

# Documentation for the symplectic methods

Robin Leroy (eggrobin)

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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  $\varpi$  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  $BAB$ ),

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

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

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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