3.3.3 Higher Order Symplectic Methods: The Suzuki-Yoshida Method

Yoshida [398] gives an elegant method for creating a symplectic scheme of arbitrarily high order, using Trotter's results for compositions of linear operators [370]. This work is related to methods suggested by Suzuki [354] in the context of Trotter factorization of quantum operators. Consider a scheme with order $2s$ (for $s \geq 1$) and where the evolution of the system under the method is given by $\exp(h\,\hat{\tilde{\mathcal{L}}}_h)$, where

$$\hat{\mathcal{L}}_h \stackrel{\text{def}}{=} \mathcal{L}_{\tilde{H}_h} = \mathcal{L}_H + h^{2s}\tilde{\mathcal{L}}_{[2s]} + h^{2s+2}\tilde{\mathcal{L}}_{[2s+2]} + h^{2s+4}\tilde{\mathcal{L}}_{[2s+4]} + \mathcal{O}(h^{2s+6})$$

is the method's characteristic operator (with corresponding shadow Hamiltonian $\tilde{H}_h$). The linear operators $\tilde{\mathcal{L}}_{[2i]}$ are compositions of Lie derivatives, and can be computed using the symmetric BCH formula. We now consider iterating this scheme three times, first using a step of $\tau_0 h$, followed by a step of $\tau_1 h$, and finally another step with stepsize $\tau_0 h$ (where $\tau_0 h + \tau_1 h + \tau_0 h = h$). The overall effect on the system is given by a product of exponentials, as

$$\exp\left(\tau_0 h\,\hat{\mathcal{L}}_{\tau_0 h}\right)\exp\left(\tau_1 h\,\hat{\mathcal{L}}_{\tau_1 h}\right)\exp\left(\tau_0 h\,\hat{\mathcal{L}}_{\tau_0 h}\right) = \exp\left(h\,Z_h\right),$$

where, using repeated application of the BCH formula, we find

$$\begin{aligned} Z_h &= 2\tau_0\,\hat{\mathcal{L}}_{\tau_0 h} + \tau_1\,\hat{\mathcal{L}}_{\tau_1 h} + \mathcal{O}(h^{2s+2}), \\ &= (2\tau_0 + \tau_1)\,\mathcal{L}_H + (2\tau_0^{2s+1} + \tau_1^{2s+1})h^{2s}\tilde{\mathcal{L}}_{[2s]} + \mathcal{O}(h^{2s+2}). \end{aligned}$$

We have free reign over constants τ_0 and τ_1 as long as $2\tau_0 + \tau_1 = 1$. Hence we have an opportunity to annihilate the perturbation operator at order h^{2s} by choosing $2\tau_0^{2s+1} + \tau_1^{2s+1} = 0$ as well. Solving simultaneously, there exists a unique real solution

$$\tau_0 = \frac{1}{2-\kappa}, \qquad \tau_1 = -\frac{\kappa}{2-\kappa}, \qquad \kappa^{2s+1} = 2,$$

giving us a scheme of order $2s+2$. We can then proceed recursively, as this new order $2s+2$ scheme can be composed similarly to wipe out successive higher order terms.

Though the fourth-order version of the scheme was given first by Forest and Ruth [139] (and discovered independently by Yoshida [398] and Candy and Rozmus [66]), we shall simply refer to these higher-order schemes as Yoshida methods, owing to the elegant derivation of schemes of arbitrary order.

Example 3.1 Consider using velocity Verlet as the base second-order method to build a Yoshida fourth-order method from. As the scheme is second-order, we have

$s = 1$, and hence

$$\tau_0 = \frac{1}{2 - \sqrt[3]{2}}, \qquad \tau_1 = -\frac{\sqrt[3]{2}}{2 - \sqrt[3]{2}}.$$

The overall scheme is then three iterations of velocity Verlet, using stepsizes $\tau_0 h$, $\tau_1 h$ and $\tau_0 h$ respectively. We write this with subindices α, β to indicate the intermediate stages.

Yoshida fourth-order scheme (velocity Verlet):

$$\begin{aligned}
\boldsymbol{P}_\alpha &\coloneqq \boldsymbol{p} - (\tau_0 h/2)\, \nabla U(\boldsymbol{q}), \\
\boldsymbol{Q}_\alpha &\coloneqq \boldsymbol{q} + (\tau_0 h)\, \boldsymbol{M}^{-1} \boldsymbol{P}_\alpha, \\
\boldsymbol{P}_\alpha &\coloneqq \boldsymbol{P}_\alpha - (\tau_0 h/2)\, \nabla U(\boldsymbol{Q}_\alpha), \\
\boldsymbol{P}_\beta &\coloneqq \boldsymbol{P}_\alpha - (\tau_1 h/2)\, \nabla U(\boldsymbol{Q}_\alpha), \\
\boldsymbol{Q}_\beta &\coloneqq \boldsymbol{Q}_\alpha + (\tau_1 h)\, \boldsymbol{M}^{-1} \boldsymbol{P}_\beta, \\
\boldsymbol{P}_\beta &\coloneqq \boldsymbol{P}_\beta - (\tau_1 h/2)\, \nabla U(\boldsymbol{Q}_\beta), \\
\boldsymbol{P} &\coloneqq \boldsymbol{P}_\beta - (\tau_0 h/2)\, \nabla U(\boldsymbol{Q}_\beta), \\
\boldsymbol{Q} &\coloneqq \boldsymbol{Q}_\beta + (\tau_0 h)\, \boldsymbol{M}^{-1} \boldsymbol{P}, \\
\boldsymbol{P} &\coloneqq \boldsymbol{P} - (\tau_0 h/2)\, \nabla U(\boldsymbol{Q}).
\end{aligned} \tag{3.8}$$

The equations could easily be written in a simplified form, combining several of the steps. This scheme requires three new evaluations of the force ∇U per iteration, making it significantly more expensive than the vanilla second-order Verlet method. We may use this fourth-order scheme (now $s = 2$) to then find a scheme of order $2s + 2 = 6$.

We compare the symplectic methods developed so far in Fig. 3.2, for $t \in [0, 100]$ using planar phase space and the Lennard-Jones oscillator (the one degree-of-freedom problem with Hamiltonian $H(q, p) = p^2/2 + \varphi_{\mathrm{LJ}}(q)$). As anticipated, there is no visible drift in the Hamiltonian as the simulation time increases. In each case, we observe an oscillation in the fluctuation of the total energy. Additionally we compute trajectories propagated at different stepsizes, and plot the maximum deviation

$$\max |H(q_k, p_k) - H(q_0, p_0)|$$

over the entire trajectory. We can see that for an order s method, the maximum deviation in the Hamiltonian is of order s, as is expected from the analysis. Yoshida fourth-order schemes are tested using both the position and velocity Verlet schemes

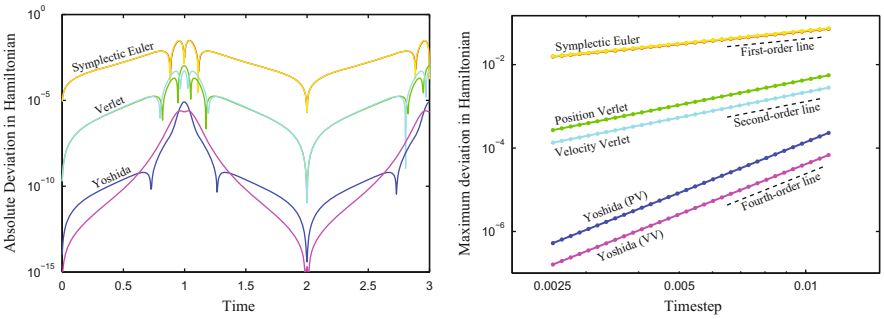

Fig. 3.2 We compare the symplectic Euler, Verlet and Yoshida schemes in application to a Lennard-Jones oscillator. The plot shows the absolute deviation in the computed Hamiltonian (*left*) as a function of time, for each scheme at a fixed timestep $h = 0.005$. Moreover we simulate the system using different stepsizes and compute for each stepsize the maximum deviation in the Hamiltonian (*right*), comparing the results with guide lines associated to various powers of the step size. The scheme used as the "base" method for the Yoshida composition methods is denoted in the parenthesis (either position or velocity Verlet)

as their base second-order methods (the base method is denoted in parenthesis in Fig. 3.2), giving similar results.

Of course we need not stop at a fourth-order scheme: we can use the constructed method to target any higher order terms we wish by composing the new scheme in a symmetric form and proceeding identically to the above.

These methods are not the best possible choices among schemes that alternate solving the terms of the splitting [260, 277], either in the sense of having the greatest stability or in the sense of having the smallest leading error coefficients. We can view the Suzuki-Yoshida methods as one type of general composition scheme [260, 277, 326]:

$$\begin{aligned}\mathscr{F}_h = \exp(\alpha_1 h\mathcal{L}_T) \circ \exp(\beta_1 h\mathcal{L}_U) \circ \exp(\alpha_2 h\mathcal{L}_T) \circ \exp(\beta_2 h\mathcal{L}_U) \circ \cdots \circ \\ \exp(\alpha_k h\mathcal{L}_T) \circ \exp(\beta_k h\mathcal{L}_U).\end{aligned}$$

The coefficients of these methods can be optimized according to many criteria, for example to reduce the coefficients associated to certain types of elementary differentials appearing in the leading error term [260], or to have maximal performance for particular families of applications, such as celestial mechanics [37, 127]. For many applications, for example celestial mechanics, such high order methods, and improved variants, are extremely useful, but in the setting of molecular dynamics, it is often found that second-order methods provide a 'good enough' option for numerical integration, the computational price-tag of higher order methods outweighing potential numerical gains. After all, the potential energy functions used in the ODEs are not perfect reflections of the laws of physics, and past a certain point using a high order method merely finds a better solution to an approximate model. Furthermore, most molecular simulations are performed at large timestep,

where the asymptotic error analysis (for $h \to 0$) may be less relevant. Nevertheless there are applications in molecular modelling where higher accuracy is needed in certain parts of a calculation in order to provide optimal sampling. An example will be found in the isokinetic stochastic integrator of Chap. 8.

For more discussion of higher order integrators, refer to [139, 164, 227, 259, 260, 262, 277, 290]. Of particular relevance for molecular dynamics is the excellent numerical study of [153].

3.3.4 The Takahashi-Imada Method

Recall the Takahashi-Imada method introduced in the last chapter,

$$\begin{aligned}\hat{\boldsymbol{P}} &:= \boldsymbol{p} - (h/2)\nabla\tilde{U}(\boldsymbol{q}),\\ \boldsymbol{Q} &:= \boldsymbol{q} + h\boldsymbol{M}^{-1}\hat{\boldsymbol{P}},\\ \boldsymbol{P} &:= \hat{\boldsymbol{P}} - (h/2)\nabla\tilde{U}(\boldsymbol{Q}),\end{aligned}$$

with modified potential energy function

$$\tilde{U}(\boldsymbol{q}) = U(\boldsymbol{q}) - \frac{h^2}{24}\nabla U(\boldsymbol{q})^T\boldsymbol{M}^{-1}\nabla U(\boldsymbol{q}).$$

One might recognize the modification as being proportional to one part of the commutator expansion in the Verlet method, in fact

$$\nabla U(\boldsymbol{q})^T\boldsymbol{M}^{-1}\nabla U(\boldsymbol{q}) = \{U,\{U,T\}\}.$$

This is certainly not a coincidence. If we replace the potential U by $\tilde{U}$ in the Verlet expansion, we have

$$\begin{aligned}\tilde{H}_h &= T + \tilde{U} + \frac{h^2}{12}\left(\{T,\{T,\tilde{U}\}\} - \frac{1}{2}\{\tilde{U},\{\tilde{U},T\}\}\right) + \mathcal{O}(h^4)\\ &= T + U - \frac{h^2}{24}\{U,\{U,T\}\} + \frac{h^2}{12}\left(\{T,\{T,\tilde{U}\}\} - \frac{1}{2}\{\tilde{U},\{\tilde{U},T\}\}\right) + \mathcal{O}(h^4)\\ &= H + \frac{h^2}{12}\left(\{T,\{T,\tilde{U}\}\} - \{\tilde{U},\{\tilde{U},T\}\}\right) + \mathcal{O}(h^4)\\ &= H + \frac{h^2}{12}\left(\boldsymbol{p}^T\boldsymbol{M}^{-1}U''\boldsymbol{M}^{-1}\boldsymbol{p} - \nabla U^T\boldsymbol{M}^{-1}\nabla U\right) + \mathcal{O}(h^4).\end{aligned}$$

Introducing coordinate transformations