2.3 Integration schemes

We discuss, in this section, some of the algorithms that can be used to integrate Newton's equations of motion for an N-body system. One common technique develops low order solutions using the time Taylor series expansion of the position and the velocity $\vec{r}_i, \vec{v}_i$ around $\Delta t = 0$. A more general technique, called Trotter expansion, uses the so-called Liouville operator. Other integration schemes may be used and we will briefly discuss advantages and disadvantages.

2.3.1 Euler algorithm

Consider a Taylor expansion of the particle trajectories, truncated to the third order, so that we retain all the terms with a physical significance

$$\vec{r}(t+\Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2 + O(\Delta t^3) \tag{2.29}$$

This is the so-called Euler algorithm. It is much worse with respect to all the other algorithms that will derived later on virtually all accounts. In particular, it is not reversible or area preserving and suffers from severe energy drifts. It is not recommended.

2.3.2 Verlet Algorithm

The simplest (but good) integration scheme is the Verlet algorithm. Consider the Taylor expansion up to the fourth order for $\vec{r}_i(t+\Delta t)$ and $\vec{r}_i(t-\Delta t)$:

$$\begin{aligned}
\vec{r}_i(t+\Delta t) &= \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2}\vec{a}_i(t)\Delta t^2 + \frac{1}{6}\frac{d^3\vec{r}_i(t)}{dt^3}\Delta t^3 + O(\Delta t^4) \\
\vec{r}_i(t-\Delta t) &= \vec{r}_i(t) - \vec{v}_i(t)\Delta t + \frac{1}{2}\vec{a}_i(t)\Delta t^2 - \frac{1}{6}\frac{d^3\vec{r}_i(t)}{dt^3}\Delta t^3 + O(\Delta t^4)
\end{aligned} \tag{2.30}$$

with $\vec{v}_i(t) = d\vec{r}_i/dt$ and $\vec{a}_i(t) = d^2\vec{r}_i/dt^2$ that, when summed up and rearranged, gives

$$\vec{r}_i(t+\Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t-\Delta t) + \vec{a}_i(t)\Delta t^2 + O(\Delta t^4) \tag{2.31}$$

The positions are accurate up to the fourth order in Δt. Note that the velocities are not calculated explicitly in this procedure but can be derived knowing the trajectory

$$\vec{v}_i(t) = \frac{\vec{r}_i(t+\Delta t) - \vec{r}_i(t-\Delta t)}{2\Delta t} + O(\Delta t^2) \tag{2.32}$$

which is accurate only up to order Δt^2. Hence, quantities depending on the velocity are not so accurate. Further, the position of the particles at $t+\Delta t$ depends on the position at time t as well as at time $t-\Delta t$. As such, we have a problem of initialization: we cannot directly apply Eq. (2.31) using standard initial conditions, i.e. a set of coordinates and velocities. As for other "high order" numerical solvers, the problem is solved by using lower order solvers for the first step, such as, given $\vec{r}_i(0)$ and $\vec{v}_i(0)$,

$$\vec{r}_i(\Delta t) \approx \vec{r}_i(0) + \vec{v}_i(0)\Delta t + \frac{\vec{a}_i(0)}{2}\Delta t^2 \tag{2.33}$$

where $\vec{a}_i(0)$ should be computed from the coordinates $\vec{r}_i(0)$. Once this approximate step is done, the forces (hence $\vec{a}_i(\Delta t)$) can be calculated and Eq. (2.31) can be used iteratively. The technique just presented turns

out to be appropriate for obtaining algorithms that are accurate to second order in time for Hamiltonian systems and that preserves the time reversal symmetry of the equation of motions. If, on the other hand, higher order in accuracy is requested, this technique requires spatial derivatives of forces that are in general computationally expensive. Moreover, when applied to non-Hamiltonian systems the Taylor series approach generally yields schemes which do not preserve the invariant phase space measure.

2.3.3 Leap Frog Algorithm

Several algorithm are equivalent to the Verlet scheme. The simplest among these is the so-called Leap Frog algorithm, that evaluates the velocity at half-integer steps and uses these velocities to compute the new positions. To derive the algorithm from the Verlet scheme, we start by defining the velocities at half-integer time steps at follows:

$$\begin{aligned} \vec{v}(t - \Delta t/2) &\equiv \frac{\vec{r}(t) - \vec{r}(t - \Delta t)}{\Delta t} \\ \vec{v}(t + \Delta t/2) &\equiv \frac{\vec{r}(t + \Delta t) - \vec{r}(t)}{\Delta t} \end{aligned} \tag{2.34}$$

From the latter equation we obtain an expression for the new positions, based on the old positions and velocities

$$\vec{r}(t + \Delta t) = \vec{r}(t) + \vec{v}(t + \Delta t/2)\Delta t \tag{2.35}$$

and from the Verlet algorithm we get an expression for the update of the velocities

$$\vec{v}(t + \Delta t/2) = \vec{v}(t - \Delta t/2) + \frac{f(t)}{m}\Delta t \tag{2.36}$$

As the Leap Frog algorithm is derived from the Verlet, it gives rise to identical trajectories. Note that the velocities are not defined at the same time as the positions. This means that kinetic and potential energy are not defined at the same time, and hence we cannot compute the total energy directly in the Leap From scheme.

2.3.4 Velocity Verlet Algorithm

An alternative recast of the algorithm, where positions and velocity are simultaneously updated, is the Velocity Verlet. This algorithm will look like a Taylor expansion, with a different update of the velocity with respect to the Euler scheme.

$$\vec{r}(t + \Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t + \frac{\vec{f}(t)}{2m}\Delta t^2 \tag{2.37}$$

$$\vec{v}(t + \Delta t) = \vec{v}(t) + \frac{\vec{f}(t) + \vec{f}(t + \Delta t)}{2m}\Delta t \tag{2.38}$$

Note that we compute the new velocities only after we have computed the new positions and, from these, the new forces.
The velocity Verlet can be translated into the following pseudo-code:

- A momentum translation by an amount (**half a kick**)

$$\vec{p}(t) + \frac{\Delta t}{2}\vec{f}(t) \longrightarrow \vec{p}(t + \Delta t/2) \tag{2.39}$$

- A position translation by an amount (**drift**)

$$\vec{r}(t) + \Delta t\vec{v}(t + \Delta t/2) = \vec{r}(t) + \frac{\vec{p}(t)}{m}\Delta t + \frac{\vec{f}(t)}{2m}\Delta t^2 \tag{2.40}$$

  using the momentum obtained in step 1.

- Computation of the forces for $\vec{r} = \vec{r}(t + \Delta t)$.

- A momentum translation by an amount (**half a kick**)

$$\vec{p}(t + \Delta t/2) + \frac{\Delta t}{2}\vec{f}(t + \Delta t) \longrightarrow \vec{p}(t + \Delta t) \tag{2.41}$$

The physical interpretation is that two impulses of equal size are imparted to the particles just before and just after each time t and that between these time points the particles drift with constant velocity.
We will derive the algorithm later; we show now that the scheme is equivalent to the Verlet algorithm. Note that

$$\vec{r}(t + 2\Delta t) = \vec{r}(t + \Delta t) + \vec{v}(t + \Delta t)\Delta t + \frac{\vec{f}(t + \Delta t)}{2m}\Delta t^2 \tag{2.42}$$

and Eq. (2.37) can be written as

$$\vec{r}(t) = \vec{r}(t + \Delta t) - \vec{v}(t)\Delta t - \frac{\vec{f}(t)}{2m}\Delta t^2 \tag{2.43}$$

and by addition we have

$$\vec{r}(t + 2\Delta t) + \vec{r}(t) = 2\vec{r}(t + \Delta t) + (\vec{v}(t + \Delta t) - \vec{v}(t))\,\Delta t + \frac{\vec{f}(t + \Delta t) - \vec{f}(t)}{2m}\Delta t^2 \tag{2.44}$$

Substitution of Eq.(2.38) yields the Verlet algorithm.

2.3.5 Velocity Verlet Algorithm: Trotter expansion

A different approach is based on the Liouville operator formulation of classical mechanics and it is the one we will discuss here. Let us focus first on Hamiltonian systems only. We now that these systems are characterized by certain fundamental properties such as the symplectic property and time reversibility. For simplicity let us begin by examining a simple one-particle system in one dimension for which the equation of motion are

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} = F(q(t)). \tag{2.45}$$

Recall that any function $O(q, p)$ evolves in time according to

$$\frac{dO}{dt} = \{O, H\} \tag{2.46}$$

where the Poisson brackets are

$$\{O, H\} = \frac{\partial O}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial O}{\partial p}\frac{\partial H}{\partial q}. \tag{2.47}$$

Clearly, if $O(q, p) = q$ we have

$$\frac{dq}{dt} = \dot{q} = \{q, H\} = \frac{\partial q}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial q}{\partial p}\frac{\partial H}{\partial q} = \frac{\partial H}{\partial p} \tag{2.48}$$

since q does not depend on p. Similarly, if $O(q,p) = p$

$$\frac{dp}{dt} = \dot{p} = \{p, H\} = \frac{\partial p}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial p}{\partial p}\frac{\partial H}{\partial q} = -\frac{\partial H}{\partial q} \tag{2.49}$$

The Hamiltonian equations can be cast in a more compact form by defining the two-dimensional phase space $\Gamma = (q,p)$:

$$\frac{d\Gamma}{dt} = \{\Gamma, H\}. \tag{2.50}$$

One can then define an operator $\hat{L}$ acting on Γ by

$$i\hat{L}\Gamma = \{\Gamma, H\}. \tag{2.51}$$

The operator $\hat{L}$ is known as the Liouville operator i.e a differential operator given by

$$i\hat{L} = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}. \tag{2.52}$$

For the the more general case of a N particle system in $d = 1$ the phase space $\Gamma = (q_1, p_1, \cdots, q_N, p_N)$ and

$$i\hat{L} = \sum_{k=1}^{N}\left[\frac{\partial H}{\partial p_k}\frac{\partial}{\partial q_k} - \frac{\partial H}{\partial q_k}\frac{\partial}{\partial p_k}\right]. \tag{2.53}$$

With the Liouville operator the equations of motions can be written in operator form as

$$\frac{d\Gamma}{dt} = i\hat{L}\Gamma \tag{2.54}$$

whose formal solution is

$$\boxed{\Gamma(t) = e^{i\hat{L}t}\Gamma(0).} \tag{2.55}$$

where $\Gamma(0) = (q_1(0), p_1(0), \cdots, q_N(0), p_N(0))$. The *unitary* operator $\exp\left(i\hat{L}t\right)$ is called the *classical propagator* and the presence of i furnishes an immediate analogy with the quantum mechanical propagator $\exp\left(-i\hat{H}t/h\right)$. Unfortunately Eq. (2.55) is not of very practical use since the analytical evaluation of $\exp\left(i\hat{L}t\right)$ can be done for very few simple cases. This can be seen by first noting that, according to eq. (2.52), $i\hat{L}$ is (for one particle system) of the form

$$i\hat{L} = i\hat{L_1} + i\hat{L_2} \tag{2.56}$$

where

$$i\hat{L_1} = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} = \dot{q}\frac{\partial}{\partial q} \qquad i\hat{L_2} = -\frac{\partial H}{\partial q}\frac{\partial}{\partial p} = \dot{p}\frac{\partial}{\partial p} \tag{2.57}$$

where in the last terms we have used the Hamiltonian equations of motion. Hence, for any phase space function $g(q,p)$ it follows that

$$\left(i\hat{L_2}\right)\left(i\hat{L_1}\right)g(q,p) = -\frac{\partial H}{\partial q}\frac{\partial}{\partial p}\left[\frac{\partial H}{\partial p}\frac{\partial g}{\partial q}\right] = -\frac{\partial H}{\partial q}\frac{\partial^2 H}{\partial p^2}\frac{\partial g}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial H}{\partial p}\frac{\partial^2 g}{\partial p \partial q} \tag{2.58}$$

$$\left(i\hat{L_1}\right)\left(i\hat{L_2}\right)g(q,p) = \frac{\partial H}{\partial p}\frac{\partial}{\partial q}\left[-\frac{\partial H}{\partial q}\frac{\partial g}{\partial p}\right] = -\frac{\partial H}{\partial p}\frac{\partial^2 H}{\partial q^2}\frac{\partial g}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial q}\frac{\partial^2 g}{\partial p \partial q}. \tag{2.59}$$

Therefore, for any phase space function $g(q,p)$

$$\left(i\hat{L_1}i\hat{L_2} - i\hat{L_2}i\hat{L_1}\right)g(q,p) \neq 0 \tag{2.60}$$

or

$$\left[i\hat{L}_1, i\hat{L}_2\right] \neq 0 \tag{2.61}$$

Since $i\hat{L}_1$ and $i\hat{L}_2$ do not commute, the classical propagator $\exp\left(i\hat{L}\right)$ *cannot* be factorized as $\exp\left(i\hat{L}_1\right)\exp\left(i\hat{L}_2\right)$. In particular by Taylor expanding the two expressions it is possible to show that

$$e^{i\hat{L}t} = e^{i\hat{L}_1 t} e^{i\hat{L}_2 t} e^{i[\hat{L}_1, \hat{L}_2]t}. \tag{2.62}$$

On the other hand there is a theorem that can be use to factorize the classical propagator. This is the *Trotter theorem*, which states that

$$\exp\left(i\hat{L}t\right) = \exp\left[(i\hat{L}_1 + i\hat{L}_2)t\right] = \lim_{M\to\infty}\left[\exp\left(\frac{i\hat{L}_2 t}{2M}\right)\exp\left(\frac{i\hat{L}_1 t}{M}\right)\exp\left(\frac{i\hat{L}_2 t}{2M}\right)\right]^M. \tag{2.63}$$

The Trotter theorem is the starting point for generating practical numerical integrators. Indeed let us consider the approximation to $\exp\left[(i\hat{L}_1 + i\hat{L}_2)t\right]$ obtained by choosing M large but still finite:

$$\exp\left[(i\hat{L}_1 + i\hat{L}_2)t\right] \approx \left[\exp\left(\frac{i\hat{L}_2 t}{2M}\right)\exp\left(\frac{i\hat{L}_1 t}{M}\right)\exp\left(\frac{i\hat{L}_2 t}{2M}\right)\right]^M. \tag{2.64}$$

By taking the $1/M$ power in both sides we have

$$\exp\left[(i\hat{L}_1 + i\hat{L}_2)t/M\right] \approx \exp\left(\frac{i\hat{L}_2 t}{2M}\right)\exp\left(\frac{i\hat{L}_1 t}{M}\right)\exp\left(\frac{i\hat{L}_2 t}{2M}\right). \tag{2.65}$$

Defining $\Delta t = t/M$ for M finite we obtain a single-time-step approximation to the propagator of the form

$$\exp\left[(i\hat{L}_1 + i\hat{L}_2)\Delta t\right] \approx \exp\left(\frac{i\hat{L}_2 \Delta t}{2}\right)\exp\left(i\hat{L}_1 \Delta t\right)\exp\left(\frac{i\hat{L}_2 \Delta t}{2}\right). \tag{2.66}$$

Let $\tilde{U}(\Delta t)$ be the right side of the previous equation. It represents an approximation of the classical propagator. It is easy to see that $\tilde{U}^\dagger(\Delta t) = \tilde{U}(-\Delta t) = \tilde{U}^{-1}(-\Delta t)$. Hence, $\tilde{U}(\Delta t)$ is *unitary* and therefore it preserves the time-reversibility of the dynamics. Moreover, by performing a Taylor expansion, it can be shown that $\tilde{U}(\Delta t)$ is accurate up to order Δt^2:

$$\begin{aligned}
&\exp\left(\frac{i\hat{L}_2\Delta t}{2}\right)\exp\left(i\hat{L}_1\Delta t\right)\exp\left(\frac{i\hat{L}_2\Delta t}{2}\right)\\
=\;& \left[1 + \frac{\Delta t}{2}i\hat{L}_2 + \frac{\Delta t^2}{8}(i\hat{L}_2)^2\cdots\right] + \left[1 + \Delta t i\hat{L}_1 + \frac{\Delta t^2}{2}(i\hat{L}_2)^2\cdots\right] + \left[1 + \frac{\Delta t}{2}i\hat{L}_2 + \frac{\Delta t^2}{8}(i\hat{L}_2)^2\cdots\right]\\
=\;& 1 + (i\hat{L}_1 + i\hat{L}_2)t + \frac{1}{2}\left[(i\hat{L}_1)(i\hat{L}_2) + (i\hat{L}_2)(i\hat{L}_1) + \frac{1}{2}(i\hat{L}_2)^2 + \frac{1}{4}(i\hat{L}_2)^2 + (i\hat{L}_1)^2 + \frac{1}{4}(i\hat{L}_2)^2\right]\Delta t^2 + \cdots\\
=\;& 1 + i\hat{L}\Delta t + \frac{1}{2}(i\hat{L}_1 + i\hat{L}_2)^2\Delta t^2 + \cdots
\end{aligned} \tag{2.67}$$

Hence there is equivalence up to second order in Δt i.e.

$$\exp\left(i\hat{L}\Delta t\right) = \exp\left(\frac{i\hat{L}_2\Delta t}{2}\right)\exp\left(i\hat{L}_1\Delta t\right)\exp\left(\frac{i\hat{L}_2\Delta t}{2}\right) + O(\Delta t^3). \tag{2.68}$$

We now look at the action of the approximate Liouville operator on the phase space (q,p). First let us remind the identity

$$e^{c\frac{\partial}{\partial q}}q = q + c \tag{2.69}$$

that can be obtained by simply Taylor expanding the left side :

$$\left[1 + c\frac{\partial}{\partial q} + \frac{1}{2}c^2\frac{\partial^2}{\partial q^2} + \cdots\right]q = q + c \tag{2.70}$$

since all derivatives higher than the first order derivative go to 0 when acting on q. This identity can be used to obtain a more one:

$$e^{c\frac{\partial}{\partial q}}g(q,p) = g(q+c,p). \tag{2.71}$$

Indeed

$$e^{c\frac{\partial}{\partial q}}g(q,p) = \sum_{k=0}^{\infty}\frac{1}{k!}\left[c\frac{\partial}{\partial q}\right]^k g(q,p) = \sum_{k=0}^{\infty}c^k g^{(k)}(q,p) \tag{2.72}$$

and the last line is just the Taylor series expansion of $g(q+c,p)$. Similar identities are valid for the action of $\exp(c\partial/\partial p)$ on p and on $h(q,p)$.//For simplicity let us now consider the classical Hamiltonian

$$H = \frac{p^2}{2m} + U(q) \tag{2.73}$$

In this case $\partial H/\partial p = p/m$ and $\partial H/\partial q = -dU/dq = F(q)$. With the above identities it is possible to evaluate the action of $\tilde{U}(\Delta t)$ on q:

$$\tilde{U}(\Delta t)q = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}e^{\Delta t\frac{\partial H}{\partial p}\frac{\partial}{\partial q}}e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}q = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}e^{\Delta t\frac{\partial H}{\partial p}\frac{\partial}{\partial q}}q \tag{2.74}$$

and since the second operator changes q to $q + \Delta t\frac{\partial H}{\partial p}$ we get:

$$\tilde{U}(\Delta t)q = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}\left(q + \Delta t\frac{\partial H}{\partial p}\right). \tag{2.75}$$

Since the last operator has no effect on q but acts on p by changing it into $p - \frac{\Delta t}{2}\frac{\partial H}{\partial q} = p + \frac{\Delta t}{2}\dot{p}$ we get

$$\begin{aligned}\tilde{U}(\Delta t)q &= q + \frac{\Delta t}{m}\left(p - \frac{\Delta t}{2}\frac{\partial H}{\partial q}\right)\\ &= q + \Delta t\frac{p}{m} + \frac{\Delta t^2}{2m}F(q)\end{aligned} \tag{2.76}$$

Starting from the initial conditions $(q(0),p(0))$ we then have

$$\tilde{U}(\Delta t)q(0) \equiv q(\Delta t) = q(0) + \Delta t\frac{p(0)}{m} + \frac{\Delta t^2}{2m}F(q(0)). \tag{2.77}$$

The action of $\tilde{U}(\Delta t)$ on p is

$$\tilde{U}(\Delta t)p = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}e^{\Delta t\frac{\partial H}{\partial p}\frac{\partial}{\partial q}}e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}p. \tag{2.78}$$

The first operator changes p to $p - \frac{\Delta t}{2}\frac{\partial H}{\partial q} = p + \frac{\Delta t}{2}\dot{p} = p + \frac{\Delta t}{2}F(q)$ giving

$$\tilde{U}(\Delta t)p = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}e^{\Delta t\frac{\partial H}{\partial p}\frac{\partial}{\partial q}}\left(p + \frac{\Delta t}{2}F(q)\right). \tag{2.79}$$

The next operator changes $F(q)$ into $F(q+\Delta t\frac{p}{m})$ and has no effect on p:

$$\tilde{U}(\Delta t)p = e^{-\frac{\Delta t}{2}\frac{\partial H}{\partial q}\frac{\partial}{\partial p}}\left[p+\frac{\Delta t}{2}F\left(q+\frac{\Delta t}{m}p\right)\right]. \tag{2.80}$$

Finally the last operator changes p into $p+\frac{\Delta t}{2}F(q)$ in all the places where it occurs:

$$\begin{aligned}\tilde{U}(\Delta t) &= p+\frac{\Delta t}{2}F(q)+\frac{\Delta t}{2}F\left(q+\frac{\Delta t}{m}\left(p+\frac{\Delta t}{2}F(q)\right)\right)\\ &= p+\frac{\Delta t}{2}\left[F(q)+F\left(q+\frac{\Delta t}{m}p+\frac{\Delta t^2}{2m}F(q)\right)\right]\end{aligned} \tag{2.81}$$

that can be written as

$$p(\Delta t) = p(0)+\frac{\Delta t}{2}\left[F(q(0))+F(q(\Delta t))\right] \tag{2.82}$$

Combining the evolutions for q and p we get

$$\begin{aligned}q(\Delta t) &= q(0)+\Delta t\frac{p(0)}{m}+\frac{\Delta t^2}{2m}F(q(0))\\ p(\Delta t) &= p(0)+\frac{\Delta t}{2}\left[F(q(0))+F(q(\Delta t))\right].\end{aligned} \tag{2.83}$$

Symplecticity An important property of the map generated by the operator $\tilde{U}(\Delta t)$ is that it preserves the invariant phase space measure. In other words the map is *symplectic*. This is equivalent to say that the Jacobian of the map

$$J\left((q(\Delta t),p(\Delta p);(q(0),p(0))\right) = \frac{\partial\left(q(\Delta t),p(\Delta t)\right)}{\partial(q(0),p(0))} \tag{2.84}$$

is equal to one. This is easy to show since the Jacobian of the transformation from $\{q(0),p(0)\}$ to $\{q(\Delta t),p(\Delta t)\}$ is the product of the Jacobian of the three transformations

$$e^{\dot{p}\partial/\partial p\Delta t/2}f(q(0),p(0)) = f\left[q(0),\left(p(0)+\frac{\Delta t}{2}\dot{p}(0)\right)\right] \tag{2.85}$$

$$e^{\dot{q}\partial/\partial q\Delta t}f\left(q(0),\left(p(0)+\frac{\Delta t}{2}\dot{p}(0)\right)\right) = f\left[\left(q(0)+\Delta t\dot{q}\left(\frac{\Delta t}{2}\right)\right),\left(p(0)+\frac{\Delta t}{2}\dot{p}(0)\right)\right] \tag{2.86}$$

$$\begin{aligned}&e^{\dot{p}\partial/\partial p\Delta t/2}f\left[\left(q(0)+\Delta t\dot{q}\left(\frac{\Delta t}{2}\right)\right),\left(p(0)+\frac{\Delta t}{2}\dot{p}(0)\right)\right]\\ =\ & f\left[\left(q(0)+\Delta t\dot{q}\left(\frac{\Delta t}{2}\right)\right),\left(p(0)+\frac{\Delta t}{2}\dot{p}(0)+\frac{\Delta t}{2}\dot{p}(\Delta t)\right)\right]\end{aligned} \tag{2.87}$$

For example for the first transformation the Jacobian is

$$\begin{vmatrix}\frac{\partial p'}{\partial p} & \frac{\partial p'}{\partial q}\\ \frac{\partial q}{\partial p} & \frac{\partial q}{\partial q}\end{vmatrix} = \begin{vmatrix}1 & 0\\ 0 & 1\end{vmatrix} = 1 \tag{2.88}$$

where $p' = p+\frac{\Delta t}{2}\dot{p}$. Note that the symplectic nature of the map ensures that the error of the map is bounded, i.e., there will be no exponential growth in the energy conservation error which can affect the long-time statistical behaviour of the dynamics. The Trotter theorem is powerful not only because it shows directly that the algorithm is symplectic and time-reversible but also because the same evolution can be obtained by viewing the approximate operator $\tilde{U}(\Delta t)$ as a combination of three sequential updates without requiring the closed form expression of eq. (2.83). Indeed

$$\tilde{U}(\Delta t) \equiv \exp\left(\frac{i\hat{L}_2\Delta t}{2}\right)\exp\left(i\hat{L}_1\Delta t\right)\exp\left(\frac{i\hat{L}_2\Delta t}{2}\right) \tag{2.89}$$

can be see as the combination of

$$\begin{aligned}
\exp\left(\frac{i\hat{L}_2(q,p)\Delta t}{2}\right)(q,p) &\rightarrow (q',p') \\
\exp\left(i\hat{L}_1(q',p')\Delta t\right)(q',p') &\rightarrow (q'',p'') \\
\exp\left(\frac{i\hat{L}_2(q'',p'')\Delta t}{2}\right)(q'',p'') &\rightarrow (q(\Delta t),p(\Delta t))
\end{aligned} \tag{2.90}$$

If we now use the expressions for $i\hat{L}_1$ and $i\hat{L}_2$ we get :

$$\begin{aligned}
e^{\frac{\Delta t}{2}\dot{p}\partial/\partial p}\begin{pmatrix} q \\ p \end{pmatrix} &= \begin{pmatrix} q(0) \\ p(0)+\frac{\Delta t}{2}F(q(0)) \end{pmatrix} = \begin{pmatrix} q' \\ p' \end{pmatrix} \\
e^{\Delta t\dot{q}\partial/\partial q}\begin{pmatrix} q' \\ p' \end{pmatrix} &= \begin{pmatrix} q'+\Delta t\dot{q}' \\ p' \end{pmatrix} = \begin{pmatrix} q' \\ p' \end{pmatrix} \\
e^{\frac{\Delta t}{2}\dot{p}\partial/\partial p}\begin{pmatrix} q'' \\ p'' \end{pmatrix} &= \begin{pmatrix} q'' \\ p''+\frac{\Delta t}{2}F(q'') \end{pmatrix} = \begin{pmatrix} q(\Delta t) \\ p(\Delta t) \end{pmatrix}
\end{aligned} \tag{2.91}$$

Finally, notice that, following this route, Eq. (2.40) gets the more general form

$$q(t)+\Delta t v(t+\Delta t/2) = q(t)+\Delta t\frac{\partial H}{\partial p}\Big|_{p=p(t+\Delta t/2)} \tag{2.92}$$

Time reversibility The condition of being time reversible requires that only even-ordered decomposition must be used and that the operators $e^{\hat{L}_1\Delta t}$ and $e^{\hat{L}_2\Delta t}$ enter symmetrically in the decomposition. For example, the time reversibility property of the second order decomposition

$$e^{(\hat{L}_1+\hat{L}_2)\Delta t} = e^{\hat{L}_2\Delta t/2}e^{\hat{L}_1\Delta t}e^{\hat{L}_2\Delta t/2} \equiv \tilde{U}(\Delta t) \tag{2.93}$$

can be shown by the property

$$\tilde{U}(\Delta t)\tilde{U}(-\Delta t) = e^{\hat{L}_2\Delta t/2}e^{\hat{L}_1\Delta t}e^{\hat{L}_2\Delta t/2}e^{-\hat{L}_2\Delta t/2}e^{-\hat{L}_1\Delta t}e^{-\hat{L}_2\Delta t/2} = 1. \tag{2.94}$$

Similarly, $\tilde{U}(-\Delta t)\tilde{U}(\Delta t) = 1$. Hence each time step in the temporal evolution is reversible leading to a time reversible trajectory.

2.3.6 Other & Higher Order Algorithms

For most Molecular Dynamics applications, Verlet-like algorithms are perfectly adequate. However, higher order algorithms makes it possible to use a longer time step without loss of (short-term) accuracy or they can be helpful if higher accuracy is required.
We first mention two schemes that yield the same trajectories as the Verlet algorithm but provide better estimates for the velocity. The first is the so-called Beeman algorithm

$$\vec{r}(t+\Delta t) = \vec{r}(t)+\vec{v}(t)\Delta t+\frac{4\vec{f}(t)-\vec{f}(t-\Delta t)}{6m}\Delta t^2 \tag{2.95}$$

$$\vec{v}(t+\Delta t) = \vec{v}(t)+\frac{2\vec{f}(t+\Delta t)+5\vec{f}(t)-\vec{f}(t-\Delta t)}{6m}\Delta t \tag{2.96}$$

By eliminating $\vec{v}(t)$ from Eq. (2.95) using Eq. (2.96), it is easy to show that the positions satisfy the Verlet algorithm. However, the velocities are more accurate than the original Verlet algorithm; as a consequence,

the total energy conservation looks better. A disadvantage of the Beeman algorithm is that the expression for the velocity does not possess time-reversal symmetry. This can be corrected and leads to the so-called velocity-corrected Verlet algorithm for which both position and velocity error is $O(\Delta t^4)$.
It is derived as follows: write a Taylor expansion for $\vec{r}(t+2\Delta t)$, $\vec{r}(t+\Delta t)$, $\vec{r}(t-\Delta t)$ and $\vec{r}(t-2\Delta t)$

$$\begin{aligned}
\vec{r}(t+2\Delta t) &= \vec{r}(t) + 2\vec{v}\Delta t + \frac{\vec{a}}{4}(2\Delta t)^2 + \frac{\dot{\vec{a}}}{3!}(2\Delta t)^3 + \dots \\
\vec{r}(t+\Delta t) &= \vec{r}(t) + \vec{v}\Delta t + \frac{\vec{a}}{4}\Delta t^2 + \frac{\dot{\vec{a}}}{3!}\Delta t^3 + \dots \\
\vec{r}(t-\Delta t) &= \vec{r}(t) - \vec{v}\Delta t + \frac{\vec{a}}{4}\Delta t^2 - \frac{\dot{\vec{a}}}{3!}\Delta t^3 + \dots \\
\vec{r}(t-2\Delta t) &= \vec{r}(t) - 2\vec{v}\Delta t + \frac{\vec{a}}{4}(2\Delta t)^2 - \frac{\dot{\vec{a}}}{3!}(2\Delta t)^3 + \dots
\end{aligned}$$

By combining these equations, we can write

$$12\vec{v}(t)\Delta t = 8\left[\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)\right] - \left[\vec{r}(t+2\Delta t) - \vec{r}(t-2\Delta t)\right] + O(\Delta t^4) \tag{2.97}$$

or, equivalently

$$\vec{v}(t) = \frac{\vec{v}(t+\Delta t/2) + \vec{v}(t-\Delta t/2)}{2} + \frac{\Delta t}{12}\left[\vec{a}(t-\Delta t) - \vec{a}(t+\Delta t)\right] + O(\Delta t^4) \tag{2.98}$$

Note that this velocity can be computed only after the next step, i.e. we must know the positions and forces at $t+\Delta t$ to compute the velocity at time t.
In general, higher order schemes require more storage and are either not time reversible or not symplectic (non area preserving). This is true in particular of the so-called predictor-corrector algorithm. The basic idea is to use information about the position and its first n derivatives at time $t+\Delta t$. We then compute the forces (and the accelerations) at the predicted positions; we find that these accelerations are *not* equal to the values that we predicted and, thus, we adjust our predictions. Further, on the basis of the observed discrepancy, we try to improve our estimation of the positions. This latter step is usually the "corrector" part of the algorithm. The one reported is one possible form.
Consider the Taylor expansion (for simplicity, in 1D)

$$x(t+\Delta t) = x(t) + \frac{dx}{dt}\Delta t + \frac{d^2x}{dt^2}\frac{(\Delta t)^2}{2!} + \frac{d^3x}{dt^3}\frac{(\Delta t)^3}{3!} + \dots \tag{2.99}$$

using the short-hand notation: $x_1(t) = \frac{dx}{dt}\Delta t$, $x_2(t) = \frac{d^2x}{dt^2}\frac{\Delta t^2}{2!}$, $x_3(t) = \frac{d^3x}{dt^3}\frac{\Delta t^3}{3!}$, we can write the following predictions for $x(t+\Delta t)$:

$$\begin{aligned}
x(t+\Delta t) &= x(t) + x_1(t) + x_2(t) + x_3(t) \\
x_1(t+\Delta t) &= x_1(t) + 2x_2(t) + 3x_3(t) \\
x_2(t+\Delta t) &= x_2(t) + 3x_3(t) \\
x_3(t+\Delta t) &= x_3(t)
\end{aligned} \tag{2.100}$$

Having $x(t+\Delta t)$ we can compute the forces at the predicted positions, thus compute $x_2(t+\Delta t)$; we denote $\Delta x_2 \equiv x_2^{\text{corrected}} - x_2^{\text{predicted}}$. We estimate corrected values for x and its derivatives as

$$x_n^{\text{corrected}} = x_n^{\text{predicted}} + C_n \Delta x_2 \tag{2.101}$$

where the C_n are constants, fixed for a given order algorithm. The values are chosen to yield an optimal compromise between accuracy and stability. For example, a fifth order algorithm has: $C_0 = 19/120$, $C_1 =$

$3/4$, $C_2 = 1$, $C_3 = 1/2$, $C_4 = 1/12$.
Finally, higher order integration schemes can be implemented using higher order decomposition, such as the fourth-order Suzuki-Trotter decomposition:

$$e^{(\hat{L_1}+\hat{L_2})\Delta t} = \prod_{i=1}^{5} e^{p_i \hat{L_1} \Delta t/2} e^{p_i \hat{L_2} \Delta t} e^{p_i \hat{L_1} \Delta t/2} + O(\Delta t^5) \tag{2.102}$$

where $p_1 = p_2 = p_4 = p_5 \equiv p = \frac{1}{4-4^{1/3}}, p_3 = 1 - 4p$. It is composed by 15 exponential operators. However, consecutive operators with L_1 in the exponent can be combined yielding to a total of 11 operators. Another fourth-order scheme is based on the so called Forest-Routh decomposition

$$e^{(\hat{L_1}+\hat{L_2})\Delta t} = e^{p\hat{L_1}\Delta t/2} e^{p\hat{L_2}\Delta t} e^{(1-p)\hat{L_1}\Delta t/2} e^{(1-2p)\hat{L_2}\Delta t} e^{(1-p)\hat{L_1}\Delta t/2} e^{p\hat{L_2}\Delta t} e^{p\hat{L_1}\Delta t/2} + O(\Delta t^5) \tag{2.103}$$

where $p = 1/(2-2^{2^{1/3}})$. Because this decomposition involves 7 operators instead of 11, the cpu time required for one integration step using eq.(2.103) is less then using eq.(2.102). On the other hand, truncation errors arising from the use of eq. (2.103) are much larger.