Involution and Constrained Dynamics II: The Faddeev-Jackiw Approach

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Abstract. We study the symplectic approach to first-order systems with constraints from the point of view of the formal theory of differential equations. We concentrate especially on systems without first class constraints and give a geometric interpretation of an approach recently proposed by Barcelos-Neto and Wotzasek. We further study the numerical properties of this approach. We also comment on some problems concerning the application to field theories.

Short title: Involution and Constrained Dynamics II

September 26, 1995

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1. Introduction

We showed in the previous article [35] of this series that many methods for the analysis of systems with constraints can mathematically be identified with completing the equations of motion to an involutive system. In this article we specialize on systems described by Lagrangians which are linear in the velocities.

Starting with an article by Floreanini and Jackiw [18] about the quantization of self-dual fields in two dimensions these systems have recently found some attention in the literature. Especially their circumvention of the classical Dirac algorithm [14] sparked some discussion [9, 12]. Faddeev and Jackiw explained this approach, sometimes also called the symplectic formalism, in a later article [15] in more detail. Actually it can already be found in the classical textbook of Sudarshan and Mukunda [37]. Thus "Faddeev-Jackiw approach" is somewhat a misnomer, but we stick to this name, as it is meanwhile widely used.

The main interest in these systems arises from the fact that they yield the Dirac bracket [14] in a very simple way [21, 23]. Barcelos-Neto and Wotzasek [4, 5] showed later how this property can be carried over to systems subject only to second class constraints via an extension of the configuration space.

Most of the present article will concentrate on this approach. Besides showing how it appears from the point of view of the involution analysis, we will give a geometric interpretation and show that the main idea lying behind it is transforming the second class constraints into first class ones. We will also study the numerical properties of this approach and show that the arising equations of motion are more stable than the standard formulation and thus less affected by the discretization error of the numerical approximation.

We assume in the sequel that the reader is familiar with the material presented in Ref. [35] in order to avoid a tedious repetition. We also continue to use the notations introduced there. The article is organized as follows: The next section presents the FaddeevJ̄ackiw approach in the case of a regular system. Section 3 discusses the techniques introduced by Barcelos-Neto and Wotzasek for second class constraints and the following section contains a geometric interpretation of it. After some examples in section 5 we study the implications of this approach for the numerical integration of the equation of motions. Section 7 points out some problems in the application to field theories. Finally, some conclusions are given.

2. First-Order Lagrangians

The symplectic formalism treats Lagrangians which are linear in the velocities:

$$L(q^i, \dot{q}^i) = a_i(q)\dot{q}^i - V(q)\,. \tag{1}$$

The corresponding Euler-Lagrange Equations are

$$\mathcal{R}_1 \,:\, \left\{ A_{ij}\dot{q}^j - \frac{\partial V}{\partial q^i} = 0\,, \qquad i = 1, \ldots, N \right. \tag{2}$$

where the matrix A is given by cross-derivatives of the a_i

$$A_{ij} = \frac{\partial a_j}{\partial q^i} - \frac{\partial a_i}{\partial q^j}\,. \tag{3}$$

Obviously, $\mathcal{R}_1$ is an involutive first-order equation provided this matrix is non-singular. Hence from the formal point of view there is no need to consider any constraints; the system is unconstrained.

If one follows the Dirac algorithm, one is forced to introduce N constraints, as all canonically conjugate momenta are independent of the velocities. Mathematically, this corresponds to insisting on treating (2) as a *second-order* differential equation. Since $\mathcal{R}_1$ is involutive, its prolongation is involutive, too, and no secondary constraints arise. Furthermore, all constraints are second class, for (2) represents a finite-type system [35].

The FaddeevJackiw approach is based on the observation that it is unnecessary to introduce the canonically conjugate momenta, because (2) possesses already the structure of a Hamiltonian system with Hamiltonian V provided we define the Poisson bracket by

$$\{q^i, q^j\} = (A^{-1})^{ij} . \tag{4}$$

Hence the name symplectic formalism. This definition makes sense as long as the matrix A is non-singular. Cronström and Noga [13] demonstrated recently, how one can explicitly construct the corresponding canonical coordinates.

We show later in the more general case of a system with second class constraints that exactly the same bracket structure arises, if one eliminates the second class constraints using Dirac brackets [14]. In the regular case this was already noted by Govaerts [21] and much earlier by Hojman and Urrutia [23].

In the case of a singular matrix A, we have "true" constraints. Faddeev and Jackiw [15] resort then to Darboux's theorem to eliminate them explicitly. If this elimination is too complicated, they recommend to apply the usual Dirac algorithm. At least for the construction of all constraints, there is no need for this. Since systems of ordinary differential equations always possess involutive symbols, the completion algorithm presented in Ref. [35] never raises the order of the system. Thus we can always obtain an involutive *first-order* system as equations of motion.

The only point is that it is no longer possible to use the matrix A to define a symplectic structure. But even if one wants to follow Dirac's approach, it is computationally much simpler to complete a first-order system and to prolong it to second order afterwards than the other way round. The true constraints are algebraic equations even in the Lagrangian formalism, and the other constraints are just prolongations of them.

For counting the degrees of freedom we can employ the same approach as in Ref. [35]. Independent of the existence of true constraints, our completion algorithm applied to (2) terminates with a system of the following form

$$\mathcal{R}_1^{(s)} : \begin{cases} \dot{q}^l = \psi(q^i, \dot{q}^k) , & l = 1, \dots, \bar{N},\ k > \bar{N},\ i = 1, \dots N \\ \phi_\alpha(q^i) = 0 , & \alpha = 1, \dots, \bar{M} \end{cases} \tag{5}$$

where $\dim \ker A = M \leq \bar{M} \leq \bar{N} \leq N$ and s denotes the number of iterations in the algorithm. This yields a Cartan character $\alpha_1^{(1)} = N - \bar{N}$.

$\dim \mathcal{R}_1^{(s)} = 2N - \bar{N} - \bar{M} = N + \alpha_1^{(1)} - \bar{M}$, as the dimension of the first-order jet bundle is $2N$. Arguing as in Ref. [35] we note that the general solution of our equations of motion has this number of arbitrary Taylor coefficients of zeroth and first order. But it depends on $\alpha_1^{(1)}$ arbitrary gauge functions, thus we must subtract this number to get the number of coefficients describing an initial state. Since for different choices of the gauge functions the evolution of the same initial state will differ, we must subtract again $\alpha_1^{(1)}$.

We conclude that a physical state is described by $\bar{N} - \bar{M}$ Taylor coefficients of zeroth and first order. This number is thus twice the number of degrees of freedom. Expressing the numbers $\bar{N}, \bar{M}$ by the intrinsically defined values $\dim \mathcal{R}_1^{(s)}$ and $\alpha_1^{(1)}$ we find the same expression for the number of degrees of freedom as we derived in Ref. [35] for the Hamiltonian equations of motion of a general system

$$F = \dim \mathcal{R}_1^{(s)} - 2\alpha_1^{(1)} . \tag{6}$$

It depends on the constraint structure whether one gains something by transforming a general Lagrangian into a first-order one by extending the configuration space. This amounts essentially to transforming higher-order Euler-Lagrange Equations into a first-order system. One obtains of course the same number of degrees of freedom, since this reduction does not change the Cartan characters [30, 32]. Computationally one might save a few steps compared to the Dirac algorithm, especially if second class constraints are present.

3. Second Class Constraints

For systems having only second class constraints one can use an idea of Barcelos-Neto and Wotzasek [4, 5] to compute the Dirac brackets in a direct manner. Thus we consider now the case that the matrix A has not maximal rank. Let a basis of its null space be given by the vectors v_α^i, i.e.

$$v_\alpha^i(q) A_{ij}(q) = 0 , \quad \alpha = 1, \ldots, M . \tag{7}$$

This implies the existence of M "primary" constraints†

$$\phi_\alpha = v_\alpha^i \frac{\partial V}{\partial q^i} = 0 . \tag{8}$$

Introducing M additional coordinates λ^α and continuing with the modified Lagrangian

$$\tilde{L}(q^i, \dot{q}^i, \lambda^\alpha) = \left(a_i + \lambda^\alpha \frac{\partial \phi_\alpha}{\partial q^i} \right) \dot{q}^i - V \tag{9}$$

we obtain new equations of motion

$$\tilde{\mathcal{R}}_1 : \begin{cases} A_{ij}\dot{q}^j + \dfrac{\partial \phi_\alpha}{\partial q^i}\dot{\lambda}^\alpha - \dfrac{\partial V}{\partial q^i} = 0 , \\ \dfrac{\partial \phi_\alpha}{\partial q^i}\dot{q}^i = 0 . \end{cases} \tag{10}$$

Equivalently, we could write $\tilde{L} = a_i \dot{q}^i - \dot{\lambda}^\alpha \phi_\alpha - V$, since this differs from (9) only by a total derivative. This approach will be used in the case of field theories (cf. section 7).

Let us assume that the second set of equations in (10) is independent of the original equations of motions (2), i.e. the prolongation of the constraints leads to new ones.

† It could of course happen, that M varies on the configuration space. But we assume that it is constant.

(10) can be written again in the form of (2) on the enlarged configuration space, if we introduce the $(N+M)\times(N+M)$ matrix $\tilde{A}$

$$\begin{aligned}
&\tilde{A}_{ij} = \frac{\partial a_i}{\partial q^j} - \frac{\partial a_j}{\partial q^i}\,, \\
&\tilde{A}_{i\alpha} = -\tilde{A}_{\alpha i} = \frac{\partial \phi_\alpha}{\partial q^i}\,, \qquad\qquad \begin{array}{l} i,j = 1,\dots,N\,, \\ \alpha,\beta = N+1,\dots,N+M\,, \end{array} \\
&\tilde{A}_{\alpha\beta} = 0\,.
\end{aligned} \tag{11}$$

If the matrix $\tilde{A}$ is regular, one can use it to define a symplectic structure. Otherwise one repeats the process. There are two possible outcomes: either one obtains after a finite number of iterations a regular matrix or the process stops, because the constraints do not generate new ones. We concentrate on the first case and assume for simplicity that already $\tilde{A}$ has maximal rank.

From the point of view of formal theory this assumption implies that the modified Euler-Lagrange Equations $\tilde{\mathcal{R}}_1$ are involutive. Indeed they are now even normal, as contraction of the first set of equations with the vectors v^i_α leads to the equations

$$v^i_\alpha \frac{\partial \phi_\beta}{\partial q^i}\dot{\lambda}^\beta - \phi_\alpha = 0\,. \tag{12}$$

The condition on the rank of $\tilde{A}$ implies that the matrix

$$B_{\alpha\beta} = v^i_\alpha \frac{\partial \phi_\beta}{\partial q^i} \tag{13}$$

has maximal rank. Thus we can obtain by a simple linear transformation the solved form usually found in the standard existence and uniqueness theorems for ordinary differential equations.

This implies further that we are dealing with a finite type system. We have already seen in Ref. [35] that this is characteristic for systems subject only to second class constraints. The appearance of first class constraints is always connected with gauge symmetries and thus with arbitrary functions in the general solution. However, such functions cannot occur in the solution of a normal system of ordinary differential equations.

To prove that the inverse of $\tilde{A}$ yields indeed the correct Dirac brackets we compute them in the standard way [14]. As already mentioned, there are N primary constraints

$$\psi_i = p_i - a_i(q) = 0\,. \tag{14}$$

The total Hamiltonian of the system is given by

$$H_T = V(q) + u^i\psi_i\,. \tag{15}$$

with some multipliers u^i. The primary constraints lead to the consistency conditions

$$\{\psi_i, H_T\} = A_{ij}u^j - \frac{\partial V}{\partial q^i} = 0\,. \tag{16}$$

They are identical with the EulerLagrange Equations (2), if we identify the multipliers u^j with the velocities $\dot{q}^j$.

If the matrix A is non-singular, these secondary constraints can be used to determine all multipliers u^i and the Dirac algorithm stops here. In the case of a singular matrix we can solve only for some of them, as contraction with v^i_α yields the "true" constraints ϕ_α. Their consistency conditions

$$\{\phi_\alpha, H_T\} = u^i \frac{\partial \phi_\alpha}{\partial q^i} \tag{17}$$

allow us to determine the remaining multipliers under the above assumptions. Thus tertiary constraints do not appear.

To determine the Dirac bracket we must compute the structure constants of the Poisson algebra generated by the constraints:

$$\begin{aligned} \{\psi_i, \psi_j\} &= A_{ij}\,, \\ \{\psi_i, \phi_\alpha\} &= -\frac{\partial \phi_\alpha}{\partial q^i}\,, \\ \{\phi_\alpha, \phi_\beta\} &= 0\,. \end{aligned} \tag{18}$$

The right hand sides are the entries of the matrix $\tilde{A}$ defined above by the modified Lagrangian $\tilde{L}$. In order to see that this yields essentially the same symplectic structure as the first-order approach we compute the Dirac brackets of the configuration space coordinates q^i. Since the "true" constraints ϕ_α depend only on the q^i, we find

$$\begin{aligned} \{q^i, q^j\}^* &= -\{q^i, \psi_k\}\,(\tilde{A}^{-1})^{kl}\,\{\psi_l, q^j\} \\ &= \delta^i_k\,(\tilde{A}^{-1})^{kl}\delta^j_l = (\tilde{A}^{-1})^{ij} \end{aligned} \tag{19}$$

in perfect agreement with (4). The generalization to the case that further extensions of the configuration space are necessary (i.e. tertiary and higher constraints appear in the Dirac algorithm) is straightforward.

4. Geometric Interpretation

Barcelos-Neto and Wotzasek omit in their articles [4, 5] a discussion of the precise relation between the equations of motion (2) derived from the original Lagrangian L and those (10) obtained from the modified one $\tilde{L}$. This is, however, quite important for understanding the meaning of the multipliers λ^α.

For this purpose we introduce vectors w^i_ρ, $\rho = M+1, \dots, N$ such that $\{v^i_\alpha, w^i_\rho\}$ form a linearly independent set. Under the above assumptions we find the following local representation of the equation $\mathcal{R}^{(1)}_1$ obtained from completing (2) consisting only of independent equations

$$\mathcal{R}^{(1)}_1 : \begin{cases} w^i_\rho\left(A_{ij}\dot{q}^j - \dfrac{\partial V}{\partial q^i}\right) = 0\,, & \rho = M+1, \dots, N\,, \\ \dfrac{\partial \phi_\alpha}{\partial q^i}\dot{q}^i = 0\,, & \alpha = 1, \dots, M\,, \\ \phi_\alpha = 0\,, & \alpha = 1, \dots, M\,. \end{cases} \tag{20}$$

Similarly we obtain a local description of $\tilde{\mathcal{R}}_1$ containing under our assumptions only independent equations, too,

$$\tilde{\mathcal{R}}_1 : \begin{cases} w^i_\rho \left(A_{ij}\ddot{q}^j + \dfrac{\partial \phi_\alpha}{\partial q^i}\dot{\lambda}^\alpha - \dfrac{\partial V}{\partial q^i} \right) = 0\,, & \rho = M+1,\dots,N\,, \\ \dfrac{\partial \phi_\alpha}{\partial q^i}\dot{q}^i = 0\,, & \alpha = 1,\dots,M\,, \\ B_{\alpha\beta}\dot{\lambda}^\beta + \phi_\alpha = 0\,, & \alpha = 1,\dots,M\,. \end{cases} \tag{21}$$

Although both represent finite type systems, note the crucial difference that $\tilde{\mathcal{R}}_1$ is normal and does not contain any algebraic equations. This entails especially a relaxation of the found constraints: we do no longer require that $\phi_\alpha = 0$ but only $\phi_\alpha = const$! Furthermore, while the solution space of $\mathcal{R}_1^{(1)}$ is $(N-M)$-dimensional, $\dim \tilde{\mathcal{R}}_1 = N + M$. But this discrepancy is removed as soon as we require that $\lambda^\alpha(t) \equiv const$, because then both systems are identical and possess of course the same solutions.

This is best seen by considering the initial value problem for $\tilde{\mathcal{R}}_1$. If the initial data $(q^i_0, \lambda^\alpha_0)$ are chosen such that $\phi_\alpha(q^i_0) = 0$, then because of the regularity of $B_{\alpha\beta}$ the corresponding solution of $\tilde{\mathcal{R}}_1$ will always stay on the submanifold described by $\lambda^\alpha = \lambda^\alpha_0$ and thus project on a solution of $\mathcal{R}_1^{(1)}$. The choice of the λ^α_0 is unimportant, as $\tilde{\mathcal{R}}_1$ is invariant under translations in λ^α.

The differential parts of both systems are almost identical. The only difference lies in the additional term in the first set of equations in $\tilde{\mathcal{R}}_1$. Solving the third set of equations for $\dot{\lambda}^\alpha$, we can write this term in the form $-(B^{-1})^{\alpha\beta}\phi_\beta \frac{\partial \phi_\alpha}{\partial q^i}$. Thus it vanishes on the constraint manifold and it can be interpreted as the components of a vector field normal to the constraint manifold. Its effect will be discussed in more detail in section 6.

Geometrically, the approach of Barcelos-Neto and Wotzasek can be understood as embedding of the original system into a larger one such that the second class constraints become first class ones. Recall that the idea behind the definition of the Dirac brackets is the introduction of a *degenerate* Poisson structure such that the second class constraints become distinguished functions (sometimes also called Casimir functions), i.e. the Dirac bracket of any functions with a second class constraint vanishes strongly.

If we compute the Poisson bracket derived from $\tilde{A}$ of any function $F(q^i, \lambda^\beta)$ defined on the extended configuration space with the constraints $\phi_\alpha(q^i)$ we obtain using (11)

$$\{F, \phi_\alpha\} = \frac{\partial F}{\partial q^i}\frac{\partial \phi_\alpha}{\partial q^j}(\tilde{A}^{-1})^{ij} + \frac{\partial F}{\partial \lambda^\beta}\frac{\partial \phi_\alpha}{\partial q^j}(\tilde{A}^{-1})^{\beta j} = \frac{\partial F}{\partial \lambda^\alpha}\,. \tag{22}$$

Thus as expected the Poisson bracket of any function independent of the multipliers λ^α with a constraint vanishes. This implies especially that the Poisson bracket of two constraints vanishes; they are now first class!

The above mentioned invariance under translations in λ^α represents therefore the invariance under the gauge transformations generated by the constraints. Reduction with respect to this gauge symmetry recovers the original configuration space.

The interpretation becomes more complicated, if $\tilde{\mathcal{R}}_1$ is not yet involutive, i.e. further multipliers must be introduced. Then we can no longer conclude that all multipliers remain constant for initial values satisfying the constraints. One must distinguish the prolongations of which constraints are taken as independent equations.

For these the algorithm has terminated and the corresponding multipliers remain constant. The others lead to further constraints ("the next generation") and their multipliers satisfy more complicated equations of motion.

However, the transition of the constraints from second class to first class also happens in this more general situation. The argument is exactly as above in (22). The Poisson bracket of any observable $F(q^k)$ independent of the multipliers with any of the constraints vanishes, since

$$\{F(q^k), \phi_\alpha(q^k)\} = \frac{\partial F}{\partial q^i}\frac{\partial \phi_\alpha}{\partial q^j}(\tilde{A}^{-1})^{ij} \tag{23}$$

and one can easily see that even if ϕ_α is a "higher generation" constraint, one always obtains $\partial\phi_\alpha/\partial q^i = \tilde{A}_{i\alpha}$ and thus the expression on the right hand side is zero. But the corresponding gauge transformations become more complicated.

We demonstrate this behaviour on an important class of constrained systems. They are described by Lagrangians of the form

$$L_2(\dot{q}^i, q^i, \mu^\alpha) = \frac{1}{2}M_{ij}(q^k)\dot{q}^i\dot{q}^j - V(q^k) + \mu^\alpha\phi_\alpha(q^k) \tag{24}$$

where $M_{ij}(q^k)$ is a symmetric, positive definite mass matrix. The holonomic constraints $\phi_\alpha(q^k)$ are introduced via the multipliers μ^α. Such systems occur e.g. in multi-body dynamics, the modelling of robots etc. Introducing additional coordinates v^i we can rewrite L_2 as an equivalent first-order Lagrangian

$$L_1(\dot{q}^i, q^i, v^i, \mu^\alpha) = M_{ij}v^i\dot{q}^j - \frac{1}{2}M_{ij}v^iv^j - V + \mu^\alpha\phi_\alpha\,. \tag{25}$$

It is easy to see that the first step of the algorithm of section 3 leads simply to replacing the multipliers μ^α with the derivatives of some new multipliers. For simplicity, we continue to denote them with μ^α. Then we need a second step which introduces the constraints on the velocities into the Lagrangian. After that the algorithm stops with the Lagrangian

$$\tilde{L}_1(\dot{q}^i, q^i, v^i, \dot{\mu}^\alpha, \dot{\lambda}^\alpha) = M_{ij}v^i\dot{q}^j - \frac{1}{2}M_{ij}v^iv^j - V + \dot{\mu}^\alpha\phi_\alpha + \dot{\lambda}^\alpha\frac{\partial\phi_\alpha}{\partial q^i}v^i\,. \tag{26}$$

The corresponding equations of motion are

$$\begin{aligned}
M_{ij}\dot{v}^j + \frac{\partial M_{ij}}{\partial q^k}v^j\dot{q}^k + \frac{1}{2}\frac{\partial M_{kj}}{\partial q^i}v^kv^j + \frac{\partial V}{\partial q^i} - \dot{\mu}^\alpha\frac{\partial\phi_\alpha}{\partial q^i} - \dot{\lambda}^\alpha\frac{\partial^2\phi_\alpha}{\partial q^i\partial q^j}v^j &= 0\,,\\
M_{ij}\left(\dot{q}^j - v^j\right) + \dot{\lambda}^\alpha\frac{\partial\phi_\alpha}{\partial q^i} &= 0\,,\\
\frac{\partial\phi_\alpha}{\partial q^i}\dot{q}^i &= 0\,,\\
\frac{\partial^2\phi_\alpha}{\partial q^i\partial q^j}v^i\dot{q}^j + \frac{\partial\phi_\alpha}{\partial q^i}\dot{v}^i &= 0\,.
\end{aligned} \tag{27}$$

By taking suitable linear combinations we can derive the following differential equations for the multipliers λ^α

$$(M^{-1})^{ij}\frac{\partial\phi_\alpha}{\partial q^i}\frac{\partial\phi_\beta}{\partial q^j}\dot{\lambda}^\beta = \frac{\partial\phi_\alpha}{\partial q^i}v^i\,. \tag{28}$$

The right hand side contains the velocity constraints. Thus as before λ^α remains constant as long as the constraints are satisfied. In contrast, μ^α will generally not remain constant, but satisfies a rather complicated differential equation.

5. Examples

We demonstrate these ideas on a simple system [3, 24] with a three-dimensional configuration space whose dynamics is determined by the Lagrangian†

$$L = (q_2 + q_3)\dot{q}_1 + k\dot{q}_3 + \frac{1}{2}(k^2 - 2q_2q_3 - q_3^2) \tag{29}$$

where k is a constant. In the formal analysis we start with the Euler-Lagrange Equations. After a trivial algebraic manipulation they can be written as

$$\mathcal{R}_1 \,:\, \begin{cases} \dot{q}_2 + \dot{q}_3 = 0\,, \\ \dot{q}_1 - q_3 = 0\,, \\ q_2 = 0\,. \end{cases} \tag{30}$$

Obviously this equation becomes involutive after one projection adding the integrability condition $\dot{q}_2 = 0$. It is also trivial to integrate it in closed form:

$$q_1(t) = at + b\,, \quad q_2(t) = 0\,, \quad q_3(t) = a \tag{31}$$

with two integration constants a, b.

For the Dirac analysis we need the canonically conjugate momenta

$$p_1 = q_2 + q_3\,, \quad p_2 = 0\,, \quad p_3 = k\,. \tag{32}$$

These are at the same time the primary constraints. The total Hamiltonian is

$$H_T = \frac{1}{2}(q_3^2 + 2q_2q_3 - k^2) + u_1(p_1 - q_2 - q_3) + u_2p_2 + u_3(p_3 - k)\,. \tag{33}$$

This leads to the secondary constraints $u_2 + u_3 = 0$, $q_3 = u_1$ and $q_2 = 0$. Their consistency conditions determine the multipliers $u_2 = u_3 = 0$. Hence we have four second class constraints $p_2 = q_2 = 0$ and $p_3 = k, q_3 = p_1$. By direct inspection one sees that there is only one dynamical degree of freedom, namely (q_1, p_1), having as Dirac bracket its standard Poisson bracket.

In the symplectic formalism one finds in the first step the "true" constraint $q_2 = 0$ and continues with the modified Lagrangian $\tilde{L} = L + \lambda\dot{q}_2$. From it we derive the matrix $\tilde{A}$

$$\tilde{A} = \begin{pmatrix} 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{34}$$

where the columns and rows are labeled by q_1, q_2, q_3, λ. This matrix is obviously invertible and yields the correct bracket, if we identify q_3 with the momentum p_1.

If we compute, however, the equations of motion, we obtain after some trivial manipulations

$$\tilde{\mathcal{R}}_1 \,:\, \begin{cases} \dot{q}_3 = 0\,, \\ \dot{q}_2 = 0\,, \\ \dot{q}_1 - q_2 - q_3 = 0\,, \\ \dot{\lambda} - q_2 = 0\,. \end{cases} \tag{35}$$

† Note that the calculations in Ref. [24] are *not* correct!

As expected the equation $q_2 = 0$ is missing and the solution space is consequently larger

$$q_1(t) = (\bar{a} + \bar{c})t + \bar{b}\,, \quad q_2(t) = \bar{c}\,, \quad q_3(t) = \bar{a}\,, \quad \lambda(t) = \bar{c}t + \bar{d} \tag{36}$$

with four integration constants $\bar{a}, \bar{b}, \bar{c}, \bar{d}$. But as soon as we require that $\lambda(t) \equiv const$ we recover the correct solution, as this implies $\bar{c} = 0$ and $\bar{d}$ appears only in $\lambda(t)$.

This example also serves well to demonstrate the difference between first- and second-order formalism. Actually it stems from a slightly more complicated system where k is not treated as constant but as an additional coordinate [22]. But the real starting point is the following system of second-order equations

$$\ddot{x} = -\dot{y}\,, \quad \ddot{y} = -y\,. \tag{37}$$

One can prove that these equations neither are nor can be transformed into the Euler-Lagrange Equations of some Lagrangian [23]. But if we rewrite the system as a first-order one

$$\dot{x} = z\,, \quad \dot{y} = w\,, \quad \dot{z} = -w\,, \quad \dot{w} = -y\,, \tag{38}$$

a Lagrangian exists, namely

$$L = (y + z)\dot{x} + w\dot{z} + \frac{1}{2}(w^2 - 2yz - z^2)\,. \tag{39}$$

(Actually every first-order system of ordinary differential equations which is solved for the derivatives can be derived from such a linear Lagrangian, as the corresponding Helmholtz conditions are always (locally) solvable [23]).

A normal form can be obtained by setting

$$q^1 = x\,, \quad q^2 = z\,, \quad p_1 = y + z\,, \quad p_2 = w\,. \tag{40}$$

Note, however, that we are now using as configuration space coordinates x and $\dot{x}$, if we compare with the original second-order system. In first-order systems the distinction between configuration and phase space begins to blur. This is the basis of the symplectic formalism.

As a second example we consider the planar pendulum in Cartesian coordinates. For simplicity, we set all constants like length, mass, gravitational acceleration, etc. to 1. Its Lagrangian is

$$L_2(\dot{x}, \dot{y}, x, y, \mu) = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - y + \frac{\mu}{2}(x^2 + y^2 - 1)\,. \tag{41}$$

We can transform it to a first-order one as in section 4. We are thus lead to compare the following two formulations of the equations of motion: The standard approach yields after completion to involution the system

$$\mathcal{R}_1 : \begin{cases} \dot{p}_x = \mu x\,, & \dot{p}_y = \mu y\,, \\ \dot{x} = p_x\,, & \dot{y} = p_y\,, \\ x^2 + y^2 = 1\,, & x p_x + y p_y = 0\,, \\ \mu = -\dfrac{p_x^2 + p_y^2 - y}{x^2 + y^2}\,. & \end{cases} \tag{42}$$

(27) applied to the Lagrangian (41) leads to the following formulation of the equation of motion

$$\tilde{\mathcal{R}}_1 : \begin{cases} \dot{p}_x - x\dot{\mu} - p_x\dot{\lambda} = 0\,, & \dot{p}_y - y\dot{\mu} - p_y\dot{\lambda} + g = 0\,, \\ \dot{x} - p_x + x\dot{\lambda} = 0\,, & \dot{y} - p_y + y\dot{\lambda} = 0\,, \\ x\dot{x} + y\dot{y} = 0\,, & x\dot{p}_x + y\dot{p}_y + p_x\dot{x} + p_y\dot{y} = 0\,. \end{cases} \tag{43}$$

The multipliers μ, λ satisfy the differential equations

$$\begin{aligned} \dot{\mu} &= \frac{y - p_x^2 - p_y^2}{x^2 + y^2}\,, \\ \dot{\lambda} &= \frac{xp_x + yp_y}{x^2 + y^2}\,. \end{aligned} \tag{44}$$

As predicted the right hand side of the equation for λ vanishes as long as the velocity constraint is not violated. The expression for $\dot{\mu}$ is the same as one obtains in the Dirac analysis of L_2 for the multiplier μ (cf. (42)). Thus we have indeed just replaced this original μ by the derivative of a new multiplier, also denoted by μ.

Inverting the matrix $\tilde{A}$ derived from the Lagrangian (41) yields the following structure matrix for the symplectic structure (the columns and rows are labeled $p_x, p_y, x, y, \mu, \lambda$)

$$\tilde{A}^{-1} = \frac{1}{x^2 + y^2} \begin{pmatrix} 0 & xp_y - yp_x & y^2 & -xy & -p_x & x \\ yp_x - xp_y & 0 & -xy & x^2 & -p_y & y \\ -y^2 & xy & 0 & 0 & x & 0 \\ xy & -x^2 & 0 & 0 & y & 0 \\ p_x & p_y & -x & -y & 0 & 1 \\ -x & -y & 0 & 0 & -1 & 0 \end{pmatrix}. \tag{45}$$

One can easily check that the upper left 4×4 sub-matrix contains indeed the Dirac brackets of x, y, p_x, p_y as computed with the standard Dirac approach [16].

6. Some Numerical Considerations

In the language of numerical analysis, the equations of motion of a constrained model form a differential-algebraic system [10]. Such systems are much harder to solve numerically than normal systems. The "distance" of a differential-algebraic system to a normal system is measured by the so-called (differentiation) *index*. In the language of the formal theory, this index can be interpreted as the number of prolongations which are needed to render the system involutive [25, 29].

The difficulty arises from the fact that although all analytical solutions lie on the constraint manifold, the discretization error of any numerical method will lead to approximations not on it. If one applies standard methods for ordinary differential equations, one observes usually a significant drift away from the constraint manifold and obtains thus rapidly physically worthless solutions.

The construction presented in section 3 is an example of an index reduction or constraint stabilization technique. Many different approaches for this reduction can be found in the literature (see e.g. [8, 19, 20, 26]), as most numerical methods cannot be applied reasonably to problems with an index higher than one or two. Most of them differentiate the constraints and add the result at a suitable place with some multipliers.

Usually this addition is done in an *ad hoc* manner at the level of the differential equations. In contrast, the technique of section 3 performs the modification at the level of the Lagrangian. Thus one can speak of a *symplectic index reduction*, as one obtains a normal system with a symplectic structure.

This entails that symplectic integrators [11, 31] can be applied for the numerical solution. But usually these are constructed only for Darboux coordinates, i.e. they assume that the standard Poisson bracket is used. Feng and Wang [17] showed how symplectic integrators can also be derived in more general coordinates. However, their construction requires essentially the transformation to Darboux coordinates, although in an extended space.

Since the symplectic structure depends on the concrete Lagrangian under consideration, it is necessary to derive a special integrator for each system. Thus it seems doubtful whether one can numerically exploit the symplectic structure of the first-order equations of motion with the presently known techniques.

Nevertheless, the approach of Barcelos-Neto and Wotzasek is of interest for the numerical integration of constrained systems. In section 4 we mentioned already that at the level of the differential equations this approach leads to the addition of a term which represents a vector field normal to the constraint surface. We study now the effect of this term on the numerical integration.

As long as the numerical solution remains on the constraint manifold this term vanishes. But if the discretization error leads to a deviation from this manifold, there are two possibilities: this term can either lead to an amplification of the error, if it points away from the manifold, or it tries to counter the error, if it points towards the manifold.

Essentially the vector field represents a linear combination of the normal vector fields $\partial\phi_\alpha/\partial q^i$. The coefficients are of the form $-(B^{-1})^{\alpha\beta}\phi_\beta$. (8,13) imply that the matrix $B_{\alpha\beta}$ can be written

$$B_{\alpha\beta} = v^i_\alpha v^j_\beta \frac{\partial^2 V}{\partial q^i \partial q^j} + v^i_\beta \frac{\partial v^i_\alpha}{\partial q^i}\frac{\partial V}{\partial q^j}\,. \tag{46}$$

In general, it is difficult to make statements about this matrix; especially not much is known about the eigenvectors v^i_α. But the situation is much simpler in the neighborhood of a minimum of the potential V. There we can neglect the second term in (46) and in the first term the Hessian of V is positive definite. In a suitably chosen coordinate system, the eigenvectors can be taken as the unit vectors $e^i_\alpha = \delta^i_\alpha$ (define some of the new coordinate as $\bar{q}^\alpha = \phi_\alpha(q)$). In these coordinates, $B_{\alpha\beta}$ is also positive definite.

A symmetric, positive definite matrix is diagonalizable with positive real eigenvalues. Thus with a further change of coordinates we can transform it into diagonal form with only positive entries. In this form the inverse can be readily computed. Since its entries are also positive, we deduce that our vector field points under the made assumptions *towards* the constraint manifold.

Although this derivation holds only in the neighborhood of minima of the potential, we conjecture that the formulation of the equation of motions obtained in section 3 is numerically more stable than the standard formulation based on a simple completion to an involutive system. As soon as a drift off the constraint manifold occurs, an additional "force" drives the system back on this manifold.

We demonstrate this effect on a standard example in the theory of differential-algebraic equations by considering again the planar pendulum in Cartesian coordinates. To show the stabilizing effect we choose initial data consistent with the constraints and integrate both sets of equations of motions (42) and (43), respectively, numerically. Since we are only interested in the drift off the constraint manifold, we take only the differential part of (42) into account, i.e. we do not apply any special method for differential-algebraic systems.

As discussed in section 4 our approach stabilizes mainly the velocity constraint. But it is a well-known empirical fact in multi-body dynamics that this suffices to eliminate the essential source of instability. A theoretical explanation of this observation was given by Alishenas [1, 2] using a perturbation analysis.

Both systems were numerically integrated over approximately three periods using the standard fourth-order Runge-Kutta method with constant step size. Figures 1-4 contain logarithmic representations of the integration error, the violation of energy conservation and of the residuals of the position and velocity constraints, respectively.† The calculation were done for the initial values $x = 0, y = -1, p_x = 2, p_y = 0$ using a step size of $h = 0.1$.

One can see that after about two periods the integration breaks down, as the integration error (estimated by comparing with the results for half the step size) is of the same magnitude as the computed values.‡ With a step size of $h = 0.01$ it is possible to integrate both formulation over three periods. With that value system (43) could even be integrated over four periods.

It is interesting to note that although the difference in the integration error is not that big (about half a power of ten), the physically relevant errors are one to two orders of magnitude smaller. The outcome is especially striking for the position constraint residual (figure 3). Whereas in the standard formulation it grows approximately proportional to $t^{1.4}$, it remains almost constant in the stabilized formulation until the breakdown of the integration.

The figures show only the logarithms of the errors. It is quite instructive to study the values with their signs. In the standard formulation the constraint residuals have always the same sign after perhaps some initial oscillations. Usually one finds a drift to smaller and smaller values for the distance from the origin. In contrast, in the stabilized formulation the trajectories oscillate around the constraint manifold under the influence of this additional "force", it has become a kind of attractor.

Table 1 shows how the errors for both approaches depend on the step size. The values are for $t = 10$. Δ_I denotes the integration error; Δ_E is the deviation from the correct energy; Δ_p, Δ_v denote the position and velocity constraint residuals, respectively. Obviously, the stabilizing effect occurs at any step size. Note the significant improvement for $h = 0.01$: the errors improved by up to five orders of magnitude compared with $h = 0.1$!

† The solid line (labeled "inv") shows the values for the standard formulation, i.e. system (42); the dashed line (labeled "fj") shows the outcome for system (43).

‡ The growth of the integration error depends strongly on the initial values. Alishenas [1] uses $x = 1, y = 0, p_x = p_y = 0$ and reports a cubic growth. But figure 1 shows for our initial values an exponential growth!

Table 1. Errors at $t = 10$ for different step sizes

	Involution			Faddeev-Jackiw		
h	0.1	0.05	0.01	0.1	0.05	0.01
Δ_I	0.21	1.7×10^{-2}	3.2×10^{-5}	5.5×10^{-2}	1.4×10^{-3}	4.1×10^{-7}
Δ_E	2.5×10^{-4}	1.8×10^{-5}	2.9×10^{-8}	2.4×10^{-5}	6.2×10^{-7}	1.3×10^{-7}
Δ_p	7.3×10^{-4}	4.9×10^{-5}	8.2×10^{-8}	6.7×10^{-6}	2.1×10^{-7}	6.8×10^{-11}
Δ_v	3.9×10^{-5}	2.6×10^{-6}	4.4×10^{-9}	4.6×10^{-6}	4.3×10^{-7}	8.5×10^{-10}

7. Field Theory

Barcelos-Neto and Wotzasek [4] apply their method also to field theories. Then the equations of motion are partial differential equations. We have shown in Ref. [35] that even the classical Dirac approach may get problems, if the field equations are over-determined. The reason for this effect is that some constraints may arise as purely spatial integrability conditions, whereas Dirac considers only the temporal evolution of the constraints. The approach presented in section 3 suffers from exactly the same problem.

As a simple example consider the following slight modification of the class of linear Lagrangian densities considered in Ref. [35]

$$\mathcal{L}[\phi, \nu, \mu, \lambda] = \nu\partial_t\phi + \mu[\partial_x\phi - f(\phi)] + \lambda[\partial_y\phi - g(\phi)]\,. \tag{47}$$

Obviously, ν, μ, λ are just multipliers. The functions f, g are arbitrary but fixed. The corresponding Euler-Lagrange Equations are

$$\mathcal{R}_1 \,:\, \begin{cases} \partial_t\nu + \partial_x\mu + \partial_y\lambda + \mu f'(\phi) + \lambda g'(\phi) = 0\,, \\ \partial_t\phi = 0\,, \\ \partial_x\phi - f(\phi) = 0\,, \\ \partial_y\phi - g(\phi) = 0\,. \end{cases} \tag{48}$$

It is straightforward to show that this system is involutive, if and only if the functions f, g satisfy the integrability condition

$$f'g - fg' = 0\,, \tag{49}$$

i.e. if $f(\phi) = cg(\phi)$ for some constant c.

For the symplectic formalism we must first construct the matrix A. If we order the fields ϕ, ν, μ, λ, it is given by

$$A = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\,. \tag{50}$$

Thus there exist two eigenvectors and we obtain the two obvious constraints

$$\Omega_1 = \partial_x\phi - f(\phi)\,, \quad \Omega_2 = \partial_y\phi - g(\phi)\,. \tag{51}$$

Following the same steps as in the finite-dimensional case, we are lead to consider the modified Lagrangian density

$$\tilde{\mathcal{L}} = \nu\partial_t\phi + (\mu + \partial_t\alpha)[\partial_x\phi - f(\phi)] + (\lambda + \partial_t\beta)[\partial_y\phi - g(\phi)] \tag{52}$$

where α, β are the new multipliers. But we gain nothing by this transformation, as the new constraints represent the temporal prolongation of the original ones and vanish due to the field equation $\phi_t = 0$.

Thus the algorithm of Barcelos-Neto and Wotzasek terminates here without finding condition (49). Their conclusion would be that since no new constraints have occurred but the matrix $\tilde{A}$ is still singular, the system is subject to first class constraints. This is of course indeed correct, as we have the obvious "gauge invariance" under translations of the multipliers.

But this result is completely irrelevant, if f, g do not satisfy (49), because then the field equations are inconsistent. In a more general situation even their conclusion of the existence of first class constraints might be wrong, as the overlooked constraint could lead to further ones such that the final system contains only second class constraints.

We must therefore conclude that this method does not fulfill the first task of any approach to constrained theories, namely checking the consistency of the field equations. The reason for the failure of the algorithm of Barcelos-Neto and Wotzasek lies in the fact that they use in the construction of the modified Lagrangian only one multiplier. By using D multipliers λ^μ, if D denotes the dimension of space-time, and adding a term of the form $\partial_\mu \lambda^\mu \Omega$ for each constraint Ω, one can enforce the generation of *all* integrability conditions.

In our example, one indeed produces the consistency condition (49) this way. The price is, however, the introduction of six multipliers. They remain all arbitrary in the field equations and correspond therefore to gauge symmetries. In order to construct Dirac brackets these must be explicitly fixed.

8. Conclusion

As in our previous article [35] we have shown that the symplectic formalism can be well understood by taking the point of view of the formal theory of differential equations. At the level of point mechanics the identification of the various approaches to constrained systems with the completion of the equations of motion to an involutive system may be of more theoretical interest than practical importance. But we have shown that in the case of field theories it is sometimes difficult to circumvent the involution analysis.

We have seen that from the point of view of differential equations the idea behind the approach of Barcelos-Neto and Wotzasek [4, 5] is rendering the equations of motion normal by extending the configuration space. This construction is only possible for second class constraints, as a normal system of ordinary differential equations is of finite type, whereas in systems with gauge symmetries the general solution always contains arbitrary functions [33, 34].

From a more physical point of view their approach can be understood as a transformation of the second class constraints into first class ones in the extended configuration space. In the simplest case the corresponding gauge transformations are just translations in the additional coordinates and the extended configuration space foliates in identical copies of the original one.

Such a "conversional approach" to second class constraints is not new. Batalin and collaborators [7, (and references therein)] have developed an approach with the same goal. There is, however, a number of significant differences between the here presented technique and that of Batalin *et al* .

They also introduce additional coordinates, so-called ghosts, but with a different

Grassmann parity. Thus their phase space is always a supermanifold. They construct new constraints in form of a power series in the ghost variables, whereas we leave the constraints unchanged and modify instead the symplectic structure. They can also handle the case that first class constraints are present [6], which is currently not possible in the Faddeev-Jackiw framework without an explicit gauge fixing.

Montani and Wotzasek [27, 28] have shown how one can construct the generators of gauge symmetries from the null vectors of the symplectic matrix A in the case of systems with first class constraints. Nevertheless, the only way to obtain the Dirac brackets seems to be to completely fix the gauge and thus to render all constraints second class. This is a considerable disadvantage of this approach for systems with both types of constraints.

The symplectic formalism is sometimes computationally more effective than the standard Dirac approach, even if one has to rewrite a higher-order Lagrangian as a first-order one. For this reason it is currently fairly popular. However, we believe that it has certain disadvantages in the case of field theories. Proving the consistency of the field equations can become rather cumbersome and may lead to a proliferation of multipliers. Furthermore, the formalism is not covariant, as it is based on the selection of velocities and requires the fixing of all gauge symmetries.

We have shown that the method of Barcelos-Neto and Wotzasek has interesting numerical properties and can be seen in the context of what numerical analysts call constraint stabilization. In this language we can formulate the general idea as follows. Physically, all dynamics happens on the constraint surface. The ambient space is an artifact of the modelling and the dynamics is not uniquely defined there. Thus we can change the system in the ambient space as we like as long as we take care that on the constraint surface the same dynamics arise.

The problem is to find a change such that the arising equations of motion are more stable against the drift off the constraint manifold. Our modification of the Lagrangian makes this manifold to a kind of attractor for nearby trajectories. Since it was guided by the idea to maintain a symplectic structure, it can unfortunately not be generalized to arbitrary differential-algebraic systems.

A somewhat related approach was presented by Simeon [36]. He includes not only the velocity constraints but also the constraints at acceleration level into the Lagrangian (which is then second-order!). After a further transformation of the equation of motions he obtains a system of differential equations containing an explicit projection on the (velocity) constraint manifold.

The philosophy behind such approaches is rather to modify the differential equations then using special techniques for differential-algebraic systems. A typical method there is e.g. to perform after each step of the numerical integration a *numerical* projection on the constraint manifold. We accomplish more or less the same effect via an equivalent reformulation of the equations of motion.

Acknowledgments

The author is grateful to R.W. Tucker for many fruitful discussions. He thanks the School of Physics and Materials, Lancaster University, for a postgraduate grant. This work was partially supported by Deutsche Forschungsgemeinschaft.

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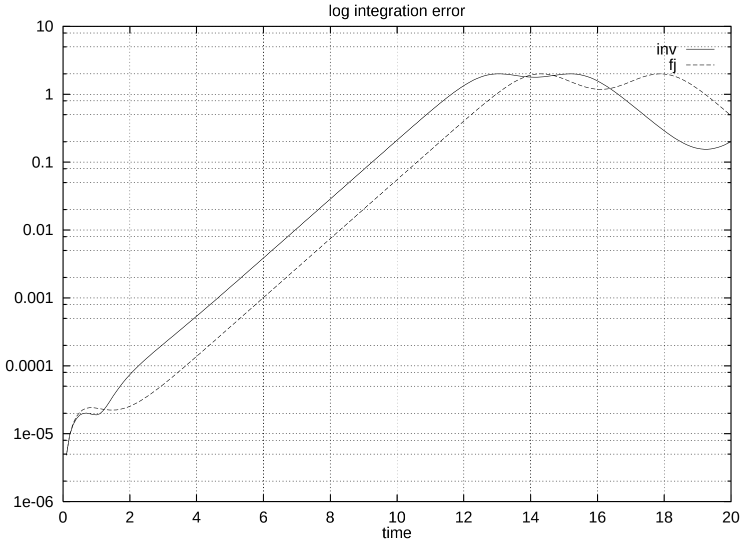

Figure 1. Estimation of integration error

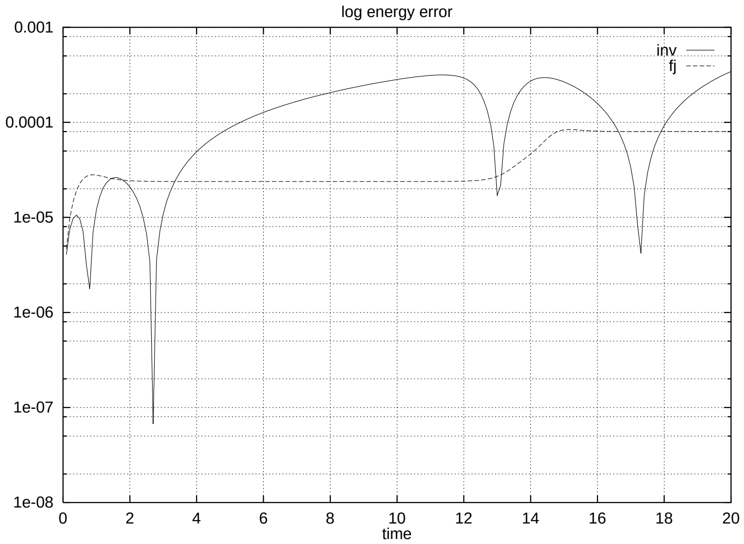

Figure 2. Energy conservation

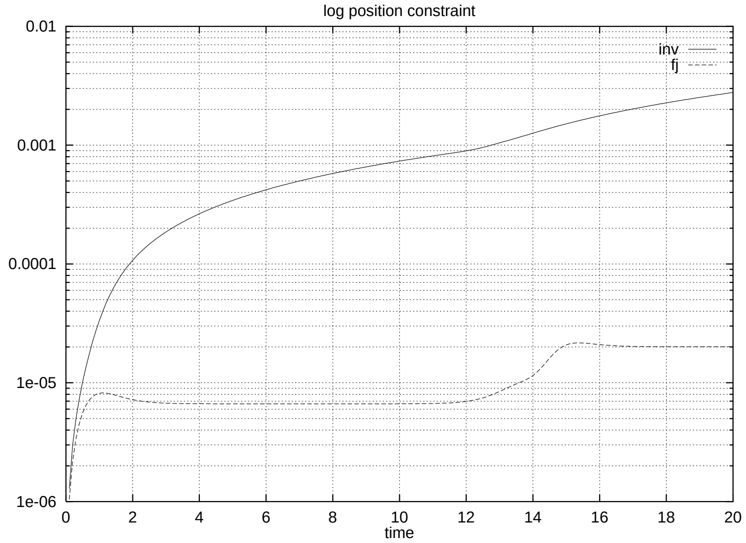

Figure 3. Position constraint residual

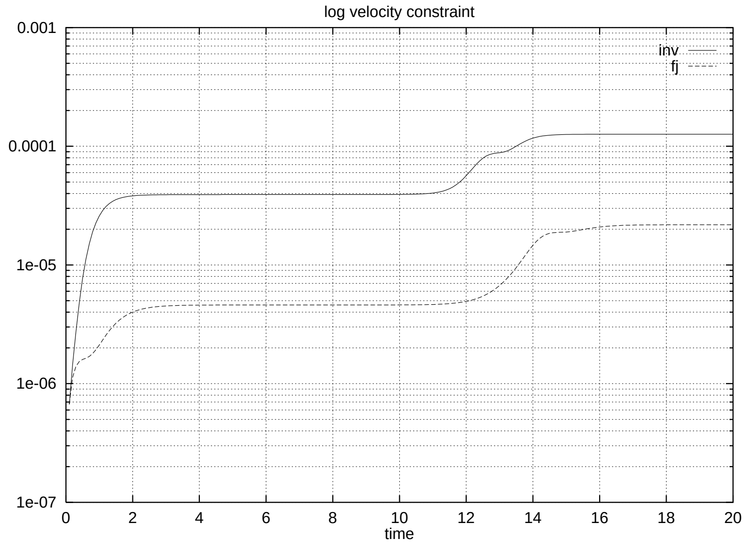

Figure 4. Velocity constraint residual