

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

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

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

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

2 Relation to Hamiltonian mechanics.

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

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

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

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

(1.3) follows from Hamilton's equations with

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

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*

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

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 all such derivatives vanish. \square