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Geometric integrators in mechanics – the need for computer algebra tools

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In this contribution we will describe some objects of the generalized geometry that appear naturally in the qualitative analysis of mechanical systems. In particular we will discuss the Dirac structures within the framework of the systems with constraints as well as of the port-Hamiltonian systems.

From the mathematical point of view, Dirac structures generalize simultaneously symplectic and Poisson structures. As for mechanics, the idea is to design numerical methods that preserve these structures and thus guarantee good physical behaviour in the simulation.

Then, we will present a framework which is even more general – the one of differential graded manifolds (also called Q-manifolds), and discuss some possible ways of using them for the “structure preserving integrators” in mechanics.

For all of the mentioned constructions we will explain the problems that arise in generic situations – most of them are open, but we think they are suitable for handling with various computer algebra approaches.

Key words and phrases: geometric mechanics, graded and generalized geometry, geometric integrators.

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Геометрические интеграторы в механике – важность методов компьютерной алгебры

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В этой работе мы описываем некоторые объекты так называемой обобщенной геометрии, возникающие естественным образом при качественном анализе уравнений, описывающих механические системы. В частности, мы обсудим структуры Дирака в рамках систем со связями и порт-Гамильтоновых систем.

С точки зрения фундаментальной математики, структуры Дирака одновременно обобщают симплектические и Пуассоновы структуры. Что касается механики, идея состоит в построении численных методов, сохраняющих эти структуры, и таким образом гарантирующих адекватные физические характеристики модели.

Затем мы опишем еще более общий формализм градуированной геометрии и дифференциальных градуированных многообразий (Q-многообразий). Мы обсудим возможности их использования для построения интеграторов “сохраняющих структуры” для задач механики.

Для всех вышеупомянутых конструкций мы опишем типичные возникающие задачи (в основном, нерешенные), для которых мы считаем уместным использование методов компьютерной алгебры.

Ключевые слова: геометрическая механика, градуированная и обобщенная геометрия, геометрические интеграторы.

1. Introduction

This paper is one in a series of works devoted to geometric formulation of contemporary mechanics. By this we mean a search for algebro-geometric structures relevant and convenient for deriving the equations governing mechanical systems and eventually studying their behaviour. The aim of the project is twofold: on the one hand spelling out the “hidden” structure of the equations describing mechanical systems may give serious hints about their properties; on the other hand one obtains an extra piece of information for design and optimization of numerical methods adapted for reliable simulation of those.

Some more or less recent works by our team and collaborators have proved this geometric approach to be very fruitful from various perspectives: taking into account conservation laws, symmetries, constraints improves the quality of numerical methods and hence the results of simulations as well as the qualitative understanding of the properties of the system. The goal of this paper is to show that in this process of “geometrizing” of mechanics the computer algebra algorithms are convenient and sometimes unavoidable.

We will address some constructions that were spotted as promising for a large class of mechanical systems, namely, the port-Hamiltonian formalism, Dirac structures, and differential graded manifolds. The following section (2) is devoted to the description of those, and after that (sections 3, 4) we provide some examples. We are obviously not going into technicalities and definitions but rather convey some ideas. However an interested reader may follow the references for details, and we give enough information to understand the issues related to computer algebra, that can be addressed directly. We end up by formulating a couple of open (at least up to our knowledge) problems.

2. Geometric preliminaries

Probably one of the first example showing the importance of geometric methods in mechanical simulations is related to symplectic integrators ([1, 2]) – they are relevant for finite dimensional conservative mechanical systems. The idea behind the method is to construct a discretization of the dynamics that preserves the symplectic structure – a differential 2-form ω defined on the phase space of the system. This form is closed and non-degenerate, it is a generalization of the area form in dimension higher than 2. The preservation of ω guarantees the conservation of the Hamiltonian function that will oscillate in a small neighborhood around the initial value of total energy of the system. The phenomenon persists also for large time intervals, in contrast to other methods even of higher order. The upshot is: a physical property (conservation of energy) is taken into account implicitly via the consideration of a geometric structure (ω). A natural application is for instance Molecular Dynamics, where one is precisely interested in long trajectories – the popular methods are based on the Verlet’s scheme (e.g. “velocity leapfrog”), which is symplectic.

A natural generalization is to consider systems with *dissipation* or *interaction with the medium*, or sub-systems *coupled* to each other. Another important class would be *systems with constraints*, i.e. not all the variables are independent – there are some relations between them. In contrast to the conservative case, the situation is less clear both from geometric and numerical points of view. It turns out that for both cases *Dirac structures* may be useful.

Dirac structures ([3]), are the sub-bundles of an object called *generalized tangent bundle* (or Pontryagin bundle) $\mathbb{T}M = TM \oplus T^*M$ with some properties. More precisely, one considers couples (vector field, differential 1-form), on these couples two natural operations are defined: the Courant–Dorfmann bracket and the contraction ‘scalar product’. A Dirac structure is a subset of these couples (of maximal rank), on which the scalar product vanishes identically and which is invariant under the bracket. Omitting the last condition will result in the definition of an *almost Dirac structure*, which we will mostly use in this text. The Dirac structures were introduced by T. Courant with a

motivation to study dynamical systems, but were almost not used in this context before the works on port-Hamiltonian systems ([4, 5]) and implicit Lagrangian systems ([6–9]).

Locally the description of Dirac structures boils down to some linear algebra, but globally it can be a bit challenging since differential geometry is involved. One can bypass (or at least “hide”) the difficulties introducing the language of *graded geometry* and *Q-structures* in the context.

One defines a graded manifold by introducing a grading on the sheaf of functions on it, that is the coordinates will have “labels” – degrees responsible for commutation relations. A typical example is the shifted tangent bundle to a smooth manifold $T[1]M$ – one views the differential forms on M as polynomial functions on $T[1]M$, where the fiber-linear coordinates anti-commute, and the degree of a form corresponds to the degree of a polynomial. A *Q-structure* is a degree-1 homological (i.e. squaring to zero) vector field on a graded manifold. For $T[1]M$ the De Rham differential is an example of such a vector field. A graded manifold equipped with a *Q-structure* is thus called a *differential graded manifold* or *Q-manifold* for short.

The framework of graded geometry is very rich, it permits to give a unified description of a great deal of contemporary geometric concepts: symplectic, Poisson and Dirac structures, algebroids; it allowed to address problems from theoretical physics, study the symmetries and gauging of functionals. And as mentioned, we are interested in graded manifolds for establishing a proper formalism of contemporary mechanics. Below we will give a couple of examples where the constructions are natural.

3. Constraints in implicit Lagrangian formalism

The first example of application of the geometric structures described above are the systems with constraints within the implicit Lagrangian formalism introduced in [6, 7]. Here we make the minimal necessary presentation, the details can be found in [8] and [9]. For simplicity we will not talk about bundles, but rather about spaces, the construction being locally the same.

We consider a mechanical system initially with d degrees of freedom. The tangent and cotangent bundles from the previous section will be constructed over its phase space and will thus locally look as $\mathcal{V} = \mathbb{R}^{4d} = \mathbb{R}^{2d} \times \mathbb{R}^{2d}$. Or more precisely, the phase space is $\mathbb{R}^{2d} = \mathbb{R}^d \times V^{*d}$, that is the trivial bundle over \mathbb{R}^d with a fiber being V^* – the dual of some d -dimensional vector space. Morally, V is the space of velocities at each point and V^* corresponds to momenta; in coordinates:

$$q = (q^1, \dots, q^d)^T \in \mathbb{R}^d, v = (v^1, \dots, v^d)^T \in V^d, p = (p_1, \dots, p_d)^T \in V^{*d}.$$

The constraints on the system mean that some of the coordinates are dependent, in a simple case it means that in the first factor \mathbb{R}^d a submanifold is defined. It also means in a general case, that there is some restriction on couples (q, v) , i.e. not all the points q are permitted, and at each point q , v is not arbitrary, but belongs to a subspace $V' \subset V$. A correct mathematical way of saying this is that v belongs to a distribution Δ_q which under regularity conditions may be seen as the kernel of a set of linear forms α^a . This will be the *input data*: the permitted vector fields $v(q) \in \Delta$ are in the kernel of given m differential 1-forms $\alpha^a(q)$, $a = 1, \dots, m$, and the dynamics is governed by a Lagrangian which is a function $L: \mathbb{R}^{2d} = \mathbb{R}^d \times V^d \rightarrow \mathbb{R}$.

Then the constraint set is a subset $\tilde{\Delta} \subset \mathcal{V}$, and the differential forms $\alpha^a(q)$ generate its annihilator Δ_0 that naturally belongs to \mathcal{V}^* . Note that, since $\mathbb{R}^d \times V^*$ is a symplectic space (cf. section 2), that is equipped with a bilinear antisymmetric non-degenerate closed form ω , one can construct a mapping $\Omega^b: \mathcal{V} \rightarrow \mathcal{V}^*$. This defines the (almost) *Dirac structure* associated to the system with constraints:

$$\mathbb{D}_\Delta = \{(w, \beta) \in \mathcal{V} \times \mathcal{V}^* \mid w \in \tilde{\Delta}, \beta - \Omega^b w \in \Delta_0\}.$$

Now, from the Lagrangian, one constructs its differential which is a mapping dL from $\mathbb{R}^d \times V$ to its cotangent. And again by post-composing it with a symplectomorphism of

the appropriate double bundles, one constructs the *Dirac differential* $\mathcal{DL}: \mathbb{R}^d \times V \rightarrow \mathcal{V}^*$. It may sound too sketchy, but the important information about its local form is already present – in coordinates it reads: $\mathcal{DL}: (q, v) \rightarrow (q, \frac{\partial L}{\partial v}, -\frac{\partial L}{\partial q}, v)$. There is also a natural way to lift the evolution of the system to this extended space via a *partial vector field* X , i.e. a mapping $X: \Delta \oplus \text{Leg}(\Delta) \subset \mathbb{R}^d \times V \oplus \mathbb{R}^d \times V^* \rightarrow \mathcal{V}$, where $\text{Leg}(\Delta_Q)$ is the image of Δ by the Legendre transform.

In the notations above, the *implicit Lagrangian system* is a triple (L, Δ, X) , s.t. $(X, \mathcal{DL}) \in \mathbb{D}_\Delta$. In local coordinates this means:

$$\begin{aligned} \dot{q} &\in \Delta, & p &= \frac{\partial L}{\partial v} \\ \dot{q} &= v, & \dot{p} - \frac{\partial L}{\partial q} &\in \Delta_0 \end{aligned}$$

The first three equations are just the usual expressions of the relations between velocities and momenta, the fourth one can be rewritten as

$$\dot{p} - \frac{\partial L}{\partial q} = \sum_{a=1}^m \lambda_a \alpha^a,$$

and one recognizes immediately the Lagrange multipliers.

The previous paragraph is not just an alternative way to recover the usual formalism, each step of it admits a discrete version. Starting from the input data one defines the discretized Lagrangian is $L_d := hL(q_k, v_k)$, and the constraints are rewritten as

$$\langle \alpha_d^a, v_k \rangle = 0, \quad a = 1, \dots, m,$$

where q_k is the value of q and v_k is an approximation of the velocity, both at the k -th timestep.

To construct the numerical method out of these data, one applies the following procedure:

$$\begin{aligned} p_{k+1} &= \frac{1}{h} \frac{\partial L_d}{\partial v_k} \\ p_k - \frac{1}{h} \frac{\partial L_d}{\partial v_k} + \frac{\partial L_d}{\partial q_k} &= \sum_{a=1}^m \lambda^a \frac{\partial \langle \alpha_d^a, v_k \rangle}{\partial v_k} \\ \langle \alpha_d^a, v_k \rangle &= 0, \quad a = 1, \dots, m. \end{aligned}$$

The variables appearing explicitly are the values of p at k -th and $(k+1)$ -st step; and v_k should be some approximation of the velocity, thus bringing in q_k , for instance $v_k := \frac{q_{k+1} - q_{k-1}}{2h}$.

This approach has been successfully applied for “scholar” examples of pendula systems ([8]) and for instabilities of the the Ziegler’s column ([9]). But for more complicated examples one sees clearly the potential *calls for computer algebra*. First, one needs to obtain the above system of equations. It is certainly doable “by hand”, but is clearly not pleasant for realistic systems with complicated non-linear constraints. Second, even more challenging, it needs to be solved. We obtain $2d + m$ equations: d from each of the lines 1 and 2 of the equations above, and m from the constraints in line 3. At the k -th step the unknowns are q_{k+1} , p_{k+1} and λ , so the system we obtain is complete. It is linear in λ and p_{k+1} , but in q_{k+1} it is linear only when the constraints are holonomic, i.e. do not depend on velocities. In contrast to derivation of the equations which is done once, their solution is needed at each timestep, so it should be to be efficient. And the situation is even more intricate for higher order methods.

4. Coupling in port-Hamiltonian systems

The second example to motivate the introduction of Dirac structures is the so-called port-Hamiltonian formalism ([4]). One studies a modification of usual Hamiltonian systems adding some terms responsible for dissipation, coupling or just external forces. Consider for example a system of the following form:

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

where $\mathbf{q} \in \mathbb{R}^n$ (or M a smooth manifold) – the (generalized) coordinates, $\mathbf{p} \in \mathbb{R}^n$ (or T_q^*M) – the conjugate momenta (also sometimes called ‘impulses’ - morally the velocities). The dynamics is then fully defined by the Hamiltonian $H = H(\mathbf{q}, \mathbf{p})$ and the force \mathbf{F} . Or more generally, look at a system of the following form:

$$\dot{\mathbf{x}} = (J(\mathbf{x}) - R(\mathbf{x}))\frac{\partial H}{\partial \mathbf{x}} + g(\mathbf{x})\mathbf{f}, \quad (1)$$

with an antisymmetric matrix $J(\mathbf{x})$ and some forces given by $R(\mathbf{x})$ and \mathbf{f} – they would precisely make a difference between the Hamiltonian case and its ‘port’- generalization.

Following [5] one can recover an almost Dirac structure for any port-Hamiltonian system in a very straightforward way. So, after this cited result there was a series of papers following the same pattern: take a Hamiltonian system, add something to it (almost anything: a dissipation, some external force, a control), identify the ‘ports’, spell out the Dirac structure. Sometimes it was done “just for fun” with no direct conclusion. We would like to address the problem with a rather precise motivation. First of all, the starting point will not be Hamiltonian but just some system of differential equations, and the first step would be to find the appropriate port-Hamiltonian formulation. Then, we would go one or two steps further – the obtained structure would be used to design numerical methods that preserve it. This can be done directly from Dirac geometry or from a more general construction of Q -manifolds ([10]).

Once again, not going into the most general procedure, let us give an example of this approach. We consider a (totally simplified) model for the problem of fluid–structure interaction. The system is an infinitely long cylinder attached to a spring, subject to constant air flow orthogonal to its axis. The phenomenon that one can observe for such a system is that small vortices are formed due to perturbations, they induce oscillations of a cylinder, which in turn influences the flow. The model can be reduced ([11]) to a harmonic oscillator coupled to the Van der Pol system:

$$\begin{aligned} \ddot{y} + y &= m\Omega^2 q \\ \ddot{q} - \varepsilon(1 - q^2)\dot{q} + \Omega^2 q &= A\ddot{y} \end{aligned} \quad (2)$$

With the usual approach to lower the order of the system, and denoting $(\Omega^2 - Am\Omega^2) =: \tilde{\Omega}^2$, $\varepsilon(1 - q^2) =: a$, we can rewrite it as follows:

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 + m\Omega q \\ \dot{q}_1 &= q_2 \\ \dot{q}_2 &= -\tilde{\Omega}^2 q_1 + aq_2 - Ay \end{aligned}$$

To fit it to the form (1) denote: $H = \frac{1}{2}(x_1^2 + x_2^2) + \frac{1}{2}(\tilde{\Omega}^2 q_1^2 + q_2^2)$,

$$X = \begin{pmatrix} x_1 \\ x_2 \\ q_1 \\ q_2 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad g = \begin{pmatrix} 0 \\ m\Omega^2 q_1 \\ 0 \\ a(q_1)q_2 - Ax_1 \end{pmatrix}.$$

The following variables correspond to fluxes and efforts (see [5] for the terminology):

$$f_s = -\dot{X}, \quad e_s = \begin{pmatrix} x_1 \\ x_2 \\ \tilde{\Omega}^2 q_1 \\ q_2 \end{pmatrix}, \quad e_i = 1 \in \mathbb{R}^1, \quad f_i = m\Omega^2 q_1 x_2 - Ax_1 q_2 + a(q_1)q_2^2.$$

A simple computation shows that $\dot{H} = -e_s^T f_s = e_i f_i$.

For the geometric picture, consider a manifold M , with coordinates (x_1, x_2, q_1, q_2) , $f_s \in \Gamma(TM)$, $e_s \in \Gamma(T^*M)$, and: $f_i \in \Gamma(\mathcal{F})$, $e_i \in \Gamma(\mathcal{F}^*)$, for \mathcal{F} a trivial bundle. In the notations of section (2) $\text{T}\mathcal{M} = (TM \times \mathcal{F}) \oplus (T^*M \times \mathcal{F}^*)$.

The almost Dirac structure is given by the condition $e_s^T f_s + e_i f_i$ which is precisely the evolution of total energy from above. This is a subbundle of rank 5, given by the graph of the bivector D :

$$\begin{pmatrix} f_s \\ f_i \end{pmatrix} = D \begin{pmatrix} e_s \\ e_i \end{pmatrix},$$

where $D: T_X^*M \times \mathcal{F}^* \rightarrow T_X M \times \mathcal{F}$ in coordinates reads:

$$D = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -m\Omega^2 q_1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -a(q_1)q_2 + Ax_1 \\ 0 & m\Omega^2 q_1 & 0 & aq_2 - Ax_1 & 0 \end{pmatrix}.$$

For the description in the world of *graded geometry*, consider $T^*[1]\mathcal{M}$ with coordinates x^i (of degree 0), and p_i (fiber-linear of degree 1). The degree 1 vector field constructed from the bivector D , following for example [12], reads:

$$\begin{aligned} Q = & -p_2 \frac{\partial}{\partial x^1} + (p_1 - p_5 m\Omega^2 x^3) \frac{\partial}{\partial x^2} - p_4 \frac{\partial}{\partial x^3} + (p_3 - p_5 a(x^3)x^4 - Ax^1) \frac{\partial}{\partial x^4} + \\ & + (p_2 m\Omega^2 x^3 + p_4 a(x^3)x^4 - Ax^1) \frac{\partial}{\partial x^5} + \\ & + Ap_4 p_5 p_5 \frac{\partial}{\partial p_1} + (-m\Omega^2 p_2 p_5 + 2\epsilon x^3 x^4 p_4 p_5) \frac{\partial}{\partial p_3} - a(x^3) p_4 p_5 \frac{\partial}{\partial p_4} \end{aligned}$$

And as before, one can easily imagine the profit from *computer algebra tools* for most of the presented steps: to recover the form (1) from (2), to spell-out the Dirac structure and the associated Q -structure, and checking their properties.

5. Conclusions / Open directions

Summing up, in this paper we have discussed two situations where we expect the computer algebra tools, and in particular symbolic algorithms to be of great use. Let us note that the two applications are essentially different. In the first one, related to Dirac structure preserving integrators for systems with constraints, the approach is rather straightforward. One basically knows what to do, and the tools are there just to simplify lengthy computations. The second one is more complicated: if going through the presented example carefully, one notices that the steps are not uniquely defined. It

means, first of all, that the existence tests are appropriate, and if they succeed, there are choices to be made, so there is room for optimization.

Let us also mention that the symbolic computations in the graded setting, are (to the best of our knowledge) almost not developed. They are extremely important for applications for the problems mentioned here, as well as for other subjects like theoretical physics. Thus, extending the standard methods from differential geometry to graded setting may be a very fruitful idea.

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