Geometric Numerical Integration

3. Modified equations

Mario Fernández-Pendás
Universidad de Oviedo/Universidá d'Uviéu

BCAM, May 20-24 2019

Index course

1. Hamiltonian mechanics and numerical methods
2. Symplectic integration
3. **Modified equations**
4. Constrained mechanical systems
5. Adaptive geometric integrators

Motivation

Motivation

Modified equations are rather old[1]; however their use as a means to analyse numerical integrators has only become popular in the last twenty years, after the *emergence of geometric integration*[2].

[1] Griffiths and Sanz-Serna, “On the Scope of the Method of Modified Equations”, 1986.

[2] Sanz-Serna, “Geometric integration”, 1997.

Motivation

Example

Suppose that the system

$$\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) \tag{1}$$

is solved with Euler's rule $\mathbf{x}_{n+1} = \mathbf{x}_n + hf(\mathbf{x}_n)$, and denote by ψ_h the corresponding map $\mathbf{x} + hf(\mathbf{x})$.
Consider the **modified or shadow system**, parameterized by h,

$$\frac{d}{dt}\mathbf{x} = \tilde{f}_h(\mathbf{x}), \quad \tilde{f}_h(\mathbf{x}) = f(\mathbf{x}) - \frac{h}{2}f'(\mathbf{x})f(\mathbf{x}), \tag{2}$$

with flow $\tilde{\varphi}_t$ (for simplicity, the dependence of this flow on the parameter h is not incorporated in the notation).

Motivation

Example (Continuation)

$$\begin{aligned}\tilde{\varphi}_h(\mathbf{x}) &= \mathbf{x} + h\tilde{f}_h(\mathbf{x}) + \frac{h^2}{2}\tilde{f}_h'(\mathbf{x})\tilde{f}_h(\mathbf{x}) + \mathcal{O}(h^3) \\ &= \mathbf{x} + h\left(f(\mathbf{x}) - \frac{h}{2}f'(\mathbf{x})f(\mathbf{x})\right) + \frac{h^2}{2}\tilde{f}_h'(\mathbf{x})\tilde{f}_h(\mathbf{x}) + \mathcal{O}(h^3) \\ &= \mathbf{x} + hf(\mathbf{x}) + \mathcal{O}(h^3).\end{aligned}$$

Thus, the Euler mapping $\psi_h(\mathbf{x})$, which differs from the flow φ_h of the system (1) being solved in $\mathcal{O}(h^2)$ terms (first-order consistency), differs from the flow $\tilde{\varphi}_h$ of the modified system (2) in $\mathcal{O}(h^3)$ terms (second-order consistency).

Motivation

Example. The harmonic oscillator

Let us particularize the preceding example to the case of the harmonic oscillator. The modified system (2) is found to be

$$\frac{dq}{dt} = p + \frac{h}{2}q, \quad \frac{dp}{dt} = -q + \frac{h}{2}p,$$

and from here a simple computation yields for the radius $r = (q^2 + p^2)^{1/2}$

$$\frac{dr}{dt} = \frac{h}{2}r.$$

So that, over a time interval of length h, r is multiplied by the factor $\exp(h^2/2) = 1 + h^2/2 + \mathcal{O}(h^3)$.
This **coincides with what we found for the Euler solution of the harmonic oscillator which was not stable** (but the $\mathcal{O}(h^3)$ remainder here will not coincide with the one before, because there is an $O(h^3)$ difference between ψ_h and $\tilde{\varphi}_h$).

Motivation

Example

In (2), $\tilde{f}_h(\mathbf{x})$ **is a first-degree polynomial in** h. If $\tilde{f}_h(\mathbf{x})$ is chosen to be quadratic in h, i.e.,

$$\tilde{f}_h = f - \frac{h}{2} f' f + h^2 f_2,$$

for some f_2, **it is possible to determine** f_2 **so as to achieve** $\psi_h - \tilde{\varphi}_h = \mathcal{O}(h^4)$ for the Euler map $\psi_h(\mathbf{x}) = \mathbf{x} + hf(\mathbf{x})$.
Similarly, **taking** $\tilde{f}_h(\mathbf{x})$ **as a suitable chosen polynomial in** h **with degree** $\mu = 3, 4, \ldots$ **it is possible to achieve** $\psi_h - \tilde{\varphi}_h = \mathcal{O}(h^{\mu+2})$.

Definition

Definition

Given a (consistent) integrator ψ_h for the system (1), there exists a (unique) *formal series in powers of* h

$$\tilde{f}_h^{\infty}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + h^2 g^{[2]}(\mathbf{x}) + \cdots , \tag{3}$$

where $g^{[\mu]}$ maps the space $\mathbb{R}^D$ into itself, with the property that, for each $\mu = 0, 1, \ldots$, the flow $\tilde{\varphi}_h^{[\mu]}$ of the modified system

$$\frac{d}{dt}\mathbf{x} = \tilde{f}_h^{[\mu]}(\mathbf{x}), \quad \tilde{f}_h^{[\mu]}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + \cdots + h^{\mu} g^{[\mu]}(\mathbf{x}), \tag{4}$$

satisfies

$$\psi_h(\mathbf{x}) - \tilde{\varphi}_h^{[\mu]}(\mathbf{x}) = \mathcal{O}(h^{\mu+2}). \tag{5}$$

Furthermore, for a symmetric method, the odd-numbered $g^{[\mu]}(\mathbf{x})$ are identically zero[3]:

$$g^{[1]}(\mathbf{x}) = g^{[3]}(\mathbf{x}) = g^{[5]}(\mathbf{x}) = \cdots = 0.$$

[3] Section 4.3.3 in Leimkuhler and Reich, *Simulating Hamiltonian dynamics*, 2004. *The order of a symmetric integrator is an even integer.*

Definition

As μ increases, the solutions of the modified system (4) **provide better and better approximations to ψ_h.**

For some vector fields f and some integrators, it may happen that the formal series (3) converges for each $\mathbf{x}$ and that the flow $\tilde{\varphi}_h^{[\infty]}$ of

$$\frac{d}{dt}\mathbf{x} = \tilde{f}_h^{\infty}(\mathbf{x}) \tag{6}$$

coincides with ψ_h. In those cases, (6) provides an **exact** modified system to study ψ_h.

However, such situations are exceptional. In general, discrete dynamical systems possess features that cannot appear in flows of autonomous systems. **The lack of convergence of** (3) **makes necessary to consider the truncations in** (4) **which do not exactly reproduce ψ_h but approximate it with an error as in** (5).

It is possible, by increasing μ as h becomes smaller, to make the discrepancy $\psi_h(\mathbf{x}) - \tilde{\varphi}_h^{[\mu(h)]}(\mathbf{x})$ exponentially small with respect to h, as proved by Neishtadt[4].

[4] Section 10.1 in Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994.

Finding explicitly the modified equations

Finding explicitly the modified equations

For splitting integrators, the terms of the series (3) may be found explicitly by using the **Baker-Campbell-Hausdorff (BCH) formula**[5].

The next theorem provides a summary of some key points.

[5] Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994

Finding explicitly the modified equations

Theorem

Assume that the system $\frac{d}{dt}\mathbf{x} = f(\mathbf{x}) = f^{(A)}(\mathbf{x}) + f^{(B)}(\mathbf{x})$ *is integrated by means of any (consistent) splitting method. The series* (3) *is of the form*

$$\left(f^{(A)} + f^{(B)}\right) + hC_{1,1}[f^{(A)}, f^{(B)}]$$
$$+ h^2\left(C_{2,1}[f^{(A)}, [f^{(A)}, f^{(B)}]] + C_{2,2}[f^{(B)}, [f^{(A)}, f^{(B)}]]\right) + \cdots$$

where, for each $\mu = 1, 2, \ldots$, ***the coefficient of*** h^μ ***is a linear combination of linearly independent iterated commutators involving*** $\mu + 1$ ***fields*** $f^{(A)}, f^{(B)}$.
The coefficients $C_{i,j}$ ***are known polynomials on the coefficients*** a_k ***and*** b_l ***of the splitting integrator***.
If the splitting is palindromic, then all ***the coefficients*** $C_{2i+1,j}$ ***corresponding to odd powers of*** h ***vanish***.

Finding explicitly the modified equations

Even though the method is the same for more involved integrators, we will give the details for the particular case of the *Lie-Trotter splitting algorithm* $\psi_h = \varphi_h^{(B)} \circ \varphi_h^{(A)}$.

Finding explicitly the modified equations

Even though the method is the same for more involved integrators, we will give the details for the particular case of the *Lie-Trotter splitting algorithm* $\psi_h = \varphi_h^{(B)} \circ \varphi_h^{(A)}$.

There are two steps: (i) **flows are represented as exponentials**

Finding explicitly the modified equations

Even though the method is the same for more involved integrators, we will give the details for the particular case of the *Lie-Trotter splitting algorithm* $\psi_h = \varphi_h^{(B)} \circ \varphi_h^{(A)}$.

There are two steps: (i) **flows are represented as exponentials**, and (ii) **exponentials are combined by means of the BCH formula**.

Finding explicitly the modified equations

Associated with the vector field $f(\mathbf{x})$ in the differential system $\frac{d}{dt}\mathbf{x} = f(\mathbf{x})$ with flow φ_t, there is a **Lie derivative** D_f. This is the first-order differential operator that maps each smooth function $\chi : \mathbb{R}^D \to \mathbb{R}$ into a new function $D_f\chi : \mathbb{R}^D \to \mathbb{R}$ defined as follows:

$$(D_f\chi)(\mathbf{x}) = \sum_{i=1}^{D} f^i(\mathbf{x}) \frac{\partial}{\partial x^i} \chi(\mathbf{x}).$$

Finding explicitly the modified equations

Associated with the vector field $f(\mathbf{x})$ in the differential system $\frac{d}{dt}\mathbf{x} = f(\mathbf{x})$ with flow φ_t, there is a **Lie derivative** D_f. This is the first-order differential operator that maps each smooth function $\chi : \mathbb{R}^D \to \mathbb{R}$ into a new function $D_f\chi : \mathbb{R}^D \to \mathbb{R}$ defined as follows:

$$(D_f\chi)(\mathbf{x}) = \sum_{i=1}^{D} f^i(\mathbf{x}) \frac{\partial}{\partial x^i}\chi(\mathbf{x}).$$

The chain rule leads to the formula

$$\frac{d}{dt}\chi\left(\varphi_t(\mathbf{x})\right)\Big|_{t=0} = (D_f\chi)(\mathbf{x}),$$

which shows the meaning of $(D_f\chi)(\mathbf{x})$ **as a rate of change of** χ **along the solution** $\varphi_t(\mathbf{x})$ **of** $\frac{d}{dt}\mathbf{x} = f(\mathbf{x})$.

Finding explicitly the modified equations

By successively applying this formula to the functions $D_f\chi, D_f(D_f\chi), \ldots$, we find

$$\frac{d^k}{dt^k}\chi\left(\varphi_t(\mathbf{x})\right)\Big|_{t=0} = (D_f^k\chi)(\mathbf{x}), \quad k = 2, 3, \ldots,$$

where D_f^k is the k-th order differential operator defined inductively as

$$(D_f^k\chi)(\mathbf{x}) = \left(D_f(D_f^{k-1}\chi)\right)(\mathbf{x}), \quad k = 2, 3, \ldots$$

Finding explicitly the modified equations

By successively applying this formula to the functions $D_f\chi, D_f(D_f\chi), \ldots$, we find

$$\frac{d^k}{dt^k}\chi\left(\varphi_t(\mathbf{x})\right)\Big|_{t=0} = (D_f^k\chi)(\mathbf{x}), \quad k = 2, 3, \ldots,$$

where D_f^k is the k-th order differential operator defined inductively as

$$(D_f^k\chi)(\mathbf{x}) = \left(D_f(D_f^{k-1}\chi)\right)(\mathbf{x}), \quad k = 2, 3, \ldots$$

Therefore, the Taylor expansion of $\chi\left(\varphi_t(\mathbf{x})\right)$ at $t = 0$ reads

$$\chi\left(\varphi_t(\mathbf{x})\right) = \sum_{k=0}^{\infty} \frac{t^k}{k!}(D_f^k\chi)(\mathbf{x}),$$

or

$$\chi\left(\varphi_t(\mathbf{x})\right) = \left(\exp\left(tD_f\right)\chi\right)(\mathbf{x}).$$

This formula may be used to retrieve, at least formally, φ_t: its application with χ equal to the coordinate function $\chi(\mathbf{x}) = x^i$, $i = 1, \ldots, D$, yields the i-th component of the vector $\varphi_t(\mathbf{x})$.

Finding explicitly the modified equations

In conclusion, the equality

$$\chi \circ \varphi_t = \exp(tD_f)\chi \tag{7}$$

may be understood as a **representation of the flow of a differential system as the exponential of the Lie operator of its vector field**.

If $f^{(A)}$ and $f^{(B)}$ are vector fields, then the compositions $D_{f^{(A)}} D_{f^{(B)}}$ and $D_{f^{(B)}} D_{f^{(A)}}$ are **second-order differential operators**. However, it is easily checked that $D_{f^{(A)}} D_{f^{(B)}} - D_{f^{(B)}} D_{f^{(A)}}$ is a **first-order differential operator**.

Proposition[6]

$D_{f^{(A)}} D_{f^{(B)}} - D_{f^{(B)}} D_{f^{(A)}}$ is the Lie operator corresponding to the vector field $[f^{(A)}, f^{(B)}]$.

[6] Section 39 in Arnold, *Mathematical methods of classical mechanics*, 1989.

Finding explicitly the modified equations

If now $\varphi_t^{(A)}$, $\varphi_t^{(B)}$ are the flows corresponding to the vector fields $f^{(A)}$ and $f^{(B)}$ respectively, two applications of (7) give

$$\begin{aligned}\chi \circ \left(\varphi_s^{(B)} \circ \varphi_t^{(A)}\right) &= \left(\chi \circ \varphi_s^{(B)}\right) \circ \varphi_t^{(A)} = \exp\left(tD_{f^{(A)}}\right)\left(\chi \circ \varphi_s^{(B)}\right) \\ &= \exp\left(tD_{f^{(A)}}\right)\left(\exp\left(sD_{f^{(B)}}\right)\chi\right) \qquad (8) \\ &= \left(\exp\left(tD_{f^{(A)}}\right)\exp\left(sD_{f^{(B)}}\right)\right)\chi.\end{aligned}$$

Finding explicitly the modified equations

If now $\varphi_t^{(A)}$, $\varphi_t^{(B)}$ are the flows corresponding to the vector fields $f^{(A)}$ and $f^{(B)}$ respectively, two applications of (7) give

$$\begin{aligned}\chi \circ \left(\varphi_s^{(B)} \circ \varphi_t^{(A)}\right) &= \left(\chi \circ \varphi_s^{(B)}\right) \circ \varphi_t^{(A)} = \exp\left(tD_{f^{(A)}}\right)\left(\chi \circ \varphi_s^{(B)}\right) \\ &= \exp\left(tD_{f^{(A)}}\right)\left(\exp\left(sD_{f^{(B)}}\right)\chi\right) \qquad (8) \\ &= \left(\exp\left(tD_{f^{(A)}}\right)\exp\left(sD_{f^{(B)}}\right)\right)\chi.\end{aligned}$$

Thus, **the operator** $\exp\left(tD_{f^{(A)}}\right)\exp\left(sD_{f^{(B)}}\right)$ **represents** $\varphi_s^{(B)} \circ \varphi_t^{(A)}$ **in analogy with** (7).

Finding explicitly the modified equations

Note that the A flow acts first in the composition $\varphi_s^{(B)} \circ \varphi_t^{(A)}$ while $\exp\left(tD_{f(A)}\right)$ acts second in the product of operators $\exp\left(tD_{f(A)}\right) \exp\left(sD_{f(B)}\right)$.

Finding explicitly the modified equations

Note that the A flow acts first in the composition $\varphi_s^{(B)} \circ \varphi_t^{(A)}$ while $\exp\left(tD_{f(A)}\right)$ acts second in the product of operators $\exp\left(tD_{f(A)}\right)\exp\left(sD_{f(B)}\right)$.

Our task now is to write it as a single exponential.

Finding explicitly the modified equations

Assume for the time being that X and Y are two square matrices of the same dimension. It is well known that *the product* $\exp(X)\exp(Y)$ *of their exponentials only coincides with* $\exp(X+Y)$ *if* X *and* Y *commute*.

Finding explicitly the modified equations

Assume for the time being that X and Y are two square matrices of the same dimension. It is well known that *the product* $\exp(X)\exp(Y)$ *of their exponentials only coincides with* $\exp(X+Y)$ *if* X *and* Y *commute*.In fact, by multiplying out

$$\exp(X) = I + X + \frac{1}{2}X^2 + \frac{1}{6}X^3 + \cdots$$

and

$$\exp(Y) = I + Y + \frac{1}{2}Y^2 + \frac{1}{6}Y^3 + \cdots$$

we find

$$\exp(X)\exp(Y) = I + X + Y + \frac{1}{2}X^2 + XY + \frac{1}{2}Y^2 + \frac{1}{6}X^3 + \frac{1}{2}X^2Y + \frac{1}{2}XY^2 + \frac{1}{6}Y^3 + \cdots$$

The products in the right-hand side are all of the form X^kY^l, while the expansion of $\exp(X+Y)$ gives rise to products like YX, Y^2X, YX^2, XYX, YXY, etc.

Finding explicitly the modified equations

The **Baker-Campbell-Hausdorff (BCH) formula**[7] writes $\exp(X)\exp(Y)$ as the exponential $\exp(Z)$ of a matrix

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] + \frac{1}{12}[Y,[Y,X]] + \frac{1}{24}[X,[Y,[Y,X]]] - \frac{1}{720}[Y,[Y,[Y,[Y,X]]]] + \cdots,$$

where $[\cdot,\cdot]$ denotes the commutator, e.g., $[X,Y] = XY - YX$.

[7] Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994; Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Finding explicitly the modified equations

The **Baker-Campbell-Hausdorff (BCH) formula**[7] writes $\exp(X)\exp(Y)$ as the exponential $\exp(Z)$ of a matrix

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] + \frac{1}{12}[Y,[Y,X]] + \frac{1}{24}[X,[Y,[Y,X]]] - \frac{1}{720}[Y,[Y,[Y,[Y,X]]]] + \cdots,$$

where $[\cdot,\cdot]$ denotes the commutator, e.g., $[X,Y] = XY - YX$.

The recipe to write down the terms in the right-hand side is of no consequence for our purposes now; what is remarkable is that **this right-hand side is a combination of X, Y and iterated commutators**.

[7] Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994; Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Finding explicitly the modified equations

Now the BCH is valid, we can substitute the X and Y matrices by elements of any associative, non-commutative algebra. In particular it may be applied to the case where X **and** Y **are first-order differential operators as those considered above**.
Going back to (8), and recalling that the commutator of the Lie derivatives corresponds to the Lie bracket of the vector fields, the BCH formula with $s = t = h$ then yields

$$\varphi_s^{(B)} \circ \varphi_t^{(A)} = \exp hD_{f_h^\infty},$$

where f_h^∞ is the vector field

$$f_h^\infty = f^{(A)} + f^{(B)} + \frac{h}{2}[f^{(A)}, f^{(B)}] + \frac{h^2}{12}[f^{(A)}, [f^{(A)}, f^{(B)}]] + \cdots$$

Finding explicitly the modified equations

Now the BCH is valid, we can substitute the X and Y matrices by elements of any associative, non-commutative algebra. In particular it may be applied to the case where X **and** Y **are first-order differential operators as those considered above**.
Going back to (8), and recalling that the commutator of the Lie derivatives corresponds to the Lie bracket of the vector fields, the BCH formula with $s = t = h$ then yields

$$\varphi_s^{(B)} \circ \varphi_t^{(A)} = \exp hD_{f_h^\infty},$$

where f_h^∞ is the vector field

$$f_h^\infty = f^{(A)} + f^{(B)} + \frac{h}{2}[f^{(A)}, f^{(B)}] + \frac{h^2}{12}[f^{(A)}, [f^{(A)}, f^{(B)}]] + \cdots$$

Now, a comparison with (7) shows that $\varphi_s^{(B)} \circ \varphi_t^{(A)}$ **is formally the** h**-flow of** f_h^∞, or, in other words, that f_h^∞ **is the modified vector-field for the Lie-Trotter splitting algorithm**.

Modified equations and order

Modified equations and order

If in the series $\tilde{f}_h^{\infty}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + h^2 g^{[2]}(\mathbf{x}) + \cdots$, the functions $g^{[1]}, \ldots, g^{[\mu-1]}$, $\mu \geq 2$, vanish so that

$$\tilde{f}_h^{[\mu]}(\mathbf{x}) - f(\mathbf{x}) = h^{\mu} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+1}),$$

then, the flow $\tilde{\varphi}_h^{[\mu]}$ and the flow φ_h will satisfy

$$\tilde{\varphi}_h^{[\mu]}(\mathbf{x}) - \varphi_h(\mathbf{x}) = h^{\mu+1} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+2})$$

which, in view of $\psi_h(\mathbf{x}) - \tilde{\varphi}_h^{[\mu]}(\mathbf{x}) = \mathcal{O}(h^{\mu+2})$, implies that

$$\psi_h - \varphi_h(x) = h^{\mu+1} g^{[\mu]}(x) + \mathcal{O}(h^{\mu+2}),$$

i.e., that **the integrator** $\psi_h(x)$ **has order** μ **(or higher)**.

Modified equations and order

If in the series $\tilde{f}_h^{\infty}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + h^2 g^{[2]}(\mathbf{x}) + \cdots$, the functions $g^{[1]}, \ldots, g^{[\mu-1]}$, $\mu \geq 2$, vanish so that

$$\tilde{f}_h^{[\mu]}(\mathbf{x}) - f(\mathbf{x}) = h^{\mu} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+1}),$$

then, the flow $\tilde{\varphi}_h^{[\mu]}$ and the flow φ_h will satisfy

$$\tilde{\varphi}_h^{[\mu]}(\mathbf{x}) - \varphi_h(\mathbf{x}) = h^{\mu+1} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+2})$$

which, in view of $\psi_h(\mathbf{x}) - \tilde{\varphi}_h^{[\mu]}(\mathbf{x}) = \mathcal{O}(h^{\mu+2})$, implies that

$$\psi_h - \varphi_h(x) = h^{\mu+1} g^{[\mu]}(x) + \mathcal{O}(h^{\mu+2}),$$

i.e., that **the integrator** $\psi_h(x)$ **has order** μ **(or higher)**.
The converse is also true, because the argument may be reversed: order $\geq \mu$ implies that $g^{[1]}, \ldots, g^{[\mu-1]}$ must vanish.

Modified equations and order

If in the series $\tilde{f}_h^{\infty}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + h^2 g^{[2]}(\mathbf{x}) + \cdots$, the functions $g^{[1]}, \ldots, g^{[\mu-1]}$, $\mu \geq 2$, vanish so that

$$\tilde{f}_h^{[\mu]}(\mathbf{x}) - f(\mathbf{x}) = h^{\mu} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+1}),$$

then, the flow $\tilde{\varphi}_h^{[\mu]}$ and the flow φ_h will satisfy

$$\tilde{\varphi}_h^{[\mu]}(\mathbf{x}) - \varphi_h(\mathbf{x}) = h^{\mu+1} g^{[\mu]}(\mathbf{x}) + \mathcal{O}(h^{\mu+2})$$

which, in view of $\psi_h(\mathbf{x}) - \tilde{\varphi}_h^{[\mu]}(\mathbf{x}) = \mathcal{O}(h^{\mu+2})$, implies that

$$\psi_h - \varphi_h(x) = h^{\mu+1} g^{[\mu]}(x) + \mathcal{O}(h^{\mu+2}),$$

i.e., that **the integrator $\psi_h(x)$ has order μ (or higher)**.
The converse is also true, because the argument may be reversed: order $\geq \mu$ implies that $g^{[1]}, \ldots, g^{[\mu-1]}$ must vanish.
From $g^{[1]}(\mathbf{x}) = g^{[3]}(\mathbf{x}) = g^{[5]}(\mathbf{x}) = \cdots = 0$, **the order of a symmetric method must be an even integer**.

Modified equations and order

To sum up, we have the following result, which *makes it possible to use the series*

$$\tilde{f}_h^{\infty}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + h^2 g^{[2]}(\mathbf{x}) + \cdots \tag{9}$$

rather than the mapping ψ_h to study the order of a given integrator.

Theorem

- A (consistent) integrator has order $\geq \nu$, $\nu \geq 2$, if and only if the functions $g^{[1]}, \ldots, g^{[\nu-1]}$ appearing in (9) are identically zero.
- When the order is exactly ν, $\nu = 1, 2, \ldots$, the leading term of the truncation error is $h^{\nu+1} g^{[\nu]}(x)$.
- A (consistent) symmetric integrator has even order.

Modified equations and order

The standard way to write down the order conditions for splitting methods is provided by the previous theorem and a result from the beginning of the section:

$$\tilde{f}_h^{\infty}(\mathbf{x}) = \left(f^{(A)} + f^{(B)}\right) + hC_{1,1}[f^{(A)}, f^{(B)}] + h^2\left(C_{2,1}[f^{(A)}, [f^{(A)}, f^{(B)}]] + C_{2,2}[f^{(B)}, [f^{(A)}, f^{(B)}]]\right) + \cdots$$

Specifically, **order** $\geq \nu$ **is equivalent to** $C_{i,j} = 0$ **whenever** $i < \nu$**.**

Modified equations and order

The standard way to write down the order conditions for splitting methods is provided by the previous theorem and a result from the beginning of the section:

$$\tilde{f}_h^{\infty}(\mathbf{x}) = \left(f^{(A)} + f^{(B)}\right) + hC_{1,1}[f^{(A)}, f^{(B)}] + h^2\left(C_{2,1}[f^{(A)}, [f^{(A)}, f^{(B)}]] + C_{2,2}[f^{(B)}, [f^{(A)}, f^{(B)}]]\right) + \cdots$$

Specifically, **order $\geq \nu$ is equivalent to $C_{i,j} = 0$ whenever $i < \nu$.**

- The Lie-Trotter formula has $\nu = 1$, and the leading term of the local error is a constant multiple of $h^2[f^{(A)}, f^{(B)}]$.
- The condition $C_{1,1} = 0$ is necessary and sufficient for an integrator to have order $\nu \geq 2$. **It is automatically satisfied for palindromic formulas**.
- Strang's formula has order exactly 2. The coefficient of h^3 in the expansion of the local error is a combination of iterated commutators with three fields.
- To have order $\nu \geq 3$ we have to impose the order conditions $C_{1,1} = 0$, $C_{2,1} = 0$, $C_{2,2} = 0$.

Modified equations and geometric integrators

Modified equations and geometric integrators

The geometric properties of integrators have a clear impact on their modified systems.

If the split systems are Hamiltonian with Hamiltonian functions $H^{(A)}$ and $H^{(B)}$, then it is feasible to work with iterated Poisson brackets of $H^{(A)}$ and $H^{(B)}$ rather than with the iterated Lie brackets of $f^{(A)}$ and $f^{(B)}$. Then, the expansion used before is replaced by

$$\left(H^{(A)}+H^{(B)}\right)+hC_{1,1}\{H^{(A)},H^{(B)}\}$$
$$+h^2\left(C_{2,1}\{H^{(A)},\{H^{(A)},H^{(B)}\}\}+C_{2,2}\{H^{(B)},\{H^{(A)},H^{(B)}\}\}\right)+\cdots$$

For each μ, the modified system

$$\frac{d}{dt}\mathbf{x}=\tilde{f}_h^{[\mu]}(\mathbf{x}),\quad \tilde{f}_h^{[\mu]}(\mathbf{x})=f(\mathbf{x})+hg^{[1]}(\mathbf{x})+\cdots+h^{\mu}g^{[\mu]}(\mathbf{x})$$

is a **Hamiltonian system**.

Modified equations and geometric integrators

The geometric properties of integrators have a clear impact on their modified systems.

If the split systems are Hamiltonian with Hamiltonian functions $H^{(A)}$ and $H^{(B)}$, then it is feasible to work with iterated Poisson brackets of $H^{(A)}$ and $H^{(B)}$ rather than with the iterated Lie brackets of $f^{(A)}$ and $f^{(B)}$. Then, the expansion used before is replaced by

$$\left(H^{(A)} + H^{(B)}\right) + hC_{1,1}\{H^{(A)}, H^{(B)}\}$$
$$+ h^2\left(C_{2,1}\{H^{(A)}, \{H^{(A)}, H^{(B)}\}\} + C_{2,2}\{H^{(B)}, \{H^{(A)}, H^{(B)}\}\}\right) + \cdots$$

For each μ, the modified system

$$\frac{d}{dt}\mathbf{x} = \tilde{f}_h^{[\mu]}(\mathbf{x}), \quad \tilde{f}_h^{[\mu]}(\mathbf{x}) = f(\mathbf{x}) + hg^{[1]}(\mathbf{x}) + \cdots + h^\mu g^{[\mu]}(\mathbf{x})$$

is a **Hamiltonian system**.

This is a reflection of the fact that *splitting integrators give rise to mappings ψ_h that are symplectic*.

Modified equations and geometric integrators

Informally, we may say that all integrators change the system being integrated into a modified system; in nonsymplectic methods the change is such that the modified system is no longer Hamiltonian. **Symplectic methods are those that change Hamiltonian systems into Hamiltonian systems**.

Modified equations and geometric integrators

Informally, we may say that all integrators change the system being integrated into a modified system; in nonsymplectic methods the change is such that the modified system is no longer Hamiltonian. **Symplectic methods are those that change Hamiltonian systems into Hamiltonian systems**.

This heuristic description cannot be made entirely rigorous because, as pointed out above, the exact modified system (6) only exists in a formal sense due to the lack of convergence of the series in (3). **The existence of Hamiltonian modified system is at the basis of many favourable properties of symplectic integrators**.

Conservation of energy by symplectic integrators

Conservation of energy by symplectic integrators

As noted above, Neishtadt proved that, under suitable regularity assumptions, **the modified system may be chosen so as to ensure that its h-flow is exponentially close to the mapping ψ_h.**

For symplectic integrators, the modified system is Hamiltonian and therefore exactly preserves its own Hamiltonian function that we denote by $\tilde{H}_h$. It follows that, except for exponentially small errors, ψ_h **preserves** $\tilde{H}_h$.

On the other hand, for a symplectic integrator of order ν, **the difference between $\tilde{H}_h$ and H is $\mathcal{O}(h^\nu)$.**

These considerations make it possible to prove that **symplectic integrators preserve the value of the Hamiltonian H of the system being integrated with error $\mathcal{O}(h^\nu)$** over time intervals $0 \leq t \leq T_h$ whose length T_h increases exponentially as $h \to 0$[8].

[8] Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006.

Conservation of energy by symplectic integrators

For linear problems, **an exact modified system exists** and, using the same argument, we may conclude that the **error in energy of a symplectic integrator has an $\mathcal{O}(h^\nu)$ bound** over the infinite interval $0 \leq t < \infty$. In other words, the *energy error may be bounded independently of the number of steps taken*.

Conservation of energy by symplectic integrators

For linear problems, **an exact modified system exists** and, using the same argument, we may conclude that the **error in energy of a symplectic integrator has an $\mathcal{O}(h^\nu)$ bound** over the infinite interval $0 \leq t < \infty$. In other words, the *energy error may be bounded independently of the number of steps taken*.

This is the case of the harmonic oscillator.

Geometric integrators and the harmonic problem

Geometric integrators and the harmonic problem

We take again as a model problem the integration of the harmonic oscillator, for which a time step $(q_{n+1}, p_{n+1}) = \psi_h(q_n, p_n)$ may be expressed as

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \tilde{M}_h \begin{bmatrix} q_n \\ p_n \end{bmatrix}, \quad \tilde{M}_h = \begin{bmatrix} A_h & B_h \\ C_h & D_h \end{bmatrix}. \tag{10}$$

for suitable method-dependent coefficients A_h, B_h, C_h, D_h.
We focus on (consistent) integrators that are both **symplectic** and **reversible**. In terms of the matrix $\tilde{M}_h$, the first of these properties corresponds to $A_h D_h - B_h C_h = 1$ and, when this condition holds, reversibility is equivalent to $A_h = D_h$. Our treatment follows Blanes, Casas, and Sanz-Serna, "Numerical Integrators for the Hybrid Monte Carlo Method", 2014.

Geometric integrators and the harmonic problem

The characteristic polynomial of $\tilde{M}_h$ is of the form $\lambda^2 - 2A_h\lambda + 1$, and there are four possibilities. The first two correspond to **unstable** simulations and the other two to **stable** simulations:

- h is such that $|A_h| > 1$. In that case, $\tilde{M}_h$ has spectral radius > 1 and, therefore, the powers $\tilde{M}_h^n$ grow exponentially with n.
- $A_h = \pm 1$ and $|B_h| + |C_h| > 0$. The powers $\tilde{M}_h^n$ grow linearly with n.
- $A_h = \pm 1$, $B_h = C_h = 0$, i.e., $\tilde{M}_h = \pm I$, $\tilde{M}_h^n = (\pm I)^n$.
- h is such that $|A_h| < 1$. In that case, $\tilde{M}_h$ has complex conjugate eigenvalues of unit modulus and the powers $\tilde{M}_h^n$, $n = 0, 1, \ldots$ remain bounded.

Geometric integrators and the harmonic problem

Comparing (10) with the result of setting $t = h$ in

$$M_t = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix},$$

we see that, by consistency, $B_h = h + \mathcal{O}(h^2)$ and $C_h = -h + \mathcal{O}(h^2)$, and, therefore, $A_h = (1 + B_h C_h)^{1/2} = 1 - h^2/2 + \mathcal{O}(h^3)$.

Thus, for $h > 0$ sufficiently small, $A_h < 1$ and the integration will be stable.

The **stability interval** of the integrator is the longest interval $(0, h_{max})$ such that integrations with $h \in (0, h_{max})$ are stable.

Geometric integrators and the harmonic problem

For each h such that $|A_h| \leq 1$, it is convenient to introduce $\theta_h \in \mathbb{R}$ such that $A_h = D_h = \cos\theta_h$. For $|A_h| < 1$, we have $\sin\theta_h \neq 0$ and we may define

$$\chi_h = B_h / \sin\theta_h. \tag{11}$$

In terms of θ_h and χ_h, the matrices in (10) and its n-th power are then

$$\tilde{M}_h = \begin{bmatrix} \cos\theta_h & \chi_h \sin\theta_h \\ -\chi_h^{-1} \sin\theta_h & \cos\theta_h \end{bmatrix} \tag{12}$$

and

$$\tilde{M}_h^n = \begin{bmatrix} \cos n\theta_h & \chi_h \sin n\theta_h \\ -\chi_h^{-1} \sin n\theta_h & \cos n\theta_h \end{bmatrix}. \tag{13}$$

For a value of h in the (stable) case $A_h = \pm 1$, $B_h = C_h = 0$, one has $\sin\theta_h = 0$, so that (11) does not make sense. However the matrix $\tilde{M}_h$ is of the form (12) for any choice of χ_h[9].

[9] Typically, for such a value of h, one may avoid the indeterminacy in the value of χ_h by taking limits as $\epsilon \to 0$ in $\chi_{h+\epsilon} = B_{h+\epsilon} / \sin\theta_{h+\epsilon}$.

Geometric integrators and the harmonic problem

For a method of order ν, $\chi_h = 1 + \mathcal{O}(h^\nu)$, $\theta_h = h + \mathcal{O}(h^{\nu+1})$ as $h \to 0$.

By comparing the numerical $\tilde{M}_h^n$ in (13) with the true M_{nh}, one sees that a method with $\theta_h = h$ would have no phase error: *the angular frequency of the rotation of the numerical solution would coincide with the true angular frequency of the harmonic oscillator*.

More generally, **the difference $\theta_h - h$ governs the phase error**. According to (13), this phase error grows linearly with n.

On the other hand, a method with $\chi_h = 1$ would have no energy error: the numerical solution would remain on the correct level curve of the Hamiltonian, i.e., on the circle $p^2 + q^2 = p_0^2 + q_0^2$. **The discrepancy between χ_h and 1 governs the energy errors**. In (13), we see that these are bounded as n grows.

Geometric integrators and the harmonic problem

The preceding considerations may alternatively be understood by considering the modified Hamiltonian given in the next result.

Proposition

Consider the application to the harmonic oscillator of a (consistent) reversible, volume-preserving integrator (10) and assume that the step size h is stable, so that $\tilde{M}_h$ may be written in the form (12). Then, ψ_h exactly coincides with the h-flow of the modified Hamiltonian

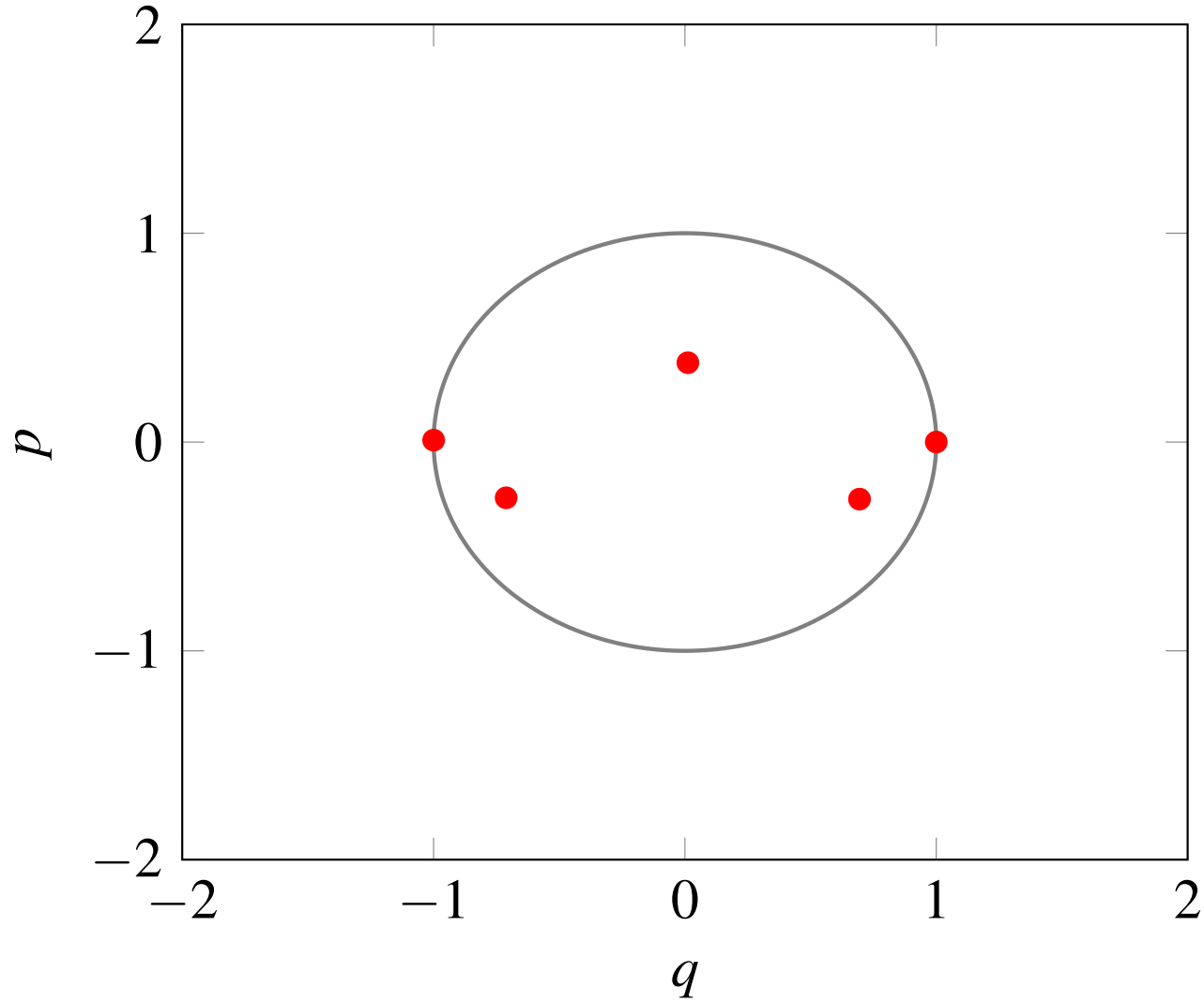
$$\tilde{H}_h = \frac{\theta_h}{2h}\left(\chi_h p^2 + \frac{1}{\chi_h} q^2\right).$$

In particular, numerical trajectories are contained in ellipses

$$\chi_h p^2 + \frac{1}{\chi_h} q^2 = \chi_h p_0^2 + \frac{1}{\chi_h} q_0^2$$

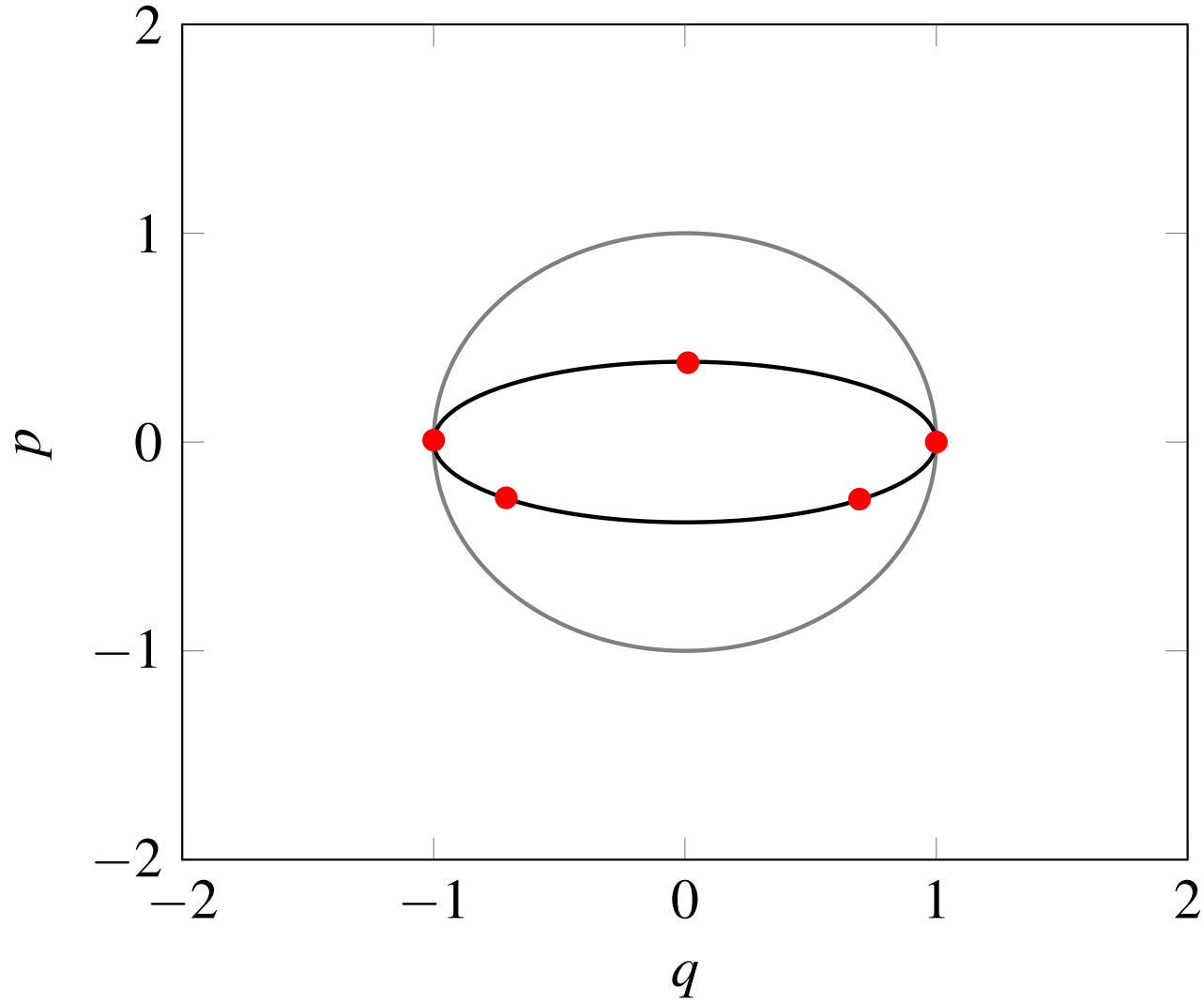
rather than in circles.

Geometric integrators and the harmonic problem



First five points along a discrete orbit of the velocity Verlet integrator initiated at $(q, p) = (1, 0)$ with $h = 1.85$. The gray contour line shows the corresponding level set of the true Hamiltonian.

Geometric integrators and the harmonic problem



Now we provide in black the associated level set of the modified Hamiltonian. It can be seen how the modified Hamiltonian is preserved.

Optimal stability of Strang's method

Optimal stability of Strang's method

Let us fix an integer N and consider consistent palindromic splitting integrators with $s = N$. Thus, it uses N evaluations of F per step.

The corresponding coefficient A_h in (10) is a polynomial of degree N in the variable $z = h^2$ (for obvious reasons, A_h is often called the **stability polynomial** of the integrator).

We pointed out above that consistency imposes the relation $A_h = 1 - z/2 + \mathcal{O}(h^2)$.

Our aim is to **identify**, among the class just described, **the polynomial** $A_h(z)$ **that satisfies** $|A_h(z)| < 1$ **for** $0 < h < h_{max}$**, with** h_{max} **as large as possible**.

Optimal stability of Strang's method

We sant to show that the desired $A_h(z)$ corresponds to the integrator

$$\psi_h = \underbrace{\psi^V_{h/N} \circ \cdots \circ \psi^V_{h/N}}_{N \text{ times}}, \tag{14}$$

where ψ^V_h is the mapping associated with the Strang/Verlet formula. Note that to carry out a step of length h with the method in (14) one just has to take N consecutive steps of length h/N of standard velocity Verlet. In other words, subject to stability, **if one wishes to take as long a step as possible with a budget of N evaluations of the force per step, the best choice is to concatenate N steps of Strang/Verlet**.

Optimal stability of Strang's method

To see the optimality of ψ_h in (14), we first note that, after expressing $\psi^V_{h/N}$ in terms of the A and B flows and merging consecutive B flows, the mapping (14) corresponds indeed to a palindromic splitting with N stages.
Then, we know that Verlet is stable for $0 < h < 2$, and this implies that (14) is stable for $0 < h/N < 2$.
In this way, (14) **has stability interval** $(0, 2N)$ and we shall prove next that *this is the longest possible*.

Optimal stability of Strang's method

Verlet with step size h/N has $A^V_{h/N} = 1 - h^2/(2N^2)$, which, in view of (12)-(13), implies that for (14) the coefficient A_h has the expression

$$\cos\theta_h = \cos\left(N\theta^V_{h/N}\right).$$

Recalling the definition $T_N(\cos\alpha) = \cos(N\alpha)$ of the *Chebyshev polynomial* T_N, we observe that for (14)

$$A_h(z) = T_N\left(1 - \frac{z}{2N^2}\right).$$

Well-known properties of T_N, imply that **no other polynomial $A_h(z)$ of degree $\leq N$ with $A_h = 1 - z/2 + \mathcal{O}(h^2)$ has modulus ≤ 1 in the interval** $-1 < 1 - z/(2N^2) < 1$, i.e., when $0 < h < 2N$.

Next session

- We will describe **constrained mechanical systems**.
- We will use this formalism for N-body systems where **holonomic constraints** are considered.
- We will present two classic **numerical methods**: SHAKE and RATTLE.
- We will show how the presented methods relate to **Hamiltonian mechanics** and to the **symplectic structure**.

- Arnold, V.I. *Mathematical methods of classical mechanics*. Vol. 60. Springer, 1989.
- Blanes, S., F. Casas, and J. M. Sanz-Serna. “Numerical Integrators for the Hybrid Monte Carlo Method”. In: *SIAM Journal of Scientific Computing* 36.4 (2014), A1556–A1580.
- Griffiths, D. and J. M. Sanz-Serna. “On the Scope of the Method of Modified Equations”. In: *SIAM Journal on Scientific and Statistical Computing* 7.3 (1986), pp. 994–1008.
- Hairer, E., C. Lubich, and G. Wanner. *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*. 2nd ed. Dordrecht: Springer, 2006.
- Leimkuhler, B. J. and S. Reich. *Simulating Hamiltonian dynamics*. Cambridge monographs on applied and computational mathematics. Cambridge: Cambridge University, 2004.

- Sanz-Serna, J. M. “Geometric integration”. In: *The state of the art in numerical analysis (York, 1996)*. Vol. 63. Oxford Univ. Press, New York, 1997, pp. 121–143.
- Sanz-Serna, J. M and M. P Calvo. *Numerical Hamiltonian problems*. 1st ed. Applied Mathematics and Mathematical Computation 7. London: Chapman & Hall, 1994.