

Documentation for the symplectic methods

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This document expands on the comments at the beginning of
integrators/symplectic_runge_kutta_nyström_integrator.hpp.

1 Differential equations.

Recall that the equations solved by this class are

$$(\mathbf{q}, \mathbf{p})' = \mathbf{X}(\mathbf{q}, \mathbf{p}, t) = \mathbf{A}(\mathbf{q}, \mathbf{p}) + \mathbf{B}(\mathbf{q}, \mathbf{p}, t) \quad \text{with } \exp h\mathbf{A} \text{ and } \exp h\mathbf{B} \text{ known and} \quad (1.1)$$
$$[\mathbf{B}, [\mathbf{B}, [\mathbf{B}, \mathbf{A}]]] = \mathbf{0};$$

the above equation, with $\exp h\mathbf{A} = \mathbb{1} + h\mathbf{A}$, $\exp h\mathbf{B} = \mathbb{1} + h\mathbf{B}$, and \mathbf{A} and \mathbf{B} known; (1.2)

$$\mathbf{q}'' = -\mathbf{M}^{-1}\nabla_{\mathbf{q}}V(\mathbf{q}, t). \quad (1.3)$$

2 Relation to Hamiltonian mechanics.

The third equation above is a reformulation of Hamilton's equations with a Hamiltonian of the form

$$H(\mathbf{q}, \mathbf{p}, t) = \frac{1}{2}\mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q}, t), \quad (2.1)$$

where $\mathbf{p} = \mathbf{M}\mathbf{q}'$.

3 A remark on non-autonomy.

Most treatments of these integrators write these differential equations as well as the corresponding Hamiltonian in an autonomous version, thus $\mathbf{X} = \mathbf{A}(\mathbf{q}, \mathbf{p}) + \mathbf{B}(\mathbf{q}, \mathbf{p})$ and $H(\mathbf{q}, \mathbf{p}, t) = \frac{1}{2}\mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q})$. It is however possible to incorporate time, by considering it as an additional variable:

$$(\mathbf{q}, \mathbf{p}, t)' = \mathbf{X}(\mathbf{q}, \mathbf{p}, t) = (\mathbf{A}(\mathbf{q}, \mathbf{p}), 1) + (\mathbf{B}(\mathbf{q}, \mathbf{p}, t), 0).$$

For equations of the form (1.3) it remains to be shown that Hamilton's equations with quadratic kinetic energy and a time-dependent potential satisfy $[\mathbf{B}, [\mathbf{B}, [\mathbf{B}, \mathbf{A}]]] = \mathbf{0}$. We introduce t and its conjugate momentum ϖ to the phase space, and write

$$\tilde{\mathbf{q}} = (\mathbf{q}, t), \quad \tilde{\mathbf{p}} = (\mathbf{p}, \varpi), \quad L(\tilde{\mathbf{p}}) = \frac{1}{2}\mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p} + \varpi.$$

(1.3) follows from Hamilton's equations with

$$H(\tilde{\mathbf{q}}, \tilde{\mathbf{p}}) = L(\tilde{\mathbf{p}}) + V(\tilde{\mathbf{q}}) = \frac{1}{2}\mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p} + \varpi + V(\mathbf{q}, t)$$

since we then get $t' = 1$. The desired property follows from the following lemma:

Lemma. *Let $L(\tilde{\mathbf{q}}, \tilde{\mathbf{p}})$ be a quadratic polynomial in $\tilde{\mathbf{p}}$, $V(\tilde{\mathbf{q}})$ a smooth function, $\mathbf{A} = \{\cdot, L\}$, and $\mathbf{B} = \{\cdot, V\}$. Then*

$$[\mathbf{B}, [\mathbf{B}, [\mathbf{B}, \mathbf{A}]]] = \mathbf{0}. \quad \square$$

Proof. It suffices to show that $\{V, \{V, \{L, V\}\}\} = 0$. It is immediate that every term in that expression will contain a third order partial derivative in the \tilde{p}_i of L , and since L is quadratic in $\tilde{\mathbf{p}}$ all such derivatives vanish. \square

See [MQ06, p. 26] for a detailed treatment of non-autonomous Hamiltonians using an extended phase space. See [McL93, p. 8] for a proof that $\{V, \{V, \{L, V\}\}\} = 0$ for arbitrary Poisson tensors.

4 Composition and first-same-as-last property

Recall from the comments that each step is computed as

$$(\mathbf{q}_{n+1}, \mathbf{p}_{n+1}) = \exp a_{r-1} h \mathbf{A} \exp b_{r-1} h \mathbf{B} \cdots \exp a_0 h \mathbf{A} \exp b_0 h \mathbf{B}(\mathbf{q}_n, \mathbf{p}_n),$$

thus, when b_0 vanishes (type ABA) or when a_{r-1} does (type BAB),

$$\begin{aligned} (\mathbf{q}_{n+1}, \mathbf{p}_{n+1}) &= \exp a_{r-1} h \mathbf{A} \exp b_{r-1} h \mathbf{B} \cdots \exp b_1 h \mathbf{B} \exp a_0 h \mathbf{A}(\mathbf{q}_n, \mathbf{p}_n), \text{ respectively} \\ (\mathbf{q}_{n+1}, \mathbf{p}_{n+1}) &= \exp b_{r-1} h \mathbf{B} \exp a_{r-2} h \mathbf{A} \cdots \exp a_0 h \mathbf{A} \exp b_0 h \mathbf{B}(\mathbf{q}_n, \mathbf{p}_n). \end{aligned}$$

This leads to performance savings.

Let us consider a method of type BAB . Evidently, the evaluation of $\exp a_0 h \mathbf{A}$ is not required, thus only $r - 1$ evaluations of $\exp \Delta t \mathbf{A}$ are required. Furthermore, if output is not needed at step n , the computation of the $(n - 1)$ th step requires only $r - 1$ evaluations of $\exp \Delta t \mathbf{B}$, since the consecutive evaluations of $\exp b_0 h \mathbf{B}$ and $\exp b_r h \mathbf{B}$ can be merged by the group property,

$$\exp b_0 h \mathbf{B} \exp b_r h \mathbf{B} = \exp(b_0 + b_r) h \mathbf{B}.$$

If the equation is of the form 1.2, the latter saving can be achieved even for dense output, since only one evaluation of \mathbf{B} is needed to compute the increments $b_r h \mathbf{B}$ and $b_0 \mathbf{B}$.

The same arguments apply to type ABA . This motivates the name of the template parameter evaluations, equal to $r - 1$ for methods of type ABA and BAB , and r otherwise.

References

- [McL93] R. I. McLachlan. ‘Symplectic integration of Hamiltonian wave equations’. In: *Numerische Mathematik* 66.1 (1993), pp. 465–492.
DOI: 10.1007/BF01385708.
- [MQ06] R. I. McLachlan and G. R. W. Quispel. ‘Geometric Integrators for ODEs’. In: *Journal of Physics A* 39 (2006), pp. 5251–5285.
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