2.3.6 Symplectic Integrators

A symplectic integrator is an approximation of the flow map that conserves the symplectic 2-form. Some first steps in the theory of symplectic integration, i.e. numerical methods explicitly designed to mimic the symplectic property of the flow map, were made by Vogalaere [98] (in 1956!) but this work went unnoticed. The first practical methods conserving the symplectic property were suggested by Ruth in 1983 [320] and followed by a number of works on a similar theme [71, 72, 129–131, 267, 353]. Later works, e.g. [132, 139, 214, 325, 398] were aimed at developing methods with higher order of accuracy or better understanding of the meaning of the symplectic property (we will discuss this aspect in the next chapter). Some symplectic integrators are found within existing families (like Runge-Kutta methods), but the most useful are typically obtained using a splitting and composition framework that allows us to build families of such methods.

In the sequel we will write $\boldsymbol{Z} = \mathscr{G}_h(\boldsymbol{z})$ to specify the starting point $\boldsymbol{z}$ and ending point $\boldsymbol{Z}$ of a step.

Alternatively, if we wish to emphasize the decomposition into positions and momenta, we write

$$\begin{bmatrix} \boldsymbol{Q} \\ \boldsymbol{P} \end{bmatrix} = \mathscr{G}_h\left(\begin{bmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{bmatrix}\right).$$

Recall that, in terms of $\boldsymbol{q}$ and $\boldsymbol{p}$, the differential equations take the form

$$\dot{\boldsymbol{q}} = \nabla_{\boldsymbol{p}} H, \qquad \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} H.$$

In molecular dynamics, the Hamiltonian is usually of the form

$$H = \boldsymbol{p}^T \boldsymbol{M}^{-1} \boldsymbol{p}/2 + U(\boldsymbol{q}),$$

with $\boldsymbol{M}$ a diagonal mass matrix, and we will concentrate on this case for the moment. In this case,

$$\dot{\boldsymbol{q}} = \boldsymbol{M}^{-1}\boldsymbol{p}, \qquad \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} U(\boldsymbol{q}) \equiv \boldsymbol{F}(\boldsymbol{q}).$$

The following scheme is a slight modification of the Euler method.

$$\boldsymbol{Q} = \boldsymbol{q} + h\boldsymbol{M}^{-1}\boldsymbol{P}, \tag{2.18}$$

$$\boldsymbol{P} = \boldsymbol{p} + h\boldsymbol{F}(\boldsymbol{q}). \tag{2.19}$$

The method is explicit: to advance the timestep, we use the second equation to compute $\boldsymbol{P}$ and then insert this in the first to get $\boldsymbol{q}$. Let the vectors $\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{Q}, \boldsymbol{P}$ have ith components q_i, p_i, Q_i, P_i, respectively; we may think of Q_i and P_i as functions of $\boldsymbol{q}$ and $\boldsymbol{p}$, then

$$\mathrm{d}Q_i = \mathrm{d}q_i + hm_i^{-1}\mathrm{d}P_i, \tag{2.20}$$

$$\mathrm{d}P_i = \mathrm{d}p_i - h\sum_{j=1}^{\mathrm{N_c}} \frac{\partial^2 U}{\partial q_j \partial q_i}\mathrm{d}q_j. \tag{2.21}$$

Computing the 2-form,

$$\mathrm{d}Q_i \wedge \mathrm{d}P_i = \mathrm{d}q_i \wedge \mathrm{d}P_i + hm_i^{-1}\mathrm{d}P_i \wedge \mathrm{d}P_i,$$

but $\mathrm{d}u \wedge \mathrm{d}u \equiv 0$ for any u, hence

$$\mathrm{d}Q_i \wedge \mathrm{d}P_i = \mathrm{d}q_i \wedge \mathrm{d}P_i,$$

and (2.21) implies

$$\mathrm{d}Q_i \wedge \mathrm{d}P_i = \mathrm{d}q_i \wedge \mathrm{d}p_i - h\sum_{j=1}^{\mathrm{N_c}} \mathrm{d}q_i \wedge \frac{\partial^2 U}{\partial q_j \partial q_i}\mathrm{d}q_j.$$

It is then a simple exercise to show that

$$\sum_{i=1}^{\mathrm{N_c}}\sum_{j=1}^{\mathrm{N_c}} \mathrm{d}q_i \wedge \frac{\partial^2 U}{\partial q_j \partial q_i}\mathrm{d}q_j = 0,$$

using the skew-symmetry of the wedge product and the fact that the Hessian matrix is symmetric. This implies that

$$\sum_{i=1}^{\mathrm{N_c}} \mathrm{d}Q_i \wedge \mathrm{d}P_i = \sum_{i=1}^{\mathrm{N_c}} \mathrm{d}q_i \wedge \mathrm{d}p_i,$$

which means that the method is symplectic.

2.3.7 The Adjoint Method

Given any numerical integrator $\mathscr{G}_h$, consider the map

$$\mathscr{G}_h^{\dagger} = \mathscr{G}_{-h}^{-1}.$$

This is popularly referred to as the *adjoint* of $\mathscr{G}_h$, although it seems something of an abuse of mathematical language to refer to it in this way. For the flow map $\mathscr{F}_h$, we know that the inverse map is precisely $\mathscr{F}_{-h}$, so $\mathscr{F}_h^\dagger = \mathscr{F}_h$, i.e. the flow map is in the normal sense "self-adjoint," i.e. *symmetric*. However, such a property does not hold in the general case. In particular, consider Euler's method

$$\boldsymbol{Z} = \boldsymbol{z} + h\boldsymbol{f}(\boldsymbol{z}).$$

The adjoint method is defined by

$$\boldsymbol{Z} = \boldsymbol{z} + h\boldsymbol{f}(\boldsymbol{Z}),$$

and where the first was explicit, the second is implicit (it is the so-called *backward Euler* method).

The method (2.18)–(2.19) is called the Symplectic Euler method. Its adjoint method has a similar structure:

$$\boldsymbol{Q} = \boldsymbol{q} + h\boldsymbol{M}^{-1}\boldsymbol{p}, \tag{2.22}$$

$$\boldsymbol{P} = \boldsymbol{p} + h\boldsymbol{F}(\boldsymbol{Q}). \tag{2.23}$$

Comparing with (2.18)–(2.19), we see that (2.22)–(2.23) is also explicit.

Given a method $\mathscr{G}_h$ with adjoint method $\mathscr{G}_h^\dagger$, it is possible to obtain the adjoint of the adjoint method $\mathscr{G}_h^{\dagger\dagger}$, but, as we might expect, the adjoint of the adjoint is the original method:

$$\mathscr{G}_h^{\dagger\dagger} = [\mathscr{G}_{-h}^\dagger]^{-1} = [\mathscr{G}_h^{-1}]^{-1} = \mathscr{G}_h.$$

2.4 Building Symplectic Integrators

Symplectic integrators may be constructed in several ways. First, we may look within standard classes of methods such as the family of Runge-Kutta schemes to see if there are choices of coefficients which make the methods automatically conserve the symplectic 2-form. A second, more direct approach is based on *splitting*. The idea of splitting methods, often referred to in the literature as *Lie-Trotter methods*, is that we divide the Hamiltonian into parts, and determine the flow maps (or, in some cases, approximate flow maps) for the parts, then compose the maps to define numerical methods for the whole system.