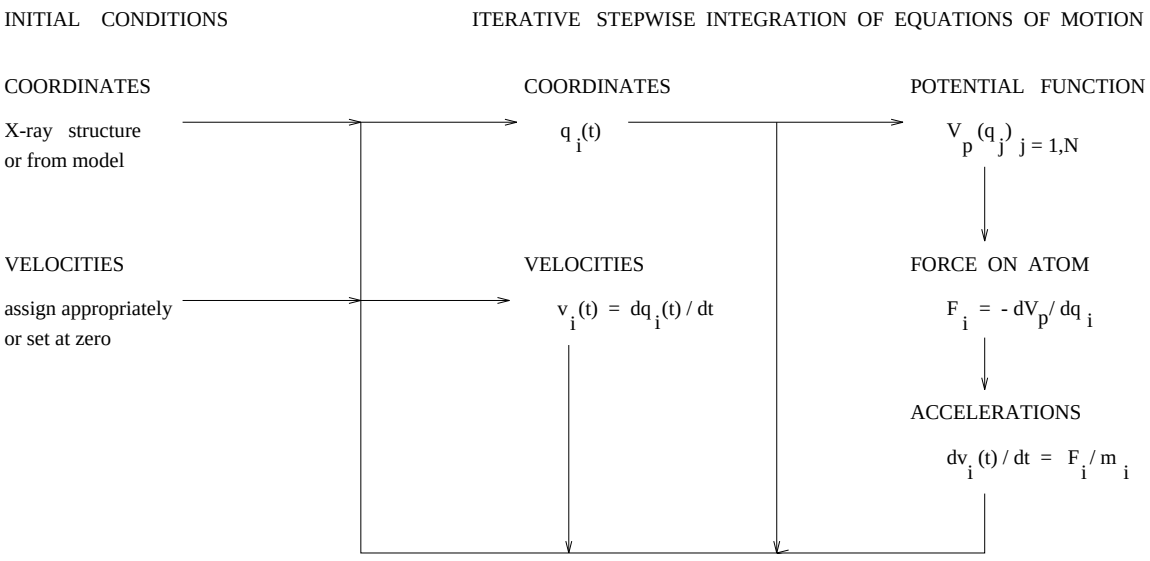
NOTES ON
MOLECULAR DYNAMICS SIMULATION



SCHEME I -- STRATEGY

At each time step new values of the positions q_i and velocities $\dot{q}_i$ for each particle in the system are calculated from the current values of the positions and velocities.

The sequence of values of q_i and $\dot{q}_i$ define the functions $q_i(t)$ and $\dot{q}_i(t)$ and constitute the trajectory of the system, i.e., the description of the motion of the system, of how it changes and fluctuates in time.

The procedure for updating the q_i and $\dot{q}_i$ is outlined in Scheme I.

Estimation of new values of the positions and velocities requires, in addition to the current values of the positions and velocities, values of the accelerations, $\ddot{q}_i = d\dot{q}_i/dt$, for each particle.

The acceleration for the ith particle is calculated from Newton's equation of motion,

$$\ddot{q}_i = \frac{F_i}{m_i} \tag{1}$$

where m_i is the mass of the ith particle and F_i is the force on it. F_i is calculated as the gradient of the potential energy,

$$F_i = -\frac{\partial V_p}{\partial q_i} \tag{2}$$

The potential function V_p takes into account interactions between the various atoms or groups of the macromolecule. It is a function of the coodinates, q_i. Typical potential functions are discussed in Chapter III of BKP and on page 999 of vanG&B. Because the positions q_i are functions of the time, V_p, F_i, and $\ddot{q}_i$ are also functions of the time and must be computed for each new set of values of q_i, i.e., for each time step.

There are various algorithms for calculating new values of the positions and velocities from the current positions and velocities and the accelerations. For a brief discussion see page 51 of BKP and page 1010 of vanG&B. The leap-frog scheme is relatively simple (vanG&B, page 1010): the position at the end of the next time step is calculated as

$$q_i(t+\Delta t) = q_i(t) + \dot{q}_i(t+\frac{\Delta t}{2})\ \Delta t \tag{3}$$

The second term of the rhs of eqn (3) contains the new estimate of the velocity, at the midpoint of the time step, calculated as

$$\dot{q}_i(t+\frac{\Delta t}{2}) = \dot{q}_i(t-\frac{\Delta t}{2}) + \ddot{q}_i(t)\ \Delta t \tag{4}$$

The first term on the rhs of eqn (4) is the current estimate of the velocity, at the midpoint of the last time step; the second rhs term contains the current estimate of the acceleration calculated as described above.

Thus one has integrated Newton's equation of motion, calculating new values for q_i and $\dot{q}_i$ for times Δt and $\Delta t/2$ beyond the current time. To obtain an accurate integration, the time step Δt is kept small, ca. 10^{-15} second, which is small compared to the characteristic times for atom motions.

The relationship between the kinetic energy of the system at time *t*, $T_k(t)$, the masses and velocities of the particles, m_i and $\dot{q}_i(t)$, and the temperature of the system at time *t*, $T(t)$, is discussed in BKP(page 34) and vanG&B (page 1008) and is given by

$$T_k(t) = \sum_{i=1}^{N} \frac{1}{2} m_i \dot{q}_i^2(t) = \frac{3}{2} N k_B T(t) \qquad (5)$$

where N is the number of particles in the system, or the number of degrees of freedom if there are constraints on the motion.

The initial conditions chosen for the coordinates and velocities of each atom are unlikely to be near the equilibrium values for the temperature desired. Equilibration of the system by interation for a number of time steps allows calculation of the temperature corresponding to the initial conditions. The velocities can then be scaled appropriately for bringing the system to within some range of a specified temperature.