



HAL
open science

Revisiting Geometric Integrators in Mechanics

Aziz Hamdouni, Vladimir Salnikov

► **To cite this version:**

Aziz Hamdouni, Vladimir Salnikov. Revisiting Geometric Integrators in Mechanics. pp.65-68, 2021.
hal-03445340

HAL Id: hal-03445340

<https://hal.science/hal-03445340>

Submitted on 21 Sep 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Revisiting Geometric Integrators in Mechanics

Aziz Hamdouni², Vladimir Salnikov^{1,2}

¹*CNRS – National Center for Scientific Research, France*

²*La Rochelle University, France*

e-mail: aziz.hamdouni@univ-lr.fr, vladimir.salnikov@univ-lr.fr

Abstract. We address the question of efficient construction of geometric integrators – numerical methods preserving some internal geometric structure of the system of equations. Such methods are of particular importance for modelling and simulation of mechanical systems, where these structures permit to control the conservation of physically relevant quantities. We focus our attention on the so called generalized geometry, for which we present an approach to design higher order Runge–Kutta style numerical methods.

Keywords: geometric integrators, constraint mechanics, Dirac structures, Runge–Kutta methods.

Motivation / Introduction

In this contribution we study the structure preserving numerical methods, also often called *geometric integrators* appearing naturally in the context of robust and reliable simulation of mechanical systems. The key idea is that the equations governing mechanical systems have some intrinsic description using the objects from modern differential and algebraic geometry, those objects serve as a “proxy” to mimic physical properties of the systems: symmetries, conservation laws, qualitative behaviour, etc... The strategy itself is not exactly new, it somehow dates back almost to the middle of the 20th century in the context of integrable systems. However very often the implementation of it amounts to some “do-it-yourself” constructions. What we discuss in this text is a part of a big project of bringing “order and method” to this strategy, namely we work on explicit descriptions of the classes of mechanical systems with the corresponding geometric structures, for which then we formulate clear algorithmic approaches to construction of appropriate numerical methods. A recent overview of the state of the art can be found in [1].

Symplectic integrators

As mentioned above, one of the folkloric examples of geometric integrators are symplectic numerical methods in the context of Hamiltonian systems. One considers the phase space of a mechanical system on which a symplectic form is naturally defined – locally this is a skew-symmetric non-degenerate (constant) bilinear form¹ ω – a multidimensional generalization of the oriented area. Given a smooth function H , this ω permits to define a Hamiltonian vector field X_H governing the dynamics of the system. It is easy to show that ω is invariant by the flow of X_H , but a more interesting property is sort of converse: a vector field preserving ω will respect the level sets of H .

Phrased this way the symplectic property naturally gives the idea of a numerical method: if a discretized flow of the system of differential equations (better) preserves the symplectic

¹In this text we will only give qualitative descriptions of the necessary geometric objects, skipping technical details, they may sound vague, but are globally correct. For more precise definitions and details a motivated reader may consult [2].

form, it conserves the energy of the system (better). However, to the best of our knowledge, the symplectic integrators were not constructed this way, they were merely discovered by chance. In some simulation of planetary systems it has been observed that neither explicit nor implicit methods produced satisfactory results in terms of stability, while a semi-implicit method did. And only after, for example in [3], the result was interpreted as above.

Let us, for pedagogical reasons, deduce the form of the symplectic Euler method. Consider a Hamiltonian system

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q},$$

defined by the Hamiltonian H and the symplectic form $\omega = dp \wedge dq$. Here q are the coordinates of the system, and p are its momenta; they are both multidimensional (vector) variables, but we omit the indices not to overload the presentation. To solve this system consider a family of first order methods

$$q^{n+1} = q^n + h \frac{\partial H}{\partial p}(q, p), \tag{1}$$

$$p^{n+1} = p^n - h \frac{\partial H}{\partial q}(q, p), \tag{2}$$

where h is the timestep, and (q, p) in the right hand sides is a point to be determined. More precisely, let

$$q = aq^n + bq^{n+1} \text{ and } p = cp^n + dp^{n+1}$$

with unknown coefficients a, b, c, d , in principal allowed to be all different. We want the symplectic form to be conserved, thus compute $dp^{n+1} \wedge dq^{n+1} - dp^n \wedge dq^n$ and determine the conditions for it to vanish up to the maximal possible power of h , for arbitrary choice of H . Plugging in the (implicit) expressions (1) and (2), and using the Taylor expansion for the right hand sides, one obtains for the linear term the condition

$$a + b - c - d = 0,$$

which is trivially satisfied due to the consistency of the method: $a + b = 1, c + d = 1$. But already the quadratic term adds to this a non-trivial condition

$$a - d = 0,$$

which precisely means that the method should be neither purely explicit nor implicit. It is satisfied by the standard symplectic Euler method, where $a = d = 1, b = c = 0$. The computation may go further and potentially produces other conditions. The same strategy can eventually be applied for higher order methods that replace (1) and (2), and as mentioned, is relevant for other geometric structures – we describe them in the next section.

Dirac structure based methods

The Hamiltonian–symplectic formalism described above is appropriate for conservative isolated mechanical systems. Since its establishment several other directions have been explored, here in particular we discuss systems with constraints. It has been observed ([4]) that the relevant geometry for those is related to Dirac structures, not going into technical details, let us just give an idea of those. For classical mechanics one can describe the system using coordinates and either velocities or momenta – that gives Lagrangian or Hamiltonian

picture respectively. Dirac structures, roughly speaking use both of them simultaneously, so the considered space is enlarged; but they also take into account that velocities and momenta are not independent, so the space is restricted back in a non-trivial way. Hence, if the system is subject to some constraints, those can be formulated in terms of velocities, or momenta, or both.

The main message of [4], reviewed in [5], is that considering the Dirac structure associated to the constraint distribution, one can apply the techniques of variational integrators to design a numerical method which preserves the constraints better than the usual one. In [5, 6] we have constructed an improvement of such a Dirac based method, and considered some applications of it. But as mentioned, this has been done rather by an “educated guess”, than by a generalizable procedure. In this text, we present a more algorithmic approach, in the style of the above symplectic discussion.

The starting point of [4, 5] is the data of a Lagrangian $L = L(q, v)$, and constraints $\varphi(q, v) = 0$, again all the variables are of appropriate dimension, but the indices are dropped. The dynamics will however be viewed in the (q, p) -space:

$$\dot{q} = v, \quad \dot{p} = \frac{\partial L}{\partial q} + \lambda \alpha, \quad (3)$$

where $\alpha = d\varphi$ – the generators of the vanishing ideal for the constraints, λ is the set of Lagrange multipliers. The constraints are rewritten as

$$\alpha(v) = 0, \quad (4)$$

and the relation of v and p is given by the Legendre transform

$$p = \frac{\partial L}{\partial v}. \quad (5)$$

These two (algebraic) conditions as well as the differential equations (3) are deduced directly from the Dirac structure.

We will now apply the Runge–Kutta type methods to solve (3). Recall that for an equation $\dot{y} = f(y)$ the method reads

$$y^{n+1} = y^n + h \sum_{i=1}^s b_i k_i, \quad k_i = f(y^n + h \sum_{j=1}^s a_{ij} k_j). \quad (6)$$

This general form of solution is applied to both equations in (3), obviously with different f . Note that the method is a priori allowed to be implicit, and the coefficients a_{ij} and b_i can and will eventually be different for the two equations.

The same procedure as for the symplectic form above is now applied to the equations (4) – (5): suppose that they are satisfied at the n -th step — compute the approximation of them for the $(n + 1)$ -st one, using the Taylor expansion — force it to be satisfied up to the maximal possible power of h . As a result, for $s = 1$, i.e. for the simplest first order Runge–Kutta method, one reproduces up to h^2 the Dirac-1 integrator spelled-out explicitly in [6]. Moreover one sees that holonomic constraints, that is not depending explicitly on v , are better preserved.

Higher order methods ($s > 1$) will be presented in detail in the extended version of this paper ([7]), together with careful benchmark tests and examples of application to mechanical systems. But already here it is important to note, that in contrast to the original approach of [4] their derivation sketched here is rather straightforward. The only arising complication is because of lengthy formal computation, potentially treated by computer algebra tools.

Conclusions / Outlook

Let us mention several remarks in conclusion.

First, the main framework discussed above – systems with constraints – seem to be a very particular class of systems. This is true from the mechanical point of view, but not exactly from the geometric perspective: for instance, apparently the Dirac structures constructed from the constraint distribution behave similarly to the ones from symplectic foliations of Poisson manifolds, this makes us think about Poisson integrators.

Second, Dirac structures also appear naturally for dissipative and coupled systems – the preservation of it by the continuous or discrete flow corresponds to power balance. We discussed some open questions on that in [2], and we can now add one more near at hand direction to them – constructing appropriate higher order discretizations.

Third, and probably conceptually the most important, is the relation of the above discussion to so called graded geometry. In fact all the above mentioned geometric constructions have a uniform and rather convenient description in terms of differential graded manifolds. We have sketched their description in [1] and [2], and mentioned some open computer algebra problems. Note here, that the discretization in the “graded world” is also a totally unexplored field that we plan to address in the nearest future.

Acknowledgments. This work is supported by the CNRS 80 Prime project “GraNum”.

References

1. *Salnikov V., Hamdouni A., Loziienko D.* Generalized and graded geometry for mechanics: a comprehensive introduction. *Mathematics and Mechanics of Complex Systems*. 2021. Vol. 9, Issue 1.
2. *Salnikov V., Hamdouni A.* Differential Geometry and Mechanics — a source of problems for computer algebra. *Programming and Computer Software*. 2020. Vol. 46, Issue 2.
3. *Verlet L.* Computer “Experiments” on Classical Fluids. *Phys. Rev.* 1967. Vol. 159(1). P. 98–103.
4. *Yoshimura H., Marsden J.E.* Dirac Structures in Lagrangian Mechanics. Part I: Implicit Lagrangian Systems. *Journal of Geometry and Physics*. 2006. Vol. 57 P. 133–156.
5. *Salnikov V., Hamdouni A.* From modelling of systems with constraints to generalized geometry and back to numerics. *Z Angew Math Mech*. 2019.
6. *Razafindralandy D., Salnikov V., Hamdouni A., Deeb A.* Some robust integrators for large time dynamics. *AMSES*. 2019. Vol. 6(5).
7. *Loziienko D., Salnikov V., Hamdouni A.* Dirac–Runge–Kutta numerical methods, final preparation, 2021.