Geometric Numerical Integration

1. Hamiltonian mechanics and numerical methods

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Motivation

- This course is devoted to the **study of numerical techniques used for simulating dynamical systems, especially conservative systems**. The emphasis of this course is on **Hamiltonian systems**

- In a dynamical simulation, **an integrator replaces a differential equation in continuous time by a difference equation defining approximate captures of the solution at discrete time steps**.

- More precisely, **geometric integrators are numerical methods that preserve geometric properties of the exact flow of a differential equation**.

Objectives

- Summary of **Hamiltonian mechanics**, and some well-known **numerical methods** and concepts related.
- Discussion of the **geometric structure of the Hamiltonians systems** and why **symplectic integrators** are interesting.
- Introduction to **modified equations** as a basic tool to study symplectic integrators.
- Summary of **constrained mechanical systems** relating them to realistic applications.
- Presentation of some recent developments in the field on molecular dynamics using **adaptive integrators**.

Index course

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

Preliminaries

Preliminaries

We are concerned with **autonomous systems** of differential equations in $\mathbb{R}^D$

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

where the function (**vector field**) f is assumed throughout to be defined in the whole of $\mathbb{R}^D$ and to be sufficiently smooth.

Preliminaries

An important role is played by the particular case

$$\frac{d}{dt}q = M^{-1}p, \qquad \frac{d}{dt}p = F(q), \tag{2}$$

where $x = (p, q) \in \mathbb{R}^D$, $D = 2d$, $q \in \mathbb{R}^d$, $p \in \mathbb{R}^d$ and M is a constant invertible matrix. So that, $f = (M^{-1}p, F(q))$.

By eliminating p, (2) is seen to be equivalent to

$$M\frac{d^2}{dt^2}q = F(q).$$

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This is not the most general autonomous system of second order differential equations in $\mathbb{R}^d$ because the derivative dq/dt does not appear in the right-hand side.

Preliminaries

When the forces depend only on the positions, **Newton's second law** for a mechanical system gives rise to differential equations of the form (2). Then, q, $(d/dt)q$, p, F are respectively the vectors of coordinates, velocities, momenta, and forces, and M is the matrix of masses.

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These are called **Hamilton equations of motion**.

Preliminaries

Definition

For a fixed real t, $\varphi_t : \mathbb{R}^D \to \mathbb{R}^D$ is the **t-flow** of the system under consideration

$$\frac{d}{dt}x = f(x), \tag{3}$$

and φ_t is the **map that associates with each $\alpha \in \mathbb{R}^D$ the value at time t of the solution of** (3) **that at the initial time 0 takes the initial value α.**

Preliminaries

Example. The harmonic oscillator

As a very simple but important example, we consider the standard **harmonic oscillator**, the system in $\mathbb{R}^2$ of the special form (2) given by

$$\frac{d}{dt}q = p, \qquad \frac{d}{dt}p = -q. \tag{4}$$

For future reference, we note that, with matrix notation, the solutions satisfy[1]:

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = M_t \begin{bmatrix} q(0) \\ p(0) \end{bmatrix}, \qquad M_t = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix}. \tag{5}$$

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

Example. The harmonic oscillator

Thus, the **flow** has the expression

$$\varphi_t(\xi, \eta) = (\xi \cos t + \eta \sin t, -\xi \sin t + \eta \cos t)\,. \tag{6}$$

When $\alpha = (\xi, \eta) \in \mathbb{R}^2$ is fixed and t varies, the right-hand side of (6) yields the solution that at $t = 0$ takes the initial value (ξ, η).
The notation $\varphi_t(\xi, \eta)$ emphasizes that, in the flow, it is **the parameter t that is seen as fixed, while $(\xi, \eta) \in \mathbb{R}^2$ is regarded as a variable**.
Geometrically, φ_t is **the clockwise rotation of angle t around the origin of the (q, p)-plane**.

Preliminaries

For a given system

$$\frac{d}{dt}x = f(x), \tag{7}$$

it is possible that for some choices of α *and* t*, the vector* $\varphi_t(\alpha) \in \mathbb{R}^D$ *is not defined*; this will happen if t is outside the interval in which the solution of (7) with initial value α exists.

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For simplicity, **we shall assume hereafter that** $\varphi_t(\alpha)$ **is always defined**.

Preliminaries

Flows possess the **group property**:

- For arbitrary real s and t,

$$\varphi_t \circ \varphi_s = \varphi_{s+t};$$

- for arbitrary real s, t and u,

$$(\varphi_t \circ \varphi_s) \circ \varphi_u = \varphi_{u+(s+t)} = \varphi_{(u+s)+t} = \varphi_t \circ (\varphi_s \circ \varphi_u);$$

- φ_0 is the indentity map;
- and, for each t,

$$(\varphi_t)^{-1} = \varphi_{-t}$$

  i.e., φ_{-t} is the inverse of the map φ_t.

Hamiltonian systems

Hamiltonian systems

Let us assume that the dimension D of

$$\frac{d}{dt}x = f(x) \tag{8}$$

is even, $D = 2d$, and let us write $x = (q, p)$ with $q, p \in \mathbb{R}^d$.

Then, the system (8) is said to be **Hamiltonian** if there is a function $H : \mathbb{R}^{2d} \to \mathbb{R}$ such that, for $i = 1, \ldots, d$, the scalar components f^i of f are given by

$$f^i(q,p) = \frac{\partial H}{\partial p^i}(q,p), \quad f^{d+i}(q,p) = -\frac{\partial H}{\partial q^i}(q,p).$$

Hamiltonian systems

Thus, the system is

$$\frac{d}{dt}q^i = \frac{\partial H}{\partial p^i}(q,p), \quad \frac{d}{dt}p^i = -\frac{\partial H}{\partial q^i}(q,p),$$

or, in vector notation[2],

$$\frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = J^{-1}\nabla H(q,p), \tag{9}$$

where

$$\nabla H = \left[\frac{\partial H}{\partial q^i}, \ldots, \frac{\partial H}{\partial q^d}, \frac{\partial H}{\partial p^1}, \ldots, \frac{\partial H}{\partial p^d}\right]^T$$

and

$$J = \begin{bmatrix} 0_{d\times d} & -I_{d\times d} \\ I_{d\times d} & 0_{d\times d} \end{bmatrix}.$$

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

Hamiltonian systems

The function H is called the **Hamiltonian**, $\mathbb{R}^{2d}$ is the **phase space**, and d is the **number of degrees of fredoom**.

[3] Bou-Rabee and Sanz-Serna, "Geometric integrators and the Hamiltonian Monte Carlo method", 2018

Hamiltonian systems

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Theorem[3]

A system of the special form

$$\frac{d}{dt}q = M^{-1}p, \quad \frac{d}{dt}p = F(q),$$

is Hamiltonian if and only if $F = -\nabla U(q)$ for a suitable real-valued function U, i.e.,

$$\frac{d}{dt}q = M^{-1}p, \quad \frac{d}{dt}p = -\nabla U(q).$$

[3] Bou-Rabee and Sanz-Serna, "Geometric integrators and the Hamiltonian Monte Carlo method", 2018

Hamiltonian systems

In the case of the theorem before,

$$H(q,p) = K(p) + U(q), \tag{10}$$

where

$$K(p) = \frac{1}{2} p^T M^{-1} p.$$

In mechanics, K and U are respectively the **kinetic** and **potential energy**, and H represents the **total energy** in the system.

The harmonic oscillator (4) provides the simplest example:

$$K = \frac{1}{2} p^2, \quad U = \frac{1}{2} q^2.$$

Hamiltonian systems

Example. The Lennard-Jones oscillator[4]

Another problem of interest is the anharmonic Lennard-Jones oscillators with Hamiltonians of the form $H(q,p) = p^2 + U(q)$, where

$$U(q) = 4\epsilon \left[\left(\frac{\sigma}{q} \right)^{12} - \left(\frac{\sigma}{q} \right)^{6} \right],$$

where ϵ is the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero (in this case $\sigma = 1$), and q is the distance between the particles.
In general, *the Lennard-Jones potential approximates the interaction between a pair of neutral atoms or molecules*.

[4] Leimkuhler and Reich, *Simulating Hamiltonian dynamics*, 2004.

Hamiltonian systems

Example. N-body problem

This model describes an homogeneous system of N bodies moving in $\mathbb{R}^3$ with masses m_i, $i = 1, \ldots, N$, interacting through a particle-particle interaction potential (**pair-potential**) $U(\mathbf{r})$, with $\mathbf{r}$ the distance between two particles. The corresponding equations of motion are

$$\frac{d}{dt}q_i = m_i^{-1}p_i, \quad \frac{d}{dt}p_i = -\sum_{i \neq j} \frac{\nabla U(r_{ij})}{r_{ij}}(q_i - q_j), \quad i = 1, 2, \ldots, N,$$

where $r_{ij} = \|q_i - q_j\|$. The Hamiltonian is

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\sum_{i=1}^{N} \frac{\|p_i\|^2}{m_i} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} U(r_{ij}). \tag{11}$$

Hamiltonian systems

Example. Molecular dynamics[5]

Molecular dynamics simulations require the solution of Hamiltonian systems with N degrees of freedom

$$\frac{d}{dt}\mathbf{q} = M^{-1}\mathbf{p}, \qquad \frac{d}{dt}\mathbf{p} = -\nabla U(\mathbf{q}),$$

where the total energy is given by (11) and U are given potential energies.
For instance, the Lennard-Jones potential is very popular in molecular dynamics (ϵ and σ are suitable constants depending on the atoms).

[5] Allen and Tildesley, *Computer Simulation of Liquids*, 1989.

Integrators

Integrators

Differential systems like the ones above have to be numerically integrated. The following works provide extensive reviews on the subject:

- Hairer, Nørsett, and Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*, 1993,
- Hairer and Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, 1996,
- Griffiths and H., *Numerical Methods for Ordinary Differential Equations: Initial Value Problems*, 2010,

Integrators

Each **one-step numerical method** or **one-step integrator** for

$$\frac{d}{dt}x = f(x) \tag{12}$$

is described by a map $\psi_h : \mathbb{R}^D \to \mathbb{R}^D$ that depends on a real parameter h called the **step size**.

Given an initial value α, and a value of h ($h \neq 0$), the integrator generates a **numerical trajectory**, $x_0, x_1, x_2, \ldots$, defined by $x_0 = \alpha$ and, iteratively,

$$x_{n+1} = \psi_h(x_n), \quad n = 0, 1, 2, \ldots$$

To compute x_{n+1} when x_n has already been found is to perform a **(time) step**.

Integrators

For each n, the vector x_n is an **approximation to the value at time $t_n = nh$ of the solution $x(t)$ of (12) with initial condition $x(0) = \alpha$**, i.e., to $\varphi_{t_n}(\alpha)$.

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Example. Euler's rule

The simplest and best known integrator, **Euler's rule**, with

$$x_{n+1} = x_n + hf(x_n), \tag{13}$$

corresponds to the mapping $\psi_h(x) = x + hf(x)$.
It uses one evaluation of f per step.

Integrators

Explicit s-stage Runge-Kutta formulas use s evaluations of f per step, $s = 1, 2, \ldots$, and are therefore s times more expensive per step than Euler's rule. Examples include **Runge's method**

$$x_{n+1} = x_n + hf\left(x_n + \frac{h}{2}f(x_n)\right)$$

with two stages.

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Remark

A method with s stages will be competitive with Euler's rule only if it gives more accurate approximations than Euler's rule when using a step size s times shorter, so as to equalize computational costs.

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Implicit Runge-Kutta integrators are also used. In them, ψ_h is defined by means of algebraic equations. For instance, the **midpoint rule** has

$$x_{n+1} = x_n + hf\left(\frac{1}{2}(x_n + x_{n+1})\right).$$

Integrators

Definition

A one-step integrator is called **symmetric** or **self-adjoint** if

$$(\psi_h)^{-1} = \psi_{-h},$$

so as to mimic the property of the exact solution flow

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The midpoint rule is a symmetric integrator. Explicit Runge-Kutta methods are never symmetric.

Integrators

For the exact solution, the sequence $x(0) = \alpha, x(t_1), x(t_2), \ldots$ satisfies $x(t_{n+1}) = \varphi_h(x(t_n))$, $n = 0, 1, \ldots$, rather than

$$x_{n+1} = \psi_h(x_n), \quad n = 0, 1, 2, \ldots$$

Thus, for the numerical integrator to make sense, **it is necessary that ψ_h is an approximation to φ_h.**

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Definition

The integrator is said to be **consistent** if, at each fixed $x \in \mathbb{R}^D$,

$$\psi_h(x) - \varphi_h(x) = \mathcal{O}(h^2), \quad h \to 0.$$

If $\psi_h(x) - \varphi_h(x) = \mathcal{O}(h^{\nu+1})$, ν a positive integer, then the integrator is (consistent) of **order** $\geq \nu$.
A method of order $\geq \nu$ that is not of order $\geq \nu + 1$ is said to *have* order ν.

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Euler's rule has order 1, the four-stage formulas of Kutta have order 4 and the midpoint rule has order 2.

Integrators

We shall see later that **the order of a symmetric integrator is an even integer**.

All integrators to be considered hereafter are assumed to be consistent.

Integrators

Definition

The vector $\psi_h(x) - \varphi_h(x)$ is called the **local error** at x: it is the *difference between the result of a single time step of the numerical method starting from* x *and the result of the application of the* h*-flow to the same point* x.

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Example. Local error for Euler's method

$$\psi_h(x) - \varphi_h(x) = (x + hf(x)) - \left(x + hf(x) + \frac{h^2}{2} f'(x)f(x) + \mathcal{O}(h^3) \right)$$

$$= -\frac{h^2}{2} f'(x)f(x) + \mathcal{O}(h^3).$$

In the expansion of the true solution flow we have used that $(d/dt)x = f(x)$ and $(d^2/dt^2)x = f'(x)(d/dt)x = f'(x)f(x)$.

Integrators

The local error does not give per se information on the **global error** at t_n, i.e., on the difference $x_n - x(t_n)$. This is because $x_n = \psi_h(x_{n-1})$ while $x(t_n)$ is the result of the application of the h-flow to $x(t_{n-1})$: ψ_h *and* φ_h *are not applied to the same point*[6]. However the following result holds:

Theorem. Global error

If the (one-step) integrator is consistent of order ν, then, for each fixed initial value $x_0 = x(0)$ and $T > 0$,

$$\max_{0 \le t_n \le T} |x_n - x(t_n)| = \mathcal{O}(h^\nu), \quad h \to 0+ .$$

Thus, the integrator is **convergent** of order ν.

[6] In order to bound the global error in terms of the local error, i.e., to obtain convergence from consistency, a stability property is needed. Hence the well-known slogan *stability + consistency imply convergence*.

The Lie bracket

The Lie bracket

If $\varphi_t^{(f)}$ and $\varphi_t^{(g)}$ denote respectively the flows of the D-dimensional systems

$$\frac{d}{dt}x = f(x), \qquad \frac{d}{dt}x = g(x),$$

in general $\varphi_s^{(g)} \circ \varphi_t^{(f)} \neq \varphi_t^{(f)} \circ \varphi_s^{(g)}$ for arbitrary t and s.

A Taylor expansion shows that, as t, s approach 0,

$$\varphi_s^{(g)}\left(\varphi_t^{(f)}(x)\right) - \varphi_t^{(f)}\left(\varphi_s^{(g)}(x)\right) = st[f,g](x) + \mathcal{O}\left(t^3 + s^3\right),$$

where the **Lie bracket** or **commutator**[7] $[f,g]$ of f and g is the mapping $\mathbb{R}^D \to \mathbb{R}^D$ that at $x \in \mathbb{R}^D$ takes the value

$$[f,g](x) = g'(x)f(x) - f'(x)g(x). \tag{14}$$

[7] Arnold, *Mathematical methods of classical mechanics*, 1989

The Lie bracket

Thus, the magnitude of $[f, g]$ **measures the lack of commutativity of the corresponding flows**. The following result holds:

Theorem

With the preceding notation, $\varphi_s^{(g)} \circ \varphi_t^{(f)} = \varphi_t^{(f)} \circ \varphi_s^{(g)}$ for arbitrary t and s if and only if the Lie bracket $[f, g](x)$ vanishes at each $x \in \mathbb{R}^D$.
If these conditions hold, we say that f and g **commute**.

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If these conditions hold, we say that f and g **commute**.

For commuting f and g, $\varphi_t^{(g)} \circ \varphi_t^{(f)} = \varphi_t^{(f)} \circ \varphi_t^{(g)}$ provides the t-flow of the system

$$\frac{d}{dt}x = f(x) + g(x).$$

The Lie bracket

Theorem. Poisson bracket of Hamiltonian functions [8]

If the fields f and g are Hamiltonian with Hamiltonian functions H and K respectively, i.e., $f = J^{-1}\nabla H$, $g = J^{-1}\nabla K$, then $[f, g]$ is also a Hamiltonian vector field.
Moreover, the Hamiltonian function of $[f, g]$ is given by $-\{H, K\}$,[9] where $\{H, K\}$ is the **Poisson bracket** of the functions H and K defined as

$$\{H, K\} = (\nabla H)^T J^{-1} \nabla K.$$

[8] Arnold, *Mathematical methods of classical mechanics*, 1989

[9] The minus sign here could be avoided by reversing the sign in the definition of the Poisson bracket.

Splitting methods

Splitting methods

- Euler's method and the other integrators mentioned above may be applied to any given autonomous system. Other techniques only make sense for particular classes of systems.

- Of special importance to us is the class of **splitting** integrators that we consider next.

- The monograph Blanes and Casas, *A Concise Introduction to Geometric Numerical Integration*, 2016 is a very good source of information.

Splitting methods

Splitting methods are applicable to cases where an autonomous system of differential equations may be split into two parts as

$$\frac{d}{dt}x = f(x) = f^{(A)}(x) + f^{(B)}(x), \tag{15}$$

in such a way that the flows $\varphi_t^{(A)}$ and $\varphi_t^{(B)}$ of the **split systems**

$$\frac{d}{dt}x = f^{(A)}(x), \qquad \frac{d}{dt}x = f^{(B)}(x), \tag{16}$$

are available analytically.

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To avoid trivial cases, *we shall hereafter assume that the Lie bracket* $[f^{(A)}, f^{(B)}]$ *does not vanish identically*.

Splitting methods

An important example are the following split systems[10]:

$$(A): \quad \frac{d}{dt}q = M^{-1}p, \quad \frac{d}{dt}p = 0 \tag{17}$$

and

$$(B): \quad \frac{d}{dt}q = 0, \quad \frac{d}{dt}p = F(q), \tag{18}$$

the flows are explicitly given by

$$\varphi_t^{(A)}(q,p) = (q + tM^{-1}p, p)$$

and

$$\varphi_t^{(B)}(q,p) = (q, p + tF(q)).$$

[10] They correspond to the Hamiltonian $H(q,p) = \frac{1}{2}p^T M^{-1}p + U(q)$, which is said to be **separable**.

Splitting methods

A simple Taylor expansion proves that the **Lie-Trotter formula**[11]

$$\psi_h = \varphi_h^{(B)} \circ \varphi_h^{(A)} \tag{19}$$

defines a first-order integrator for (15):

$$\psi_h(x) - \varphi_h(x) = \frac{h^2}{2}[f^{(A)}, f^{(B)}](x) + \mathcal{O}(h^3). \tag{20}$$

[11] Trotter, "On the Product of Semi-Groups of Operators", 1959

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Observe that the coefficient of the leading power of h is proportional to the Lie bracket.

While $f^{(A)}$ and $f^{(B)}$ contribute simultaneously to the change of x in (15), they do so successively in the Lie-Trotter integrator.

[11] Trotter, "On the Product of Semi-Groups of Operators", 1959

Splitting methods

The most popular splitting integrator for (15) corresponds to **Strang's formula**[12]

$$\psi_h = \varphi^{(B)}_{h/2} \circ \varphi^{(A)}_h \circ \varphi^{(B)}_{h/2},$$

which, as a Taylor expansion shows, has **second order accuracy**: $\psi_h(x) - \varphi_h(x) = \mathcal{O}(h^2)$ as $h \to 0$. More precisely,

$$\psi_h(x) - \varphi_h(x) = \frac{h^3}{12}[f^{(A)}, [f^{(A)}, f^{(B)}]](x) + \frac{h^3}{24}[f^{(B)}, [f^{(A)}, f^{(B)}]](x) + \mathcal{O}(h^4),$$

so that the leading term of the local error is a linear combination of two so-called *iterated Lie brackets*.

[12] Strang, "Accurate partial difference methods I: Linear cauchy problems", 1963

Splitting methods

When applied to the particular case

$$\frac{d}{dt}q = M^{-1}p, \qquad \frac{d}{dt}p = F(q), \tag{21}$$

the Strang formula yields the well-known **velocity Verlet integrator**, the method of choice in molecular dynamics:

$$\begin{aligned} p_{n+1/2} &= p_n + \frac{h}{2}F(q_n), \\ q_{n+1} &= q_n + hM^{-1}p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} + \frac{h}{2}F(q_{n+1}). \end{aligned}$$

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$$\frac{d}{dt}q = M^{-1}p, \qquad \frac{d}{dt}p = F(q), \tag{21}$$

the Strang formula yields the well-known **velocity Verlet integrator**, the method of choice in molecular dynamics:

$$\begin{aligned} p_{n+1/2} &= p_n + \frac{h}{2}F(q_n), \\ q_{n+1} &= q_n + hM^{-1}p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} + \frac{h}{2}F(q_{n+1}). \end{aligned}$$

The evaluations of F represent the bulk of the computational cost of the algorithm.

Splitting methods

When N steps of the method $\psi_h = \varphi^{(B)}_{h/2} \circ \varphi^{(A)}_h \circ \varphi^{(B)}_{h/2}$ are taken, the map that advances the numerical solution from x_0 to x_N, i.e.,

$$\psi_h^N = \underbrace{\left(\varphi^{(B)}_{h/2} \circ \varphi^{(A)}_h \circ \varphi^{(B)}_{h/2}\right) \circ \cdots \circ \left(\varphi^{(B)}_{h/2} \circ \varphi^{(A)}_h \circ \varphi^{(B)}_{h/2}\right)}_{N \text{ times}},$$

may be rewritten with the help of the group property[13] in the **leapfrog** form

$$\psi_h^N = \varphi^{(B)}_{h/2} \circ \underbrace{\left(\varphi^{(A)}_h \circ \varphi^{(B)}_h\right) \circ \cdots \circ \left(\varphi^{(A)}_h \circ \varphi^{(B)}_h\right)}_{N-1 \text{ times}} \circ \varphi^{(A)}_h \circ \varphi^{(B)}_{h/2}.$$

Now, the right hand-side only uses $N+1$ times the flow $\varphi^{(B)}_t$. In the particular case (21), the combination $\varphi^{(A)}_h \circ \varphi^{(B)}_h$ corresponds to the following formulas to advance the numerical solution:

$$\begin{aligned} p_{n+1/2} &= p_{n-1/2} + hF(q_n), \\ q_{n+1} &= q_n + hM^{-1}p_{n+1/2}. \end{aligned} \tag{22}$$

[13] $\varphi_t \circ \varphi_s = \varphi_{s+t}$

Splitting methods

Strang's method is symmetric:

$$\begin{aligned}(\psi_h)^{-1} &= \left(\varphi^{(B)}_{h/2}\right)^{-1} \circ \left(\varphi^{(A)}_{h}\right)^{-1} \circ \left(\varphi^{(B)}_{h/2}\right)^{-1} \\ &= \varphi^{(B)}_{-h/2} \circ \varphi^{(A)}_{-h} \circ \varphi^{(B)}_{-h/2} \\ &= \psi_{-h}.\end{aligned}$$

It is clear that the symmetry is a consequence of the **palindromic** structure of

$$\psi_h = \varphi^{(B)}_{h/2} \circ \varphi^{(A)}_{h} \circ \varphi^{(B)}_{h/2},$$

i.e., *the formula reads the same from left to right as from right to left*.

Splitting methods

It is possible to use splitting formulas more sophisticated than Strang's. For instance, for any choice of a real parameter b, we may consider

$$\psi_h = \varphi^{(B)}_{bh} \circ \varphi^{(A)}_{h/2} \circ \varphi^{(B)}_{(1-2b)h} \circ \varphi^{(A)}_{h/2} \circ \varphi^{(B)}_{bh}, \tag{23}$$

where, in one step, the A and B flows **act for a total duration of h units of time each to ensure consistency**.

Due to its palindromic structure, the integrator (23) is symmetric, and its order is at least two[14]. *It turns out that the order is exactly two for all choices of b*[15].

[14] Bou-Rabee and Sanz-Serna, "Geometric integrators and the Hamiltonian Monte Carlo method", 2018

[15] Blanes, Casas, and Sanz-Serna, "Numerical Integrators for the Hybrid Monte Carlo Method", 2014

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The order of splitting integrators is discussed later in relation with the concept of *modified equations*.

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[14] Bou-Rabee and Sanz-Serna, "Geometric integrators and the Hamiltonian Monte Carlo method", 2018

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Splitting methods

Three B flows and two A flows feature in (23). However, N steps of the integrator only require the computation of $2N + 1$ B flows and $2N$ A flows; this is seen by combining flows as we did above for the Strang case.

We say that (23) is a **palindromic two-stage** integrator[16]. The method (23) may be denoted by[17]

$$(b, 1/2, (1 - 2b), 1/2, b).$$

[16] But (23) is still a *one-step* integrator, because x_{n+1} is determined by x_n. The term *stage* is borrowed from the Runge-Kutta literature.

[17] Blanes, Casas, and Sanz-Serna, "Numerical Integrators for the Hybrid Monte Carlo Method", 2014 and Fernández-Pendás, Akhmatskaya, and Sanz-Serna, "Adaptive multi-stage integrators for optimal energy conservation in molecular simulations", 2016

Splitting methods

Similarly, one may consider the two-parameter family of palindromic **three-stage** splittings

$$(b, a, 1/2 - b, 1 - 2a, 1/2 - b, a, b).$$

A full description of this family is given by Campos and Sanz-Serna, "Palindromic 3-stage splitting integrators, a roadmap", 2017

This reference suggests parameter choices for various applications. **There is a unique choice of a and b resulting in a fourth-order method often associated with Yoshida's name**[18]. For all other choices, the order is $\nu = 2$.

[18] Yoshida, "Construction of higher order symplectic integrators", 1990

Splitting methods

The family of **palindromic s-stage** splitting formulas is given by

$$(b_1, a_1, b_2, a_2, \ldots, a_{s'}, b_{s'+1}, a_{s'}, \ldots, a_2, b_2, a_1, b_1),$$

if $s = 2s'$ is even, and by

$$(b_1, a_1, b_2, a_2, \ldots, b_{s'}, a_{s'}, b_{s'}, \ldots, a_2, b_2, a_1, b_1),$$

if $s = 2s' - 1$.

After imposing the consistency requirement that at each step, the A and B flows act during h units of time each, the family has $s - 1$ parameters left. **By taking s sufficiently high it is possible to achieve any desired order**[19].

[19] Section 13.1 in Sanz-Serna and Calvo, *Numerical Hamiltonian problems*, 1994

Splitting methods

Some classic examples of splitting integrators in the literature:

- Wisdom and Holman, “Symplectic maps for the n-body problem”, 1991 applied to the n-planet solar system problem.
- McLachlan, “Explicit Lie-Poisson integration and the Euler equations”, 1993 and McLachlan, “Symplectic integration of Hamiltonian wave equations”, 1993 describe different splitting and discretizations that can be applied to PDE’s arising in physics.
- Zhang, “Explicit unitary schemes to solve quantum operator equations of motion”, 1991 and Zhang, “Algorithms that preserve the volume amplification factor for linear systems”, 1993 give examples for the unitary and volume-preserving cases, respectively.

Fixed h stability

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Global errors may be bounded as in

$$\max_{0 \leq t_n \leq T} |x_n - x(t_n)| = \mathcal{O}(h^\nu), \qquad h \to 0+ .$$

However, in practice, **it is usually not possible to estimate the error constant implied in $\mathcal{O}(h^\nu)$ in the bound**.

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The literature on numerical integrators has traditionally resorted to problems where x_n and $x(t_n)$ may be written down in closed form. *The performance of the various integrators on the model problem may then be investigated analytically and is taken as an indication of their performance when applied to realistic problems*.

Fixed h stability. One degree of freedom

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$$\frac{d}{dt}q = p, \qquad \frac{d}{dt}p = -q. \tag{24}$$

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For a splitting method, a time step $(q_{n+1}, p_{n+1}) = \psi_h(q_n, p_n)$ may be expressed as

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

for suitable method-dependent coefficients A_h, B_h, C_h, D_h. The evolution over n time steps is then given by

$$\begin{bmatrix} q_n \\ p_n \end{bmatrix} = \tilde{M}_h^n \begin{bmatrix} q_0 \\ p_0 \end{bmatrix},$$

an expression to be compared with

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = M_t \begin{bmatrix} q(0) \\ p(0) \end{bmatrix}, \qquad M_t = \begin{bmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{bmatrix}.$$

Fixed h stability. One degree of freedom

If a given $h > 0$ is such that $|\tilde{M}_h^n| \to \infty$ as $n \to \infty$, **the magnitude of the numerical solution** (q_n, p_n) **will grow unboundedly, while the true solution remains bounded as** $t \to \infty$.

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If a given $h > 0$ is such that $|\tilde{M}_h^n| \to \infty$ as $n \to \infty$, the magnitude of the numerical solution (q_n, p_n) will grow unboundedly, while the true solution remains bounded as $t \to \infty$. Necessarily, global errors will be large for large n. Then, the integrator is said to be **unstable** for that particular choice of h.

Fixed h stability. One degree of freedom

Example. Euler's rule

For Euler's rule, $x_{n+1} = x_n + hf(x_n)$, we find

$$A_h = D_h = 1, \quad B_h = -C_h = h.$$

The eigenvalues of $\tilde{M}_h$ are $1 \pm ih$ with modulus $(1+h^2)^{1/2}$. Therefore, for any fixed $h > 0$, $\tilde{M}_h^n$ **grows exponentially** as n increases. Thus, **Euler's rule is unsuitable to integrate the harmonic oscillator**.

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In the step $n \to n+1$, the radius $r = (q^2 + p^2)^{1/2}$, which remains constant for the true solution, grows like

$$r_{n+1} = (1+h^2)^{1/2} r_n = \left(1 + \frac{h^2}{2} + \mathcal{O}(h^4)\right) r_n$$

for the Euler solution, so that $r_n = (1+h^2)^{n/2} r_0$.

Fixed h stability. One degree of freedom

Example. Midpoint rule

The midpoint rule, $x_{n+1} = x_n + hf\left(\frac{1}{2}(x_n + x_{n+1})\right)$, has

$$A_h = D_h = \frac{1 - \frac{h^2}{4}}{1 + \frac{h^2}{4}}, \quad B_h = -C_h = \frac{h}{1 + \frac{h^2}{4}}.$$

The characteristic equation of $\tilde{M}_h$ is

$$\lambda^2 - 2A_h\lambda + 1. \tag{25}$$

Therefore, the product of the eigenvalues is 1. For $h \neq 0$, $|A_h| < 1$ and the matrix has a pair of complex conjugate eigenvalues of unit modulus. Then, **the powers $\tilde{M}_h^n$ remain bounded as n increases and the method is stable for any h.**

Fixed h stability. One degree of freedom

Example. Strang's splitting

Let us next consider Strang's splitting, $\psi_h = \varphi_{h/2}^{(B)} \circ \varphi_h^{(A)} \circ \varphi_{h/2}^{(B)}$, applied with the splitting (17)-(18), which yields the velocity Verlet algorithm. It has

$$A_h = D_h = 1 - h^2/2, \quad B_h = h, \quad C_h = -h + h^3/4.$$

The characteristic equation is again of the form (25).

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For $h > 2$, $A_h < -1$ and the eigenvalues are real and distinct, so that one of them has modulus > 1, and therefore **the powers $\tilde{M}_h^n$ grow exponentially**.

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For $h = 2$, $\tilde{M}_h$ is a nontrivial Jordan block **whose powers grow linearly** (**weak instability**).

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For $h < 2$ the eigenvalues are complex of unit modulus and **the powers $\tilde{M}_h^n$ remain bounded**.
For $h = 2$, $\tilde{M}_h$ is a nontrivial Jordan block **whose powers grow linearly** (**weak instability**).
Thus, the integrator is unstable for $h \geq 2$ and has the stability interval $0 < h < 2$. $h > 2$ lead to large global errors.

Fixed h stability. One degree of freedom

Are values of h below the upper limit 2 satisfactory?

The answer depends on the accuracy required. The table below gives, for the initial condition $q = 1$, $p = 0$, and different stable values of h, the relative error in the Euclidean norm

$$\frac{|(q_n - q(t_n), p_n - p(t_n))|}{|(q(t_n), p(t_n))|}$$

at the final integration time, when the integration is carried out over an interval of length either one oscillation period (second column) or ten oscillation periods (third column).

h	$t = T_{per}$	$t = 10T_{per}$
$T_{per}/4$	6.49e-1	2.00e0
$T_{per}/8$	1.60e-1	1.48e0
$T_{per}/16$	4.03e-2	4.00e-1
$T_{per}/32$	1.01e-2	1.01e-1

Fixed h stability. One degree of freedom

Example

Columns are consistent with the order of convergence.

Fixed h stability. One degree of freedom

Example

Columns are consistent with the order of convergence. The last rows reveal that **the error increases linearly with** t. In the first row, the error grows more slowly than t: the numerical solution (q_n, p_n) remains close to the unit circle for all values of n and errors cannot be substantially larger than the diameter of the circle.

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If we are interested in errors below 10 % over an interval of length equal to ten oscillation periods, then h **has to be taken below** $2\pi/32 \approx 0.20$, i.e., well below the end, $h = 2$, of the stability interval.

Fixed h stability. One degree of freedom

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To provide an indication of the effect of using unstable values of h, we mention that **with** $h = \pi$ **the error after one period is** ≈ 46.4 **and after ten periods** $\approx 4.68 \times 10^{17}$.

Fixed h stability. One degree of freedom

Replacing the model (24) with the apparently more general system

$$\frac{d}{dt}q = \omega p, \qquad \frac{d}{dt}p = -\omega q, \qquad \omega > 0, \tag{26}$$

with oscillation period $2\pi/\omega$, does not really change things. Integrating (26) with step size h is equivalent to integrating (24) with step size h/ω.

Fixed h stability. Several degrees of freedom

Let us now move to the model with d **degrees of freedom**

$$\frac{d}{dt}\mathbf{q} = M^{-1}\mathbf{p}, \quad \frac{d}{dt}\mathbf{p} = -K\mathbf{q},$$

where M and K are $d \times d$, symmetric, positive-definite matrices. The Hamiltonian associated to this system is

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p} + \frac{1}{2}\mathbf{q}^T K\mathbf{q}. \tag{27}$$

In mechanics, M and K are the **mass** and **stiffness** matrices respectively.

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This model may be transformed into d uncoupled one-degree-of-freedom oscillators: we take $M = LL^T$ and diagonalize the symmetric, positive-definite matrix $L^{-1}KL^{-T}$ as $U^T L^{-1}KL^{-T}U = \Omega^2$, with U orthogonal and Ω diagonal with diagonal entries ω_i, $i = 1, \ldots, d$.

Fixed h stability. Several degrees of freedom

Proposition

With the notation as above, the (non-canonical) change of dependent variables, $\mathbf{q} = L^{-T}U\bar{\mathbf{q}}$, $\mathbf{p} = LU\Omega\bar{\mathbf{p}}$, decouples the system into a collection of d harmonic oscillators (superscripts denote components):

$$\frac{d\bar{q}^i}{dt} = \omega_i \bar{p}^i, \quad \frac{d\bar{p}^i}{dt} = -\omega_i \bar{q}^i, \quad i = 1, \ldots, d.$$

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For all integrators of practical interest, **decoupling and numerical integration commute**: carrying out the integration in the old variables $(\mathbf{q}, \mathbf{p})$ yields the same result as successively (i) changing variables in the system; (ii) integrating each of the uncoupled oscillators; (iii) translating the result to the old variables.

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Then, **stability may be analyzed under the assumption that the integration is performed in the uncoupled version**.

Fixed h stability. Several degrees of freedom

Example

Consider a particular case with $d = 2$, $M = L = I$, $\omega_1 = 1$ and $\omega_2 = 100$ and the initial condition

$$\bar{q}^1(0) = 1, \quad \bar{p}^1(0) = 0, \quad \bar{q}^2(0) = 0.01, \quad \bar{p}^2(0) = 0.$$

We wish to integrate with the velocity Verlet algorithm over $0 \leq t \leq 20\pi$ (ten periods of the slower oscillation) and aim at absolute errors of magnitude ≈ 0.1 in the Euclidean norm of the variables (q^1, q^2, p^1, p^2) or, equivalently, because here $q = U\bar{q}$ with U orthogonal, in the Euclidean norm of the variables $(\bar{q}^1, \bar{q}^2, \bar{p}^1, \bar{p}^2)$.

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For **accuracy**, it would be sufficient to take $h \approx 0.2$: it integrates the first uncoupled oscillator with the desired accuracy, and the second oscillator should not contribute significantly to the error, due to the smallness of $\bar{q}^2(t)$ and $\bar{p}^2(t)$ for all t. However, unless we take $h\omega_2 < 2$, i.e., $h < 0.02$, the errors in $\bar{q}^2(t)$ and $\bar{p}^2(t)$ will grow exponentially due to **instability**.

Fixed h stability. Several degrees of freedom

In the example above, and in many situations arising in practice, to avoid instabilities, the value of h has to be chosen much smaller than accuracy would require. These situations are called **stiff**. To deal with stiffness one may resort to suitable *implicit integrators* or *to explicit integrators with large stability intervals*.

It may seem that the initial condition in the preceding example is unnatural as the sizes of two components of $\bar{q}$ are so unbalanced. This is not so: it is easily checked that, in terms of the original energy in (27), the contributions to H of the ω_1 and ω_2 oscillations are both equal to $1/2$. Those oscillations are called **normal modes** in mechanics.

We emphasize that, while the preceding material refers to the quadratic Hamiltonian (27), one may expect that it has some relevance for Hamiltonians close to that model. However there are cases where the behaviour of a numerical integrators departs considerably from its behaviour when applied to (27).

Next session

- Maintaining the Hamiltonian framework, we will move to **geometric integration**.
- We will focus our attention on **symplectic integrators**, discussing the preservation of oriented volume.
- We will talk about the **preservation of energy** and the **canonical probability measure**.
- We will discuss **reversible systems**.

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