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

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

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

$$\boldsymbol{q}'' = -\boldsymbol{M}^{-1}\boldsymbol{\nabla}_{\boldsymbol{q}} V(\boldsymbol{q},t). \tag{1.3}$$

2 Relation to Hamiltonian mechanics.

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

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

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

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 $\boldsymbol{X} = \boldsymbol{A}(\boldsymbol{q},\boldsymbol{p}) + \boldsymbol{B}(\boldsymbol{q},\boldsymbol{p})$ and $H(\boldsymbol{q},\boldsymbol{p},t) = \frac{1}{2}\boldsymbol{p}^\top \boldsymbol{M}^{-1}\boldsymbol{p} + V(\boldsymbol{q})$. It is however possible to incorporate time, by considering it as an additional variable:

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

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 $[\boldsymbol{B},[\boldsymbol{B},[\boldsymbol{B},\boldsymbol{A}]]] = \boldsymbol{0}$. We introduce t and its conjugate momentum ϖ to the phase space, and write

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

(1.3) follows from Hamilton's equations with

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

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

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

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

□

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 in $\tilde{\boldsymbol{p}}$ all such derivatives vanish. □

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

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

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

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

This leads to performance savings.

Let us consider a method of type BAB. Evidently, the evaluation of $\exp a_0 h\boldsymbol{A}$ is not required, thus only $r-1$ evaluations of $\exp \Delta t\boldsymbol{A}$ 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 $\exp \Delta t\boldsymbol{B}$, since the consecutive evaluations of $\exp b_0 h\boldsymbol{B}$ and $\exp b_r h\boldsymbol{B}$ can be merged by the group property,

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

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

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. DOI: 10.1088/0305-4470/39/19/S01.