1 A different view of the Verlet update

We wish now to give a new look at the Verlet transformation, that is useful when discussing more general algorithms. From a theoretical point of view the transformation is obtained by combining two distinct transformations $\exp(iL_p t)$ and $\exp(iL_q t)$. We wish to discuss these two transformations in more detail.

The operator L_p can be viewed as a Liouvillian associated with the Hamiltonian $H(p,q) = U(q)$. The operator $\exp(iL_p t)$ generates the transformation

$$Q = q \qquad\qquad P = p + F(q)t;$$

It is quite easy to verify that this transformation is canonical with $H_2(P,Q) = H(p(P,Q), q(P,Q)) = H(P - F(Q)t, Q) = U(Q) = H(P,Q)$. As we have discussed in the previous lesson this implies

$$iL_p(q,p)A(Q(q,p), P(q,p)) = [iL_p(Q,P)A(Q,P)]_{Q=Q(q,p),P=P(q,p)}\,.$$

The same argument applies to L_q, which is a Liouvillian associated with $H(p,q) = p^2/(2m)$. The operator $\exp(iL_q t)$ generates the transformation

$$Q = q + \frac{pt}{m} \qquad\qquad P = p;$$

It is quite easy to verify that the transformation is canonical with $H_2(P,Q) = H(p(P,Q), q(P,Q)) = H(P, Q - Pt/m) = P^2/(2m) = H(P,Q)$. As we have discussed in the previous lesson, this implies

$$iL_q(q,p)A(Q(q,p), P(q,p)) = [iL_q(Q,P)A(Q,P)]_{Q=Q(q,p),P=P(q,p)}\,.$$

We can thus reinterpret the three steps that are relevant for the Verlet dynamics as follows. Suppose that the system is in point q_0, p_0 at time t. The first step is

$$\begin{pmatrix} p_1 \\ q_1 \end{pmatrix} = \left[\exp[iL_p(q,p)\Delta t/2] \begin{pmatrix} p \\ q \end{pmatrix}\right]_{q=q_0,p=p_0}$$

The second step corresponds to

$$\begin{pmatrix} p_2 \\ q_2 \end{pmatrix} = \left[\exp[iL_q(q,p)\Delta t]\; \exp[iL_p(q,p)\Delta t/2] \begin{pmatrix} p \\ q \end{pmatrix}\right]_{q=q_0,p=p_0}$$

which can be rewritten as

$$\begin{pmatrix} p_2 \\ q_2 \end{pmatrix} = \left[\exp[iL_q(q,p)\Delta t]\; \begin{pmatrix} p_1(q,p) \\ q_1(q,p) \end{pmatrix}\right]_{q=q_0,p=p_0}$$

Now, we use the relations we have proved to rewrite this expression as

$$\begin{pmatrix} p_2 \\ q_2 \end{pmatrix} = \left[\exp[iL_q(Q,P)\Delta t]\; \begin{pmatrix} P \\ Q \end{pmatrix}\right]_{Q=q_1,P=p_1}$$

The last step is dealt analogously so that

$$\begin{pmatrix} p_3 \\ q_3 \end{pmatrix} = \left[\exp[iL_p(Q,P)\Delta t/2] \begin{pmatrix} P \\ Q \end{pmatrix}\right]_{Q=q_2,P=p_2}$$

Of course, $p(t+\Delta t) = p_3$ and $q(t+\Delta t) = q_3$.

This argument allows us to rewrite the update in the following way:

a) We set $q_0 = q(t)$ and $p_0 = p(t)$;

b) We apply $\exp[iL_p(q,p)\Delta t/2]$ and set $q_1 = q_0$ and $p_1 = p_0 + \frac{1}{2}F(q_0)\Delta t$;

c) We apply $\exp[iL_q(q,p)\Delta t]$ and set $q_2 = q_1 + \frac{p_1}{m}\Delta t$ and $p_2 = p_1$;

d) We apply $\exp[iL_p(q,p)\Delta t/2]$ and set $q_3 = q_2$ and $p_3 = p_2 + \frac{1}{2}F(q_2)\Delta t$;

e) We set $p(t + \Delta t) = p_3$ and $q(t + \Delta t) = q_3$.

It is trivial to verify that we reobtain the standard Verlet transformation if we eliminate the intermediate variables q_1, q_2, p_1, and p_2. This approach is convenient when we approximate the evolution operator in terms of many factors. The multiple-time step algorithms represent a typical example.