^3 / \varepsilon$
Temperature	$T^* = kT / \varepsilon$
Thermal pressure coefficient	$\gamma_v^* = \gamma_v \sigma^3 / k$
Total energy	$E^* = E / N\varepsilon$
Velocity	$v^* = v\sqrt{m/\varepsilon}$

^aW. Thomson, Lecture XVI, p. 158: "The distinguishing feature of an engineer is the quickness with which he can reduce from square feet to acres, and so on. If his brain were free from that, he might do more elsewhere, and have more time to find out about the properties of matter."

The unitless (or reduced) forms for quantities are indicated by an asterisk; for example, (5.4) for the Lennard-Jones potential becomes

$$u^*(r^*) = 4 \left[\left(\frac{1}{r^*} \right)^{12} - \left(\frac{1}{r^*} \right)^6 \right] \quad (5.19)$$

where $u^* = u/\varepsilon$ and $r^* = r/\sigma$. The reduced forms for other derived quantities are given in Table 5.2.

State Condition. For equilibrium molecular dynamics performed on isolated systems, the independent thermodynamic properties are the number of molecules N , system volume V , and total energy E . Then for a one-phase system, specifying values for the number density $\rho^* = N\sigma^3/V$ and the energy per atom $E^* = E/N\varepsilon$ determines the thermodynamic state. Usually, $100 < N < 1000$, with the particular value of N taken to be large enough to properly capture the phenomena of interest yet small enough to prevent the simulation from being prohibitively expensive. Having picked N , the required value of V is obtained from the assigned density ρ^* .