Geometric numerical methods for mechanics

P. CARRÉ[a], J. BENSOAM[b]

a. IRCAM, CNRS UMR 9912, S3AM, pierre.carre@ircam.fr
b. IRCAM, CNRS UMR 9912, S3AM, joel.bensoam@ircam.fr

Abstract :

In this paper, two classes of numerical integrators are introduced and compared : Lie group methods, presented via the particular case of Runge-Kutta Munthe-Kaas integrators ; and variational methods, in which natural charts integrators and Galerkin methods are examined. Considering the case of a configuration manifold with a Lie group action, both classes of methods are studied in terms of configuration space preservation and symplectic/energy behaviour. As an example, we apply those formulations on the rigid body problem.

Mots clefs : Geometric integrators, Structure Preserving numerical methods, Variational methods.

1 Introduction

In this paper, two classes of numerical integrators preserving the Lie group structure of the system they are applied on are reviewed and compared, namely Lie group methods and variational integrators. The first will be approached via the example of the Runge-Kutta Munthe-Kaas class of integrators [9, 10, 11], and the second via the formalism introduced by Marsden *et al.* [7] We propose a numerical experiment for both types of designs on the rigid body problem in order to compare the results of simulations.

The setting of variational mechanics is central to the approach of this review, and is therefore summarized here. Let a physical system be represented by a configuration manifold Q and a Lagrangian $\mathrm{L} : TQ \to \mathbb{R}$, the action map is defined as the time integral of the Lagrangian along a path q

$$\mathcal{A}(q) = \int_0^T \mathrm{L}(q(t), \dot{q}(t))dt.$$

The first variation of the action map for an arbitrary path variation δq leads to the expression

$$\mathrm{d}\,\mathcal{A}(q)\delta q = \int_0^T \left(\frac{\partial \mathrm{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathrm{L}}{\partial \dot{q}}\right)\delta q dt + \left[\frac{\partial \mathrm{L}}{\partial \dot{q}}\delta q\right]_0^T.$$

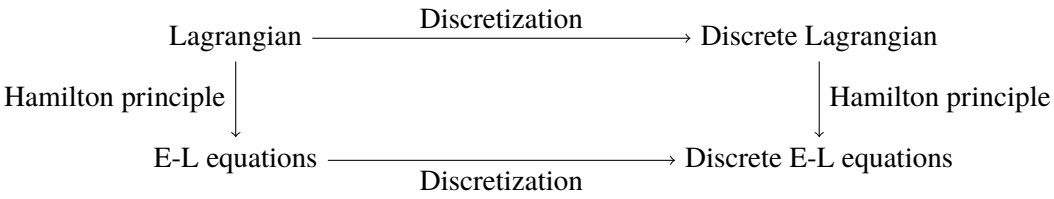
The Hamilton principle states that solutions q of the problems are critical points of the action map where q is fixed at the endpoints. Hence, such a path q must cancel the action variation for arbitrary variations δq and where $\delta q(0) = \delta q(T) = 0$, yielding the Euler-Lagrange equations from the above expression

$$\frac{d}{dt}\frac{\partial \mathrm{L}}{\partial \dot{q}} - \frac{\partial \mathrm{L}}{\partial q} = 0.$$

Solutions of the Euler-Lagange equations can be shown to preserve the so called symplectic form, which has important consequences in terms of energy behaviour. Preserving this feature in the discrete setting is desirable to design energy preserving approximations.

In addition, we will place ourselves in the case of a homogeneous configuration space Q, in which a solution is invariant by the action of an associated Lie group. It will be shown that both types of numerical integrators preserve the underlying geometric structure of the system by computing approximations that exhibit the same invariance properties than the solutions.

The difference between the two numerical integrators families comes from the discretization of the Euler-Lagrange equations into discrete counterparts. They can be summed up by the following non commutating diagram.



Runge-Kutta Munthe-Kaas methods provide a direct discretization of the Euler-Lagrange equations ensuring that discrete solutions stay on the configuration manifold. In that setting, well known and powerful tools (i.e. Runge-Kutta, Butcher series) can be applied to equations expressed on the Lie algebra to design higher order methods as well as to determine their numerical convergence. However in this case no particular property of symplecticity or energy preservation is obtained without further constraints. Alternatively, variational methods rely on providing an approximate Lagrangian and applying a discrete variational principle. In that case, the numerical solutions preserve an approximate symplectic form and shows good long time energy behaviour. However, beyond these helpful intrinsic invariance property some drawbacks may appears in the practical applications : it is difficult to define high order methods, estimating the numerical error is usually non trivial, and the constructed method are often implicit, which may increase the computational cost.

Section 2 will review the basics of the Runge-Kutta Munthe-Kaas class of methods as well as an example of numerical integrator based on the classical RK4 method. Then the general discrete variational approach is layed out in section 3 along with examples of low and high order integrators, and the case of variational integration when the configuration space is a Lie group is examined in section 4, along with formulations for simple natural charts and Galerkin numerical integrators. We present a comparison of a Runge-Kutta Munthe-Kaas method with a variational integrator based on natural charts of the Lie group in section 5, where it is applied on the rigid body problem.

2 Runge-Kutta Munthe-Kaas methods

The Runge-Kutta Munthe-Kaas methods (RKMK), presented in a series of articles [9, 10, 11], are examples of Lie group methods. They can be used for a given initial value problem

$$\dot{Y} = A(t, Y)\, Y, \qquad Y(0) = Y_0 \in \mathcal{M} \tag{1}$$

where Y is an element of a homogeneous space $\mathcal{M}$ on which a Lie group G acts. For a homogeneous space $Y = gY_0$ which means that any point of the manifold can be attained using a element $g \in G$ from

a fix point Y_0.

After presenting the fundations of Runge-Kutta Munthe-Kaas methods (2.1), we present the details of the RKMK4 integrator (2.2). An implementation of this integrator is applied on section 5 on the rigid body problem.

2.1 Principles of Runge-Kutta Munthe-Kaas methods

The idea is to use the exponential map, $\exp : \mathfrak{g} \to G$, to guess a solution of (1) on the form $Y(t) = g(t)Y_0 = \exp(\Omega(t))Y_0$. Introducing the right group action $R_g : G \to G$ and its differential TR_g, the computation of the time derivative

$$\dot{Y} = \dot{g}Y_0 = \dot{g}g^{-1}gY_0 = \dot{g}g^{-1}Y = TR_{g^{-1}}(\dot{g})Y = TR_{g^{-1}}\left(T\exp(\dot{\Omega})\right)Y,$$

shows clearly that equation (1) may be written as $\dot{Y} = \mathrm{d}^{\mathrm{R}}\exp(\dot{\Omega})Y = AY$, as soon as the right trivialized derivative of the exponential map is defined by $\mathrm{d}^{\mathrm{R}}\exp = TR_{g^{-1}} \circ T\exp$. Since $\mathrm{d}^{\mathrm{R}}\exp : \mathfrak{g} \to \mathfrak{g}$, it means that $A(t, Y) = \mathrm{d}^{\mathrm{R}}\exp(\dot{\Omega})$ belongs to the Lie algebra $\mathfrak{g}$. Inverting $\mathrm{d}^{\mathrm{R}}\exp$, a differential equation on the variable $\Omega \in \mathfrak{g}$ is then obtained

$$\dot{\Omega} = \mathrm{d}^{R}\exp^{-1}\left(A(t, Y(t))\right), \tag{2}$$

for which, we take $\Omega(0) = 0$ to ensure that $Y(0) = Y_0$. The solution $\Omega(t)$ of this equation is then finally used to compute $Y(t)$ via the exponential map. Doing so ensures that the structure of the Lie group is preserved — namely that the solution lies on G.

The application $\mathrm{d}^{\mathrm{R}}\exp$ is invertible for all Ω such that $\|\Omega\| < \pi$, and its inverse can be expressed as the series $\mathrm{d}^{\mathrm{R}}\exp_{\Omega}^{-1} = \sum_{k=0}^{\infty}(B_k/k!)\,\mathrm{ad}_{\Omega}^{k}$ where $(B_k)_{k\geq 0}$ are the Bernouilli numbers. We finally get for Ω the initial value problem

$$\dot{\Omega}(t) = A\left(t,\, \exp\left(\Omega(t)\right)Y_0\right) + \sum_{k=1}^{\infty}\frac{B_k}{k!}\,\mathrm{ad}_{\Omega}^{k}\left(A\left(t,\, \exp\left(\Omega(t)\right)Y_0\right)\right), \qquad \Omega(0) = 0. \tag{3}$$

In the general case, equation (3) cannot be solved analytically, so an approximation $\widetilde{\Omega} \approx \Omega(h)$ of Ω at time h is computed by means of a classical Runge-Kutta method. The step $Y_0 \mapsto Y_1$ is then computed as $Y_1 = \exp(\widetilde{\Omega})Y_0 \approx Y(h)$ where the order of the approximation depends on the order of the RK method.

We recall that an s stage RK method is specified by the set of coefficients $a_{ij}, b_i \in \mathbb{R}$ and $c_i = \sum_{j=1}^{s} a_{ij}$ where $i, j \in \{1, \ldots, s\}$, and is given for an initial value problem $\dot{y} = f(t, y)$, $y(t_0) = y_0$ and a time step $h \in \mathbb{R}$ by

$$k_i = f\left(t_0 + c_i h,\, y_0 + h\sum_{j=1}^{s} a_{ij}k_j\right), \quad i \in \{1, \ldots, s\}$$

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i k_i.$$

The infinite sum in (3) is not practical to work with. However, it can sometimes be replaced by an analytical expression (for example when $\mathfrak{g} = \mathfrak{so}(3)$ [2]), or by a low order polynomial while keeping the order of the RK method [1]. Otherwise, the sum is often truncated up to an order q, the RKMK methods

featuring the fundamental property that if the RK method is order p and that the truncation order checks $q \geq p-2$, then the RKMK method is order p [3].

The interest of RKMK methods over other Lie group methods such as Crouch-Grossman methods is that the order of the Runge-Kutta method is readily preserved, whereas additional order conditions have to be determined for Crouch-Grossman methods [13], adding a set of equations to the method.

2.2 The Runge-Kutta Munthe-Kaas method of order 4

The RKMK4, based on the order 4 classical RK4 method, is obtained by truncation of the sum (3) up to the term of order $q = 2$, yielding

$$\dot{\Omega} := f(t, \Omega) = A(t,\, Y) - \frac{1}{2}\,\mathrm{ad}_{\Omega}\,(A(t,\, Y)) + \frac{1}{12}\,\mathrm{ad}^2_{\Omega}\,(A(t,\, Y))$$

where we wrote $Y = \exp(\Omega) Y_n$. We recall that the classical RK4 method is described by the Butcher table

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array}$$

allowing us to define the RKMK4 method

$$k_1 = f(t_n, 0), \qquad k_2 = f(t_n + h/2, \frac{h}{2} k_1), \qquad k_3 = f(t_n + h/2, \frac{h}{2} k_2), \qquad k_4 = f(t_n + h, h\, k_3)$$

$$\widetilde{\Omega} = \frac{h}{6}\,(k_1 + 2\,k_2 + 2\,k_3 + k_4)$$

where the step $Y_n \mapsto Y_{n+1}$ is given by

$$Y_{n+1} = \exp\left(\frac{h}{6}\,(k_1 + 2\,k_2 + 2\,k_3 + k_4)\right)\, Y_n.$$

RKMK methods are straightforward and preserve the configuration space constraints. Moreover they can be designed to be explicit by taking an explicit RK method. However, as any Lie group method, they do not by default guarantee the conservation of any other property of the modelled system which might be desirable to preserve, such as symplecticity, energy, or momenta ; such a behaviour can be observed in the numerical results presented in section 5 for non symplectic and non energy preserving discrete solution of the rigid body problem obtained via an RKMK4 integrator. Nonetheless, another class of methods, based on a discrete variational principle, have these features by design.

3 Variational methods

In this section we review the fundamentals of variational methods. Those are based on the Lagrangian viewpoint of mechanics and allow for a number of properties, among which the symplectic energy and momentum preservation. After a general review of discrete variational mechanics (3.1), we derive two examples of methods : the midpoint variational method (3.2), and the high order Galerkin variational integrator (3.3). This section serves as an introduction for section 4 where we present the case of Lie group variational methods.

3.1 Discrete variational mechanics

We review here the standard formulation of the discrete variational mechanics based on the discrete Hamilton principle, as presented by Marsden and West in [8].

In order to downsize the continuous problem to a finite dimension discrete case, we only consider the set of configurations $q_k := q(kh) \in Q$ where q is the exact solution, $h \in \mathbb{R}$ an arbitrary time step and $k \in \{0, \dots, N\}$ (for the sake of simplicity, we only consider the case of a constant time step h, but the following can be generalized to the case of adaptative time steps). Variational methods will provide us with a mean to estimate the configurations q_k.

We recall from section (ref) that the exact solution q of the problem associated the Lagrangian $\mathrm{L} : TQ \to \mathbb{R}$ is given by the Hamilton principle as the extremum of the action map $\mathcal{A}(q) = \int_0^T \mathrm{L}(q(t), \dot{q}(t))dt$. This integral can be split as a sum over k, taking the expression

$$\mathcal{A}(q) = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \mathrm{L}(q(t), \dot{q}(t))dt.$$

where $t_k := kh$. In order to rephrase the problem in terms of q_k only we define the exact discrete Lagrangian $\mathrm{L}_d^E\, Q \times Q \to \mathbb{R}$ as the extremum of the Lagrangian integral over $[t_k, t_{k+1}]$ with boundary conditions $q(t_k) = q_k$ and $q(t_{k+1}) = q_{k+1}$. In other words, the exact discrete Lagrangian is equal to the action restricted to the interval $[t_k, t_{k+1}]$. We write

$$\mathrm{L}_d^E(q_k, q_{k+1}) := \underset{\substack{\tilde{q}:[t_k,t_{k+1}]\to Q \\ \tilde{q}(t_k)=q_k,\, \tilde{q}(t_{k+1})=q_{k+1}}}{\mathrm{ext}} \int_{t_k}^{t_{k+1}} \mathrm{L}(\tilde{q}(t), \dot{\tilde{q}}(t))dt = \int_{t_k}^{t_{k+1}} \mathrm{L}(q(t), \dot{q}(t))dt$$

Let the discrete path q_d denote the set of configurations $q_d := \{q_k\}_{k=0}^N$, the action map can be rewritten as a function of q_d

$$\mathcal{A}_d^E(q_d) = \sum_{k=0}^{N-1} \mathrm{L}_d^E(q_k, q_{k+1}) = \mathcal{A}(q)$$

where the action map $\mathcal{A}_d^E$ only depends explicitely on q_d and the exact solution q is given implicitely by the exact discrete Lagrangian.

Computing $\mathrm{L}_d^E(q_k, q_{k+1})$ would require knowing the exact solution q between t_k and t_{k+1}, which we don't have access to. For this reason, we introduce a discrete Lagrangian $\mathrm{L}_d : Q \times Q \to \mathbb{R}$ as an approximation of L_d^E, that is

$$\mathrm{L}_d(q_k, q_{k+1}) \approx \mathrm{L}_d^E(q_k, q_{k+1}).$$

This discrete Lagrangian is to be thought of as the result of a local optimisation problem of finiding an approximate path solving a simplified variational problem for given boundary conditions. Defining a discrete Lagrangian is a two step process : taking a subset of possible solutions for $\tilde{q}$, and providing a quadrature for the action integral restricted to $[t_k, t_{k+1}]$. There is no unique definition for L_d, and the choice for its definition will result in different numerical methods. Concrete examples are given in sections 3.2 and 3.3, where numerical integrators are derived from two different definitions for the discrete Lagrangian.

Without any additional hypothesis on the discrete Lagrangian, a number of results can be proven for methods deriving from the discrete variational principle regadless of a specific choice for L_d. We define

the discrete action $\mathcal{A}_d$ as the sum over k of the discrete Lagrangian L_d, which expression is given for a discrete path q_d as

$$\mathcal{A}_d(q_d) := \sum_{k=0}^{N-1} \mathrm{L}_d(q_k, q_{k+1}).$$

Looking for conditions on q_d to be the solution of the approximate variational problem, we compute the variation of action for variations $\delta q_d := \{\delta q_k\}_{k=0}^N$

$$\begin{aligned}
\mathrm{d}\,\mathcal{A}_d(q_d)\cdot\delta q_d &= \sum_{k=0}^{N-1} D_1\,\mathrm{L}_d(q_k,q_{k+1})\cdot\delta q_k + D_2\,\mathrm{L}_d(q_k,q_{k+1})\cdot\delta q_{k+1} \\
&= \sum_{k=1}^{N-1} \left(D_1\,\mathrm{L}_d(q_k,q_{k+1}) + D_2\,\mathrm{L}_d(q_{k-1},q_k)\right)\cdot\delta q_k \\
&\qquad + \Theta^+_{\mathrm{L}_d}(q_{N-1},q_N)\cdot(\delta q_{N-1},\delta q_N) - \Theta_{\mathrm{L}_d}(q_0,q_1)\cdot(\delta q_0,\delta q_1)
\end{aligned}$$

where we define the two Lagrangian 1-forms

$$\Theta^+_{\mathrm{L}_d}(q_0,q_1) = D_2\,\mathrm{L}_d(q_0,q_1)\,\mathrm{d}\,q_1 \qquad \Theta^-_{\mathrm{L}_d}(q_0,q_1) = -D_1\,\mathrm{L}_d(q_0,q_1)\,\mathrm{d}\,q_0.$$

Applying the Hamilton principle to the restricted problems, that is taking arbitrary variations δq_d with vankishing endpoints δq_0 and δq_N, leads by independence of the variations $\{\delta q_k\}_{k=1}^{N-1}$ to the discrete Euler-Lagrange equations (DEL) given for all $k \in \{1,\dots,N-1\}$ by

$$D_1\,\mathrm{L}_d(q_k,q_{k+1}) + D_2\,\mathrm{L}_d(q_{k-1},q_k) = 0. \tag{4}$$

Solving these equations for q_{k+1} knowing q_{k-1} and q_k provide us with the step $(q_{k-1},q_k) \mapsto (q_k,q_{k+1})$ defining the numerical method.

Symplecticity One important feature of the numerical method obtained by solving the DEL is that they are symplectic. This is otained by showing that the solutions of the numerical method preserve the discrete symplectic two-form $\Omega_{L_d} := \mathrm{d}\,\Theta^+_{\mathrm{L}_d} = \mathrm{d}\,\Theta^-_{\mathrm{L}_d}$ (see [8]). It is well known [6, 3] that discrete paths obtained via symplectic integrators also preserve energy for an approximate Lagrangian system, and thus display excellent long-time energy behaviour : the energy is approximately preserved and oscillates around the exact value. Symplecticity, and approximate energy preservation, is a design feature of variational integrators.

3.2 Variational midpoint method

We present here an example of straightforward variational method, featured in [14]. This method is build by approximating the path q by the linear interpolation between q_0 and q_1, and approximating the Lagrangian integral by the midpoint rule

$$\begin{aligned}
\tilde{q}(t) &= q_0 + t\,\frac{q_1-q_0}{h} \\
\mathrm{L}_d(q_0,q_1) &= h\,\mathrm{L}\left(\tilde{q}(h/2),\dot{\tilde{q}}(h/2)\right).
\end{aligned}$$

This yields the discrete Lagrangian

$$\mathrm{L}_d(q_0, q_1) = h\ \mathrm{L}\left(\frac{q_0+q_1}{2}, \frac{q_1-q_0}{h}\right).$$

The associated discrete Euler-Lagrange equations (4) are given for $k \in \{1, \dots, N\}$ by

$$\frac{h}{2}\frac{\partial \mathrm{L}}{\partial q}\left(q_{k-\frac{1}{2}}, \dot{q}_{k-\frac{1}{2}}\right) + \frac{\partial \mathrm{L}}{\partial \dot{q}}\left(q_{k-\frac{1}{2}}, \dot{q}_{k-\frac{1}{2}}\right) + \frac{h}{2}\frac{\partial \mathrm{L}}{\partial q}\left(q_{k+\frac{1}{2}}, \dot{q}_{k+\frac{1}{2}}\right) - \frac{\partial \mathrm{L}}{\partial \dot{q}}\left(q_{k+\frac{1}{2}}, \dot{q}_{k+\frac{1}{2}}\right) = 0 \quad (5)$$

where $q_{k+\frac{1}{2}} = \frac{q_k+q_{k+1}}{2}$ and $\dot{q}_{k+\frac{1}{2}} = \frac{q_{k+1}-q_k}{h}$. Those equations are generally implicit for q_{k+1} and have to be solved numerically.

3.3 Galerkin variational methods

The construction of Galerkin variational integrators is based on expressing simplified solutions with a set of polynomials and approximating the Lagrangian integrals with quadrature rules. They allow the design of high order schemes that are computationally effective while still retaining the preservation properties. Those methods were introduced in [8] and have since been further developed ; see for example [12, 5].

Solutions on a time interval $[t_k, t_{k+1}]$ are approximated as polynomials of degree s for an arbitrary $s \in \mathbb{N}$, that is between each pair of boudary conditions (q_k, q_{k+1}) the discrete path is interpolated as a polynomial. As shown in figure 1, interpolating solutions on $[t_k, t_{k+1}]$ are defined uniquely by specifying $s+1$ control points $0 = \alpha_0 < \cdots < \alpha_s = 1$ and corresponding configurations $\left(q^0, q^1, \dots, q^{s-1}, q^s\right) = \{q^\nu\}_{\nu=0}^s$ such that $q^0 = q_k$ and $q^s = q_{k+1}$. From now on, we focus on a fixed interval $[t_k, t_{k+1}]$ and boundary conditions (q_k, q_{k+1}) ; without loss of generality we set $t_k = 0$ and $t_{k+1} = h$. We define $q_d : [0, h] \to Q$ the interpolating polynomial on this interval depending on the configurations $\{q^\nu\}$ such that for all $\nu \in \{0, \dots, s\}$ we have $q_d(\alpha_\nu h; \{q^\mu\}) = q^\nu$. Those polynomials admit a unique decomposition on the basis of degree s Lagrange polynomials $\phi_\nu : [0, 1] \to \mathbb{R}$ defined for ν by

$$\phi_\nu(t) = \prod_{0 \le i \le s,\, i \neq \nu} \frac{t-\alpha_i}{\alpha_\nu - \alpha_i}.$$

The path q_d and its derivative are expressed in that basis by

$$q_d(t; \{q^\nu\}) = \sum_{\nu=0}^{s} q^\nu \phi_\nu(t/h), \qquad \dot{q}_d(t; \{q^\nu\}) = \frac{1}{h}\sum_{\nu=0}^{s} q^\nu \dot{\phi}_\nu(t/h). \quad (6)$$

With the set of paths well defined, one now needs to provide an approximation for the Lagrangian integral restricted to the set of interpolating polynomials q_d

$$\underset{\substack{q_d:[0,h]\to Q \\ q_d(0)=q_k,\ q_d(h)=q_{k+1}}}{\mathrm{ext}} \int_0^h \mathrm{L}(q_d, \dot{q}_d)dt. \quad (7)$$

Extremalizing this integral on the set of interpolating paths q_d with constraints $q_d(0) = q_k$ and $q_d(h) = q_{k+1}$ is exactly extremalizing it on the set of configurations $\{q^\nu\}_{\nu=0}^s$ with constraints $q^0 = q_k$ and

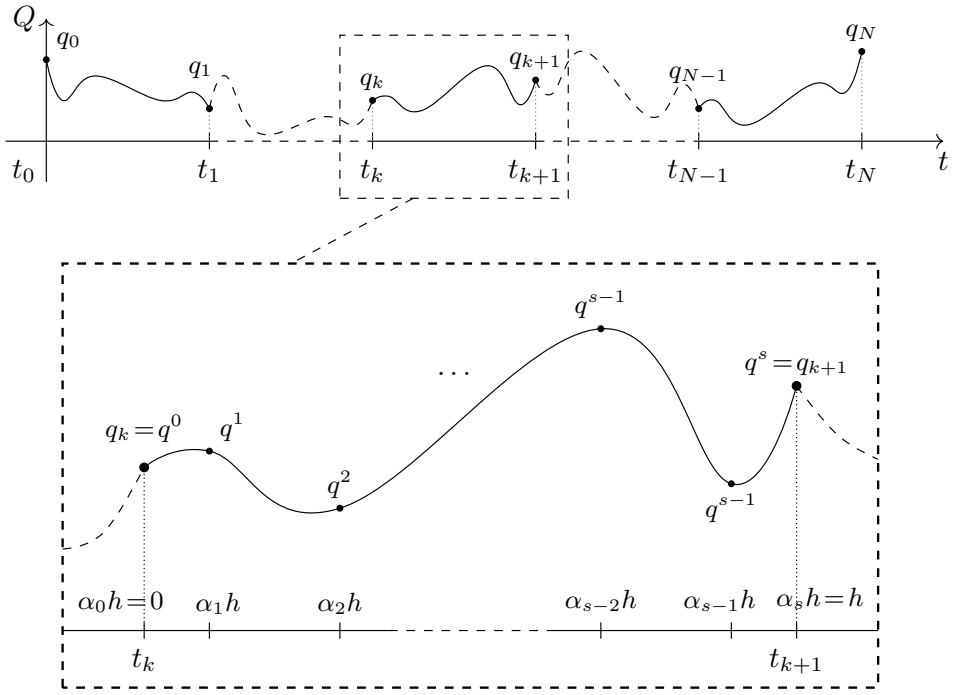


FIGURE 1 – A schematic of the curve interpolation.

$q^s = q_{k+1}$. This is why (7) can be equivalently written

$$\underset{\substack{\{q^\nu\}_{\nu=1}^{s-1} \in Q \\ q^0 = q_k,\, q^s = q_{k+1}}}{\text{ext}} \int_0^h \mathrm{L}(q_d(t;\{q^\nu\}), \dot{q}_d(t;\{q^\nu\}))dt.$$

We now provide an approximation for the integral. Let $(c_i, w_i)_{1\leq i\leq r}$ be a quadrature of the interval $[0,1]$ with quadrature points c_i associated to the weights w_i ; classical examples of widely used quadratures are given by Gauss-Legendre or Gauss-Lebatto. We refer to [12] for a discussion on the choices of quadratures and the order of the resulting methods. We define the local discrete action $\widetilde{\mathcal{A}}_d : Q^s \to \mathbb{R}$ as the quadrature associated to (c_i, w_i) of the integral $\int_0^h \mathrm{L}(q_d, \dot{q}_d)dt$, that is

$$\widetilde{\mathcal{A}}_d(\{q^\nu\}_{\nu=0}^s) := h \sum_{i=1}^r w_i \, \mathrm{L}\left(c_i h; \{q^\nu\}\right)$$

where we used the shortcut notation $\mathrm{L}(c_i h; \{q^\nu\}) = \mathrm{L}(q_d(c_i h; \{q^\nu\}), \dot{q}_d(c_i h; \{q^\nu\}))$. To find the extremal of the local action $\widetilde{\mathcal{A}}_d$, we compute the variations of action with respect to arbitrary variations δq^ν with constraint $\delta q^0 = \delta q^s = 0$,

$$\begin{aligned}
\mathrm{d}\,\widetilde{\mathcal{A}}_d(\{q^\mu\})(\{\delta q^\nu\}) &= \sum_{\nu=1}^{s-1} h \sum_{i=1}^r w_i \,\mathrm{d}\,\mathrm{L}(c_i h; \{q^\mu\})(\delta q^\nu) \\
&= \sum_{\nu=1}^{s-1} h \sum_{i=1}^r w_i \left(\frac{\partial \mathrm{L}}{\partial q}(c_i h; \{q^\mu\}) \,\mathrm{d}\, q_d(\delta q^\nu) + \frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \{q^\mu\}) \,\mathrm{d}\, \dot{q}_d(\delta q^\nu) \right) \\
&= \sum_{\nu=1}^{s-1} h \sum_{i=1}^r w_i \left(\phi_\nu(c_i) \frac{\partial \mathrm{L}}{\partial q}(c_i h; \{q^\mu\}) + \frac{1}{h} \dot{\phi}_\nu(c_i) \frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \{q^\mu\}) \right) \delta q^\nu.
\end{aligned}$$

where in line 2 we computed the differential of the path q_d and of its time derivative $\dot{q}_d$ along the variations δq^ν as

$$\begin{aligned}
\mathrm{d}\, q_d(\delta q^\nu) &= \frac{\partial q_d}{\partial q^\mu}\,\mathrm{d}\, q^\mu(\delta q^\nu) + \frac{\partial q_d}{\partial t}\,\mathrm{d}\, t(\delta q^\nu) = \delta_{\nu\mu}\phi_\mu \delta q^\nu,\\
\mathrm{d}\, \dot{q}_d(\delta q^\nu) &= \delta_{\nu\mu}\frac{1}{h}\dot{\phi}_\mu \delta q^\nu.
\end{aligned}$$

Here, since the mesh is fixed, variations δq^ν are taken along the fibre Q, hence $\mathrm{d}\, t(\delta q^\nu) = 0$.

The variations δq^ν being independent for $1 \leq \nu \leq s-1$, taking $\delta\widetilde{\mathcal{A}}_d = 0$ yields for $\nu \in \{1, \ldots, s-1\}$

$$h\sum_{i=1}^{r} w_i \left(\phi_\nu(c_i)\frac{\partial \mathrm{L}}{\partial q}(c_i h; \{q^\mu\}) + \frac{1}{h}\dot{\phi}_\nu(c_i)\frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \{q^\mu\})\right) = 0. \tag{8}$$

This allows us to define the discrete Lagrangian $\mathrm{L}_d : Q \times Q \to \mathbb{R}$ on a pair (q_k, q_{k+1}) as the extremum of the local action $\widetilde{\mathcal{A}}_d$ evaluated on $\{q^\nu\}_{\nu=0}^s$ with boudary conditions $q^0 = q_k$ and $q^s = q_{k+1}$

$$\mathrm{L}_d(q_k, q_{k+1}) = \underset{\substack{\{q_k^\nu\}_{\nu=1}^{s-1}\in Q\\ q^0=q_k,\, q^s=q^{k+1}}}{\mathrm{ext}} \widetilde{\mathcal{A}}_d(\{q^\nu\}_{\nu=0}^s) = \underset{\substack{\{q_k^\nu\}_{\nu=1}^{s-1}\in Q\\ q^0=q_k,\, q^s=q^{k+1}}}{\mathrm{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}(c_i h; \{q^\nu\}, h),$$

or equivalently to write

$$\mathrm{L}_d(q_k, q_{k+1}) = h\sum_{i=1}^{r} w_i\, \mathrm{L}(c_i h; \{\tilde{q}_k\}), \tag{9}$$

where now on we denote $\tilde{q}_k = \{\tilde{q}^\nu\}_{\nu=0}^s$ the set of extremalizing configurations where $\tilde{q}^0 = q_k$, $\tilde{q}^s = q_{k+1}$ and $\tilde{q}_k$ is solution of equations (8) for $\nu \in \{1, \ldots, N-1\}$.

We recall from section 3.1 that L_d satisfies the DEL equation (4) for $k \in \{1, \ldots, N-1\}$. The derivatives $D_1\,\mathrm{L}_d(q_k, q_{k+1}) = \frac{\partial}{\partial q_k}\mathrm{L}_d(q_k, q_{k+1})$ and $D_2\,\mathrm{L}_d(q_k, q_{k+1}) = \frac{\partial}{\partial q_{k+1}}\mathrm{L}_d(q_k, q_{k+1})$ are obtained from expression (9) as

$$\begin{aligned}
D_1\,\mathrm{L}_d(q_k, q_{k+1}) &= \frac{\partial}{\partial q^0}\mathrm{L}_d(q_k, q_{k+1}) = h\sum_{i=1}^{r} w_i \left(\phi_0(c_i)\frac{\partial \mathrm{L}}{\partial q}(c_i h; \tilde{q}_k) + \frac{1}{h}\dot{\phi}_0(c_i)\frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \tilde{q}_k)\right)\\
D_2\,\mathrm{L}_d(q_k, q_{k+1}) &= \frac{\partial}{\partial q^s}\mathrm{L}_d(q_k, q_{k+1}) = h\sum_{i=1}^{r} w_i \left(\phi_s(c_i)\frac{\partial \mathrm{L}}{\partial q}(c_i h; \tilde{q}_k) + \frac{1}{h}\dot{\phi}_s(c_i)\frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \tilde{q}_k)\right)
\end{aligned}$$

since $q_k = q^0$ and $q_{k+1} = q^s$. This yields the DEL equation for $k \in \{1, \ldots, N-1\}$

$$\begin{aligned}
h\sum_{i=1}^{r} w_i \left(\phi_0(c_i)\frac{\partial \mathrm{L}}{\partial q}(c_i h; \tilde{q}_k) + \frac{1}{h}\dot{\phi}_0(c_i)\frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \tilde{q}_k)\right)&\\
+ h\sum_{i=1}^{r} w_i \left(\phi_s(c_i)\frac{\partial \mathrm{L}}{\partial q}(c_i h; \tilde{q}_{k-1}) + \frac{1}{h}\dot{\phi}_s(c_i)\frac{\partial \mathrm{L}}{\partial \dot{q}}(c_i h; \tilde{q}_{k-1})\right) &= 0.
\end{aligned} \tag{10}$$

Finally, a step $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ of the high order Galerkin variational method is obtained by setting $q^0 = q_k$ and solving the $s-1$ equations (8) together with the DEL equation (10) for the s unknown variables $\{q^\nu\}_{\nu=1}^s$ and updating $q_{k+1} = q^s$, the set of s configurations $\tilde{q}_{k-1}$ being known from

the previous step computation. In the general case, the equations have to be solved implicitly for the s variables using a numerical solver to determine a root $(q_k^1, \dots, q_k^{s-1}, q_k^s)$ of the set of $s-1$ equations (8) and (10).

4 Lie group variational methods

This section follows the development in section 3 where we focused on discrete variational mechanics in a general setting. We now consider the case where the configuration space is a Lie group G acting on itself, and a left G-invariant Lagrangian L. That is to say $\forall \tilde{g} \in G$, $\mathrm{L}(L_{\tilde{g}} g, TL_{\tilde{g}} \dot{g}) = \mathrm{L}(g, \dot{g})$ where $L_g : G \to G$ is the group left action. In particular, for the choice $\tilde{g} = g^{-1}$, we have

$$\mathrm{L}(g, \dot{g}) = \mathrm{L}(L_{g^{-1}} g, TL_{g^{-1}} \dot{g}) = \mathrm{L}(e_G, TL_{g^{-1}} \dot{g}).$$

This allows for the definition of a reduced problem, expressed by means of a reduced Lagrangian $\ell : \mathfrak{g} \to \mathbb{R}$ now defined on the Lie algebra $\mathfrak{g}$ for a path g as

$$\ell(\xi) := \mathrm{L}(e_G, \xi)$$

where $\xi = TL_{g^{-1}} \dot{g}$. In this case the Hamilton principle leads to the Euler-Poincaré equations. The discrete counterparts provide numerical methods preserving both the symplectic structure and the G invariance. Two methods are developed in this new setting, and applied in section 5 on the rigid body problem.

4.1 Discrete variational mechanics on Lie groups

Let $\mathrm{L} : TQ \to \mathbb{R}$ be a left invariant Lagrangian, we can always design a left invariant discrete Lagrangian $\mathrm{L}_d : Q \times Q \to \mathbb{R}$ [5]. This means that for any pair $g_k, g_{k+1} \in G$ and $\tilde{g} \in G$, $\mathrm{L}_d(\tilde{g} g_k, \tilde{g} g_{k+1}) = \mathrm{L}_d(g_k, g_{k+1})$. Let us assume that our discrete Lagrangian L_d has such a property. Following [7], the discrete reduced Lagrangian $\ell_d : G \to \mathbb{R}$ is defined by choosing $\tilde{g} = g_k^{-1}$ as the left group action on $G \times G$ and composing it with the discrete Lagrangian, defining for any g_k, g_{k+1}

$$\mathrm{L}_d(g_k, g_{k+1}) = \mathrm{L}_d(e_G, g_k^{-1} g_{k+1}) = \ell_d(g_k^{-1} g_{k+1}).$$

The associated reduced discrete action is obtained as

$$\mathcal{A}_d(g_d) := \sum_{k=0}^{N-1} \ell_d(f_{k,k+1})$$

where we defined $f_{k,k+1} := g_k^{-1} g_{k+1} \in G$.

As in section 3, the variation of the discrete reduced action is computed on an arbitrary path g_d in order to look for solutions of the problem formulated by the Lagrangian by applying a Hamilton principle. The variations $\delta f_{k,k+1}$ first need to be computed :

$$\begin{aligned} \delta f_{k,k+1} &= -g_k^{-1} \delta g_k g_k^{-1} g_{k+1} + g_k^{-1} \delta g_{k+1} = TR_{f_{k,k+1}}(-g_k^{-1} \delta g_k + \mathrm{Ad}_{f_{k,k+1}} g_{k+1}^{-1} \delta g_{k+1}) \\ &= TR_{f_{k,k+1}}(-\zeta_k + \mathrm{Ad}_{f_{k,k+1}} \zeta_{k+1}) \end{aligned}$$

where $\zeta_k := g_k^{-1} \delta g_k$ and $\mathrm{Ad}_g : \mathfrak{g} \to \mathfrak{g}$ is the adjoint map in $g \in G$. Taking a path with vanishing

variation at endpoints $\delta g_0 = \delta g_N = 0$, we obtain $\zeta_0 = \zeta_N = 0$, and we compute the reuslting variation of action

$$\begin{aligned}\mathrm{d}\,\mathcal{A}_d(g_d)\delta g_d &= \sum_{k=0}^{N-1} \ell_d'(f_{k,k+1})\delta f_{k,k+1} = \sum_{k=0}^{N-1} \ell_d'(f_{k,k+1}) TR_{f_{k,k+1}}(-\zeta_k + \mathrm{Ad}_{f_{k,k+1}}\,\zeta_{k+1}) \\ &= \sum_{k=1}^{N-1} \left(\ell_d'(f_{k-1,k}) TR_{f_{k-1,k}}\,\mathrm{Ad}_{f_{k-1,k}} - \ell_d'(f_{k,k+1}) TR_{f_{k,k+1}}\right)(\zeta_k).\end{aligned}$$

The Hamilton principle applied for arbitrary independent ζ_k for $k \in \{1, \dots, N-1\}$ yields the discrete Euler-Poincaré equations (DEP) given for all $k \in \{1, \dots, N-1\}$ by

$$\ell_d'(f_{k-1,k}) TR_{f_{k-1,k}}\,\mathrm{Ad}_{f_{k-1,k}} - \ell_d'(f_{k,k+1}) TR_{f_{k,k+1}} = 0. \tag{11}$$

Solving the DEP equation (11) gives the increments $\{f_{k,k+1}\}_{k=0}^{N-1}$, from which the path g_d is obtained via the initial value g_0 and the reconstruction step $g_{k+1} = g_k f_{k,k+1}$. Since for all k, $f_{k,k+1} \in G$ and $g_0 \in G$, it is readily checked that $g_k \in G$, i.e. the discrete path remains on the Lie group. Moreover, all the properties of general variational integrators such as symplectic behaviour still hold in this setting.

4.2 Natural chart integrator

We propose here a straightforward construction for a Lie variational integrator. Following [7], we use a natural chart τ of the group G to approximate the path g.

Let $\tau : \mathfrak{g} \to G$ be a local diffeomorphism containing an open neighborhood of the identity and such that $\tau(0_\mathfrak{g}) = e_G$; typical examples for τ are given by the exponential map and the Cayley map (ref). Let $g_k, g_{k+1} \in G$ be two group elements, we define the associated Lie algebra element $\xi_{k,k+1} \in \mathfrak{g}$ by

$$g_{k+1} = g_k \tau(\xi_{k,k+1}),$$

in other words $\xi_{k,k+1}$ is the direction taken to transport g_k to g_{k+1} along the diffeomorphism τ. We recall from section 4.1 that $f_{k,k+1} = g_k^{-1} g_{k+1}$, yielding the relation

$$\xi_{k,k+1} = \tau^{-1}(f_{k,k+1}).$$

Let us now consider a time interval $[t_k, t_{k+1}]$ and a given pair of configurations (g_k, g_{k+1}). We approximate the exact path g on this interval by the interpolating curve $g_d : [0, h] \to G$, $g_d(t) = g_k \tau(t\xi_{k,k+1}/h)$. This interpolation is left G-invariant, that is for any $\tilde{g} \in G$, $g_d(t; \tilde{g}g_k, \tilde{g}g_{k+1}) = \tilde{g} g_d(t; g_k, g_{k+1})$. Indeed, for $\tilde{g} \in G$,

$$\begin{aligned} g_d(t; \tilde{g}g_k, \tilde{g}g_{k+1}) &= \tilde{g}g_k \tau\left(t\tau^{-1}\left((\tilde{g}g_k)^{-1}(\tilde{g}g_{k+1})\right)/h\right) \\ &= \tilde{g}g_k \tau\left(t\tau^{-1}\left(g_k^{-1}\tilde{g}^{-1}\tilde{g}g_{k+1}\right)/h\right) \\ &= \tilde{g}g_k \tau\left(t\tau^{-1}\left(g_k^{-1}g_{k+1}\right)/h\right) \\ &= \tilde{g} g_d(t; g_k, g_{k+1}). \end{aligned}$$

We use the shortcut notation $g_d(t) := g_d(t; g_k, g_{k+1})$ from now on.

Now that the set of discrete paths has been define, we choose the discrete Lagrangian L_d as the left

rectangle rule quadrature of the Lagrangian integral $\int_0^h \mathrm{L}(g_d(t), \dot{g}_d(t))dt$, namely

$$\mathrm{L}_d(g_k, g_{k+1}) := h\,\mathrm{L}(g_d(0), \dot{g}_d(0)).$$

This discrete Lagrangian is left G-invariant since, for any $\tilde{g} \in G$,

$$\begin{aligned}
\mathrm{L}_d(\tilde{g}g_k, \tilde{g}g_{k+1}) &= h\,\mathrm{L}\left(g_d(0; \tilde{g}g_k, \tilde{g}g_{k+1}), \dot{g}_d(0; \tilde{g}g_k, \tilde{g}g_{k+1})\right) \\
&= h\,\mathrm{L}\left(\tilde{g}g_d(0; g_k, g_{k+1}), \tilde{g}\dot{g}_d(0; g_k, g_{k+1})\right) \\
&= h\,\mathrm{L}\left(g_d(0; g_k, g_{k+1}), \dot{g}_d(0; g_k, g_{k+1})\right) \\
&= \mathrm{L}_d(g_k, g_{k+1})
\end{aligned}$$

where we used the G invariance of g_d in line 1 and of L in line 2. This allows us to define a reduced discrete lagrangian $\ell_d : G \to \mathbb{R}$ as $\ell_d(g_k^{-1}g_{k+1}) := \mathrm{L}_d(g_k, g_{k+1})$. This can still be further simplified by expressing it in terms of the reduced Lagrangian $\ell : \mathfrak{g} \to \mathbb{R}$. After noticing that $g_d^{-1}(t)\dot{g}_d(t) = \xi_{k,k+1}/h$, we write

$$\begin{aligned}
\ell_d(g_k^{-1}g_{k+1}) = \mathrm{L}_d(g_k, g_{k+1}) &= h\,\mathrm{L}(g_d(0), \dot{g}_d(0)) \\
&= h\,\mathrm{L}\left((g_d(0))^{-1}g_d(0), (g_d(0))^{-1}\dot{g}_d(0)\right) \\
&= h\,\mathrm{L}(e_G, \xi_{k,k+1}/h) = h\ell(\xi_{k,k+1}/h) \\
&= h\ell(\tau^{-1}(f_{k,k+1})/h)
\end{aligned}$$

where we used the G-invariance of L in the first line. The expression for the derivative of ℓ_d follows, given by

$$\begin{aligned}
\ell_d'(f_{k,k+1}) &= \ell'\left(\tau^{-1}(f_{k,k+1})/h\right) T_{f_{k,k+1}}\tau^{-1} \\
&= \ell'\left(\xi_{k,k+1}/h\right) T_{\tau(\xi_{k,k+1})}\tau^{-1}
\end{aligned}$$

from which we deduce the discrete Euler-Poincaré equations (11) expressed in this setting for any $k \in \{1, \ldots, N-1\}$

$$\ell'\left(\xi_{k-1,k}/h\right) \mathrm{d}^{\mathrm{R}}\tau^{-1}_{\xi_{k-1,k}} \mathrm{Ad}_{\tau(\xi_{k-1,k})} - \ell'\left(\xi_{k,k+1}/h\right) \mathrm{d}^{\mathrm{R}}\tau^{-1}_{\xi_{k,k+1}} = 0 \tag{12}$$

where we recall from section 2 the definition of the right trivialized derivative $\mathrm{d}^{\mathrm{R}}\tau_\xi^{-1} : \mathfrak{g} \to \mathfrak{g}$, $\mathrm{d}^{\mathrm{R}}\tau_\xi^{-1} := T_{\tau(\xi)}\tau^{-1}TR_{\tau(\xi)}$.

An integrator for a choice of specific chart τ can be derived from equation (12) as follows. For a given pair (g_{k-1}, g_k), the element $\xi_{k-1,k}$ is computed as $\xi_{k-1,k} = \tau^{-1}(g_{k-1}^{-1}g_k)$. The next algebra element $\xi_{k,k+1}$ is determined as the solution of equation (12), where depending on the problem it might have to be solved implicitly, with a Newton method for example. Finally, the position g_{k+1} is updated as $g_{k+1} = g_k\tau(\xi_{k,k+1})$. A numerical application of such an integrator is given in section 5 on the rigid body problem.

4.3 Galerkin variational integrators

We recall the construction of the Galerkin variational integrator in section 3.3. In order to adapt it to the new setting of 4, it is necessary to make some adjustments in order to obtain a G invariant formulation.

As done previously in section 3.3, we construct g_d the interpolating curve of the exact path g on the time interval $[t_k, t_{k+1}]$ by setting $s+1$ control points $0 = \alpha_0 < \cdots < \alpha_s = 1$ associated to the group elements $\{g^\nu\}_{\nu=0}^s \in G$ such that $g_d(\alpha_\nu h; \{g^\mu\}) = g^\nu$ for every ν. In order to construct a G invariant interpolation, we use the correspondence of the Lie group G and its algebra $\mathfrak{g}$ via a local diffeomorphism $\tau : \mathfrak{g} \to G$ containing the identity and such that $\tau(0_\mathfrak{g}) = e_G$. This allows the interpolating curve of the solution g_d to be identified with a path ξ_d on the Lie algebra, defined by the relation

$$g_d(t; \{g^\nu\}) = g^0 \tau\left(\xi_d(t; \{\xi^\nu\})\right)$$

where we define the control points $\{\xi^\nu\}_{\nu=0}^s \in \mathfrak{g}$ by

$$\xi^\nu := \xi_d(\alpha_\nu h; \{\xi^\mu\})$$

and hence are deduced from $\{g^\nu\}$ by the relation

$$\xi^\nu = \tau^{-1}((g^0)^{-1} g^\nu).$$

As in section 3.3, we define the interpolating curve $\xi_d : [0, h] \to \mathfrak{g}$ in the algebra as a degree s polynomial expressed on the basis of Lagrange polynomials ϕ_ν, yielding

$$\xi(t; \{\xi^\nu\}) = \sum_{\nu=0}^{s} \xi^\nu \phi_\nu \left(\frac{t}{h}\right).$$

Its derivative $\dot{\xi}_d = g_d^{-1} \dot{g}_d$ is computed as

$$\dot{\xi}(t; \{\xi^\nu\}) = \frac{1}{h} \sum_{\nu=0}^{s} \xi^\nu \dot{\phi}_\nu \left(\frac{t}{h}\right).$$

With this definition, we can check that g_d is G invariant, i.e. for $\tilde{g} \in \mathfrak{g}$, $g_d(t; \{\tilde{g} g^\nu\}) = \tilde{g} g_d(t; \{g^\nu\})$. Let $\tilde{g} \in \mathfrak{g}$, then

$$\begin{aligned}
g_d(t; \{\tilde{g} g^\nu\}) &= \tilde{g} g^0 \tau\left(\xi_d\left(t; \left\{\tau^{-1}\left(\left(\tilde{g} g^0\right)^{-1} (\tilde{g} g^\nu)\right)\right\}\right)\right) \\
&= \tilde{g} g^0 \tau\left(\xi_d\left(t; \left\{\tau^{-1}\left((g^0)^{-1} \tilde{g}^{-1} \tilde{g} g^\nu\right)\right\}\right)\right) \\
&= \tilde{g} g^0 \tau\left(\xi_d\left(t; \left\{\tau^{-1}\left((g^0)^{-1} g^\nu\right)\right\}\right)\right) \\
&= \tilde{g} g^0 \tau\left(\xi_d(t; \{\xi^\nu\})\right) \\
&= \tilde{g} g_d(t; \{g^\nu\}).
\end{aligned}$$

We define the discrete Lagrangian L_d in the same way we did in section 3.3. For a given quadrature $(c_i, w_i)_{1 \le i \le r}$ of the interval $[0, 1]$ we define the local discrete action $\widetilde{\mathcal{A}}_d$ associated to the configurations $\{g^\nu\}_{\nu=0}^s$ as

$$\widetilde{\mathcal{A}}_d(\{g^\nu\}_{\nu=0}^s) := h \sum_{i=1}^{r} w_i \, \mathrm{L}\left(c_i h; \{g^\nu\}\right)$$

where we used the shortcut notation $\mathrm{L}(c_i h; \{g^\nu\}) := \mathrm{L}(g_d(c_i h; \{g^\nu\}), \dot{g}_d(c_i h; \{g^\nu\}))$. This allows us

to define the discrete Lagrangian $\mathrm{L}_d : G \times G \to \mathbb{R}$ on a pair (g_k, g_{k+1}) as the extremum of the local discrete action $\widetilde{\mathcal{A}}_d$ evaluated on $\{g^\nu\}_{\nu=0}^{s}$ with $g^0 = g_k$ and $g^s = g_{k+1}$

$$\mathrm{L}_d(g_k, g_{k+1}) = \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(c_i h; \{g^\nu\}\right)$$

Defining a reduced discrete Lagrangian requires L_d to be left G-invariant. We prove this by taking an arbitrary $\tilde{g} \in \mathfrak{g}$ and computing

$$\begin{aligned}
\mathrm{L}_d(\tilde{g}g_k, \tilde{g}g_{k+1}) &= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=\tilde{g}g_k,\, g^s=\tilde{g}g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(g_d(c_i h; \{g^\nu\}, h), \dot{g}_d(c_i h; \{g^\nu\}, h)\right) \\
&= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(g_d(c_i h; \{\tilde{g}g^\nu\}, h), \dot{g}_d(c_i h; \{\tilde{g}g^\nu\}, h)\right) \\
&= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(\tilde{g}g_d(c_i h; \{g^\nu\}, h), \tilde{g}\dot{g}_d(c_i h; \{g^\nu\}, h)\right) \\
&= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(g_d(c_i h; \{g^\nu\}, h), \dot{g}_d(c_i h; \{g^\nu\}, h)\right) \\
&= \mathrm{L}_d(g_k, g_{k+1})
\end{aligned}$$

where we used the G invariance of g_d in line 2 and of L in line 3.

In order to express the equations in terms of Lie algebra elements, we define the reduced discrete Lagrangian $\ell_d(g_k^{-1}g_{k+1}) := \mathrm{L}_d(g_k, g_{k+1})$ and we rewrite the action extremal by involving the reduced Lagrangian ℓ. After recalling $f_{k,k+1} = g_k^{-1}g_{k+1}$ and checking that $\xi^0 = \tau^{-1}((g^0)^{-1}g^0) = 0_{\mathfrak{g}}$ and $\xi^s = \tau^{-1}(g_k^{-1}g_{k+1}) = \tau^{-1}(f_{k,k+1})$, we compute

$$\begin{aligned}
\ell_d(f_{k,k+1}) &= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(g_d(c_i h; \{g^\nu\}, h), \dot{g}_d(c_i h; \{g^\nu\}, h)\right) \\
&= \underset{\substack{\{g^\nu\}_{\nu=1}^{s-1}\in G \\ g^0=g_k,\, g^s=g_{k+1}}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(L_{g_k^{-1}} g_d(c_i h), TL_{g_k^{-1}}\dot{g}_d(c_i h)\right) \\
&= \underset{\substack{\{\xi^\nu\}_{\nu=1}^{s-1}\in \mathfrak{g} \\ \xi^0=0,\, \xi^s=\tau^{-1}(f_{k,k+1})}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(\tau(\xi_d(c_i h)), T_{\xi_d(c_i h)}\tau(\dot{\xi}_d(c_i h))\right) \\
&= \underset{\substack{\{\xi^\nu\}_{\nu=1}^{s-1}\in \mathfrak{g} \\ \xi^0=0,\, \xi^s=\tau^{-1}(f_{k,k+1})}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(L_{\tau(\xi(c_i h))^{-1}}\tau(\xi(c_i h)), TL_{\tau(\xi(c_i h))^{-1}} T_{\xi_d(c_i h)}\tau(\dot{\xi}_d(c_i h))\right) \\
&= \underset{\substack{\{\xi^\nu\}_{\nu=1}^{s-1}\in \mathfrak{g} \\ \xi^0=0,\, \xi^s=\tau^{-1}(f_{k,k+1})}}{\operatorname{ext}} h\sum_{i=1}^{r} w_i\, \mathrm{L}\left(e, TL_{\tau(\xi(c_i h))^{-1}} TL_{\tau(\xi(c_i h))}\, \mathrm{d}^{\mathrm{L}}\tau_{\xi_d(c_i h)}(\dot{\xi}_d(c_i h))\right)
\end{aligned}$$

$$= \underset{\substack{\{\xi^\nu\}_{\nu=1}^{s-1}\in\mathfrak{g} \\ \xi^0=0,\, \xi^s=\tau^{-1}(f_{k,k+1})}}{\text{ext}} h\sum_{i=1}^{r} w_i \,\mathrm{L}\left(e_G, \mathrm{d}^{\mathrm{L}}\,\tau_{\xi_d(c_i h)}(\dot{\xi}_d(c_i h))\right)$$

$$= \underset{\substack{\{\xi^\nu\}_{\nu=1}^{s-1}\in\mathfrak{g} \\ \xi^0=0,\, \xi^s=\tau^{-1}(f_{k,k+1})}}{\text{ext}} h\sum_{i=1}^{r} w_i \ell\left(\mathrm{d}^{\mathrm{L}}\,\tau_{\xi_d(c_i h)}(\dot{\xi}_d(c_i h))\right)$$

where we used the shortcut notation $g_d(t) = g_d(t;\{g^\nu\},h)$ and $\xi_d(t) = \xi_d(t;\{\xi^\nu\},h)$, and where the left trivialized derivative $\mathrm{d}^{\mathrm{L}}\,\tau_\xi : T_\xi\mathfrak{g} \equiv \mathfrak{g} \to \mathfrak{g}$ is defined by $\mathrm{d}^{\mathrm{L}}\,\tau_\xi = TL_{\tau(\xi)^{-1}} \circ \mathrm{d}\,\tau_\xi : \mathfrak{g} \to T_{\tau(\xi)}G \to \mathfrak{g}$. The left invariance of the Lagrangian L was used twice, in lines 1 and 3.

The discrete reduced Lagrangian ℓ_d verifies the DEP equation established in section 4.1

$$\ell_d'(f_{k-1,k})TR_{f_{k-1,k}}\,\mathrm{Ad}_{f_{k-1,k}} - \ell_d'(f_{k,k+1})TR_{f_{k,k+1}} = 0 \tag{13}$$

5 Numerical application : free rigid body dynamics

We apply the previously described methods on the free rigid body problem. Its relatively simple and well know structure, well described in [7], makes it a common choice for numerical methods testing. Examples of numerical discretizations of the rigid body problem include [3] and [2].

After presenting the rigid body formulation, we apply both RKMK4 and natural chart methods designed in sections 2.2 and 4.2 respectively, and discussed the obtained discrete solutions. We refer to [4] for an extensive discussion about the implementation of Lie Galerkin integrator and its numerical restults for the rigid body dynamics.

5.1 Free rigid body dynamics

Let $\mathbb{I}$ be the constant inertia tensor, describing the geometry of the rigid body, without loss of generality we assume it to be diagonal, that is expressed in the principal directions of the body. Let $R(t) \in G = \mathrm{SO}(3) = \{R \in GL_3(\mathbb{R}) / RR^T = I,\ \det(R) = 1\}$ be the attitude matrix of the body at time t, the left trivialized rotational speed ξ is given at time t by $\xi(t) := R^{-1}(t)\dot{R}(t) \in \mathfrak{g} = \mathfrak{so}(3)$. In the absence of external forces, the Lagrangian $\mathrm{L} : TG \to \mathbb{R}$ is simply equal to the kinetic energy

$$\mathrm{L}(R,\dot{R}) = \frac{1}{2}\,\mathrm{tr}\left(\dot{R}^T R\mathbb{I}R^T\dot{R}\right).$$

This Lagrangian is left invariant, since for any $\tilde{R} \in \mathrm{SO}(3)$

$$\begin{aligned}\mathrm{L}(\tilde{R}R,\tilde{R}\dot{R}) &= \frac{1}{2}\,\mathrm{tr}\left((\tilde{R}\dot{R})^T(\tilde{R}R)\mathbb{I}(\tilde{R}R)^T(\tilde{R}\dot{R})\right)\\ &= \frac{1}{2}\,\mathrm{tr}\left(\dot{R}^T\tilde{R}^T\tilde{R}R\mathbb{I}R^T\tilde{R}^T\tilde{R}\dot{R}\right)\\ &= \frac{1}{2}\,\mathrm{tr}\left(\dot{R}^T R\mathbb{I}R^T\dot{R}\right) = \mathrm{L}(R,\dot{R}),\end{aligned}$$

allowing us to define the reduced Lagrangian $\ell : \mathfrak{so}(3) \to \mathbb{R}$ as

$$\ell(\xi) = \frac{1}{2}\,\mathrm{tr}\left(\xi^T\mathbb{I}\xi\right).$$

The algebra $\mathfrak{so}(3) = \{\xi \in GL_3(\mathbb{R}) / \xi^T = -\xi\}$ of skew-symmetric matrices can be identified with $\mathbb{R}^3$ via the hat map $\widehat{\cdot} : \mathbb{R}^3 \to \mathfrak{so}(3)$ defined for $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T \in \mathbb{R}^3$ by

$$\widehat{\boldsymbol{\xi}} = \begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix}$$

and for any $\boldsymbol{\nu} \in \mathbb{R}^3$ we have $\widehat{\boldsymbol{\xi}}\boldsymbol{\nu} = \boldsymbol{\xi} \wedge \boldsymbol{\nu}$. With this notation, the reduced Lagrangian can be rewritten as $\ell : \mathbb{R}^3 \to \mathbb{R}3$ where

$$\ell(\boldsymbol{\xi}) = 1/2 \, \langle \mathbb{I}\boldsymbol{\xi}, \boldsymbol{\xi} \rangle \tag{14}$$

for all $\boldsymbol{\xi} \in \mathbb{R}^3$. Applying the Hamilton principle yields the Euler-Poincaré equations for the rigid body

$$\dot{\boldsymbol{\pi}} + \boldsymbol{\xi} \wedge \boldsymbol{\pi} = 0 \tag{15}$$

where $\boldsymbol{\pi} := \mathbb{I}\boldsymbol{\xi} \in \mathbb{R}^3 \equiv \mathfrak{so}^*(3)$ is the angular momentum of the body.

5.2 RKMK4

Rewritten together with the initial condition $\boldsymbol{\pi}(0) = \boldsymbol{\pi}_0$, equation (15) becomes

$$\dot{\boldsymbol{\pi}} = \begin{pmatrix} 0 & \frac{\pi_3}{I_3} & -\frac{\pi_2}{I_2} \\ -\frac{\pi_3}{I_3} & 0 & \frac{\pi_1}{I_1} \\ \frac{\pi_2}{I_2} & -\frac{\pi_1}{I_1} & 0 \end{pmatrix} \boldsymbol{\pi}, \qquad \boldsymbol{\pi}(0) = \boldsymbol{\pi}_0 \tag{16}$$

with $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3)^T$ and $\mathbb{I} = diag(I_1, I_2, I_3)$. This equation is of the form (1) where $\mathcal{M} = \mathfrak{so}(3)^*$ is the homogeneous space and $G = \mathrm{SO}(3)$ is the acting Lie group. This means that for any t the angular momentum $\boldsymbol{\pi}(t)$ has a constant norm, that is $\|\boldsymbol{\pi}(t)\| = \|\boldsymbol{\pi}_0\|$. By applying a Runge-Kutta Munthe-Kaas method, we can ensure that this property is preserved by the approximate solution.

5.3 Natural chart integrator

In order to set up the method described in section 4.2, one need to provide the local diffeomorphism $\tau : \mathfrak{so}(3) \to \mathrm{SO}(3)$. We chose to use the Cayley map cay for its simplicity of computation. For any $\xi \in \mathfrak{so}(3)$, the image $\mathrm{cay}(\xi)$ is defined by

$$\mathrm{cay}(\xi) = \left(I - \frac{\xi}{2}\right)^{-1} \left(I + \frac{\xi}{2}\right)$$

A computation (ref) gives $\mathrm{d}^{\mathrm{R}} \mathrm{cay}_{\xi}^{-1} : \mathbb{R}^3 \to \mathbb{R}^3$ in the matrix form for $\xi \in \mathfrak{so}(3)$

$$\mathrm{d}^{\mathrm{R}} \mathrm{cay}_{\xi}^{-1} = I - \frac{\xi}{2} + \frac{\boldsymbol{\xi}\boldsymbol{\xi}^T}{4}.$$

Since the map $\mathrm{Ad}_g : \mathbb{R}^3 \to \mathbb{R}^3$ is given for $g \in \mathrm{SO}(3)$ by $\mathrm{Ad}_g(\boldsymbol{\xi}) = g\boldsymbol{\xi}$ where $\boldsymbol{\xi} \in \mathbb{R}^3$, we get the discrete Euler-Poincaré equation

$$\boldsymbol{\xi}_{k,k+1}^T \mathbb{I} \left(I - \frac{\xi_{k,k+1}}{2} + \frac{\boldsymbol{\xi}_{k,k+1}\boldsymbol{\xi}_{k,k+1}^T}{4} \right) = \boldsymbol{\xi}_{k-1,k}^T \mathbb{I} \left(I - \frac{\xi_{k-1,k}}{2} + \frac{\boldsymbol{\xi}_{k-1,k}\boldsymbol{\xi}_{k-1,k}^T}{4} \right) \tau(\xi_{k-1,k})$$

which has to be solved implicitly for $\boldsymbol{\xi}_{k,k+1}$.

5.4 Numerical results

In the following, all the numerical applications have been performed for the conditions

$$\boldsymbol{\pi}_0 = \begin{pmatrix} \cos(\pi/3) & 0 & \sin(\pi/3) \end{pmatrix}^T, \qquad \mathbb{I} = \begin{pmatrix} 2/3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

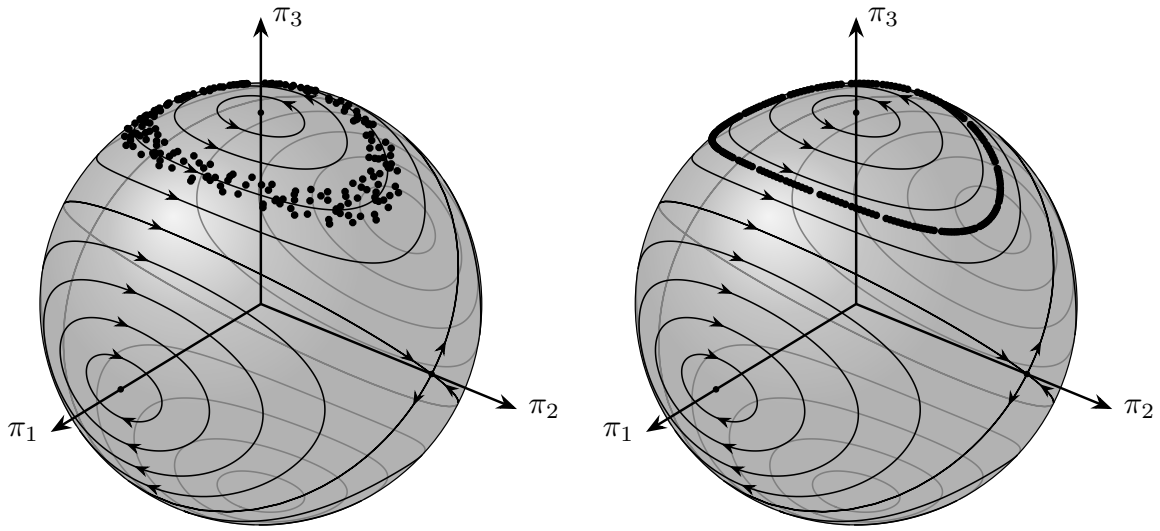


FIGURE 2 – Approximate angular momentum for RKMK4 (left) and natural chart (right) methods for $h = 0.9$.

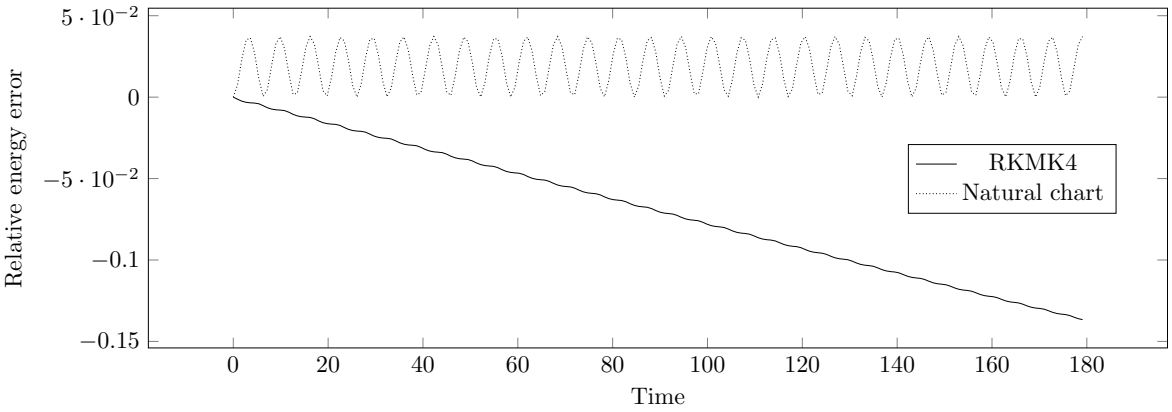


FIGURE 3 – Relative energy error for $h = 0.9$.

As expected, we observe on figure 2 that both methods preserve the Lie group structure of the solutions. This is illustrated by the fact that discrete paths for the angular momentum remain on the surface of the $\|\boldsymbol{\pi}_0\|$ radius sphere. That property is not ensured when applying direct discretization of the DEP equations ; examples of discrete paths drifting away from the sphere for the rigid body problem can be found in [3].

However, the two methods perform very differently in terms of symplecticity and consequentely energy behaviour. The RKMK4 method generates numerical errors that result over the long term in energy

dissipation. This is displayed on figure 2 by the drift of the solution towards orbits of lower energy level, i.e closer to the vertical axis. On the contrary, the natural chart method remains on a closed path crossing several orbits. Although the energy is not exactly preserved by this path, it never diverges over the long run and remains in a bounded interval. This feature is clearly illustrated in figure 3 displaying the relative energy error against time for both discrete paths.

Références

[1] F. Casas, B. Owren, Cost efficient Lie group integrators in the RKMK class, BIT, 43 (2003) 723–742.

[2] E. Celledoni, B. Owren, Lie group methods for rigid body dynamics and time integration on manifolds, Computer Methods in Applied Mechanics and Engineering, 192 (2003) 421–438.

[3] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration : Structure-Preserving Algorithms for Ordinary Differential Equations, Springer-Verlag, 2006.

[4] J. Hall, M. Leok, Lie Group Spectral Variational Integrators, Foundations of Computational Mathematics, 17 (2017) 199–257.

[5] M. Leok, Generalized Galerkin Variational Integrators, 2005.

[6] A. Lew, J.E. Marsden, M. Ortiz, M. West, Variational Time Integrators, International Journal for Numerical Methods in Engineering, 60 (2004), 153–212

[7] J.E. Marsden, T.S. Ratiu, Introduction to Mechanics and Symmetry : A Basic Exposition of Classical Mechanical Systems, 1999.

[8] J.E. Marden, M. West, Discrete Mechanics and Variational Integrators, Acta Numerica, 10 (2001) 357–514.

[9] H. Munthe-Kaas, Lie-Butcher Theory for Runge-Kutta Methods, BIT Numerical Mathematics, 35 (1995) 572–587.

[10] H. Munthe-Kaas, Runge-Kutta Methods on Lie Groups, BIT Numerical Mathematics, 38 (1998) 92–111.

[11] H. Munthe-Kaas, High Order Runge-Kutta Methods on Manifolds, Applied Numerical Mathematics, 29 (1999) 115–127.

[12] S. Ober-Blöbaum, N. Saake, Construction and Analysis of Higher Order Galerkin Variational Integrators, 2013.

[13] B. Owren, A. Marthinsen, Runge-Kutta Methods Adapted to Manifolds and Based on Rigid Frames, BIT, 39 (2001) 116–142.

[14] J.M. Wendlandt, J.E. Marsden, Mechanical Systems with Symmetry, Variational Principles, and Integration Algorithms, Current and Future Directions in Applied Mathematics, Birkhäuser Boston, 1997, pp. 219–261.