NUMERICAL ANALYSIS OF CONSTRAINED HAMILTONIAN SYSTEMS AND THE FORMAL THEORY OF DIFFERENTIAL EQUATIONS

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Abstract. We show how the formal theory of differential equations provides a unifying framework for some aspects of constrained Hamiltonian systems and of the numerical analysis of differential algebraic equations, respectively. This concerns especially the Dirac algorithm for the construction of all constraints and various index concepts for differential algebraic equations.

1. Introduction

Constrained Hamiltonian systems arise in many fields, e. g. in multi-body dynamics or molecular dynamics. As it is rarely possible to solve them analytically, their numerical integration is of great importance. Due to the existence of the constraints, the equations of motion form a differential algebraic equation, i. e. a system comprising differential and algebraic equations.

The straightforward application of standard numerical methods to differential algebraic equations is usually not possible. One reason is the existence of hidden constraints or integrability conditions. These are further algebraic equations satisfied by any solution of the original system but not part of it. They make especially a consistent initialization rather difficult.

Physicists have developed various methods to deal with constrained Hamiltonian systems, although they are usually more interested in their quantization than in numerical computations. The Dirac theory [13, 14] provided not only the first solution but represents still one of the most important approaches. The Dirac algorithm constructs all hidden constraints in a simple manner. A geometric version based on differential equations was presented in [28].

Various authors developed independently geometric frameworks for the treatment of differential algebraic equations (or more generally implicit differential equations) [32, 33, 46]. These include algorithms for the construction of all integrability conditions, as this is important for an existence and uniqueness theory. Despite the fact that mechanical systems with constraints represent one of the main sources for differential algebraic equations, the relation between these formalisms and the Dirac theory has apparently never been studied in detail.

The purpose of this article is to point out that the mentioned physical and numerical theories, respectively, are special cases of the general problem of completion of a non-normal system of differential equations. First solutions of this problem,

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even for systems of partial differential equations, were presented already at the beginning of the century, namely the Janet-Riquier theory [21] and the Cartan-Kähler theory [11]. We will use the formal theory of differential equations [30] which combines elements of both theories.

We consider here only finite-dimensional systems, i. e. ordinary differential equations, although the full potential of the formal theory shows only in the infinite-dimensional case. But the formal theory of ordinary differential equations is much simpler than that of partial differential equations, as one can dispense with the analysis of the symbol and the problem of δ-regularity does not appear. This also explains why it has been rediscovered so many times!

It should be obvious from these remarks that this is a theoretical article. Its goal is not to propose new integration methods for constrained systems but rather to help to clarify some of the basic concepts. For that reason we will use a fairly informal style and omit rigorous proofs. They will appear elsewhere together with a detailed treatment of the infinite-dimensional case.

The article is organized as follows: the next section gives a brief introduction into the formal analysis of ordinary differential equations. Section 3 discusses the application of this theory to Hamiltonian systems with constraints. In the following section some aspects of differential algebraic equations are considered from the point of view of the formal theory. Section 5 combines the results of the two previous ones and studies the numerical analysis of constrained systems. Before finally some conclusions are given, Section 6 shortly reviews available computer algebra tools for calculations like the here presented ones.

2. Formal Theory of Differential Equations

We consider only (first order) ordinary differential equations, as this leads to considerable simplifications in the theory. Nevertheless it is worth while pointing out that almost all results can be extended to partial differential equations. For a detailed introduction into the formal theory we refer to [30].

Jet bundles [37] provide an intrinsic geometric basis for the formal theory, but for our purposes it suffices to work in local coordinates. We denote the space of dependent variables by X with coordinates x_i, $(1 \leq i \leq n)$ and the space of the independent variable by T with coordinate t. For derivatives with respect to t we use dots. Local coordinates of the first order jet bundle $\mathcal{J}_1(T,X)$ are $(t, x_i, \dot{x}_i)$.

The construction of higher order jet bundles is similar. For example, to obtain $\mathcal{J}_2(T,X)$ one simply adds the second order derivatives $\ddot{x}_i$ as further coordinates. The natural projection $\pi_2 : \mathcal{J}_2(T,X) \to \mathcal{J}_1(T,X)$ simply "forgets" these additional coordinates. Similarly, we introduce the projection $\pi_1 : \mathcal{J}_1(T,X) \to T \times X$.

A system of ordinary differential equations $\phi_\tau(t, x_i, \dot{x}_i) = 0$ $(1 \leq \tau \leq r)$ may be considered as a (fibered) submanifold $\mathcal{R}_1 \subset \mathcal{J}_1(T,X)$. Note that $\mathcal{R}_1$ as a geometric object is independent of the chosen coordinates of $\mathcal{J}_1(T,X)$. The functions ϕ_τ are only one possible local representation of $\mathcal{R}_1$. Any other generating set of the ideal spanned by the ϕ_τ will lead to the same submanifold (even if its cardinality is not r), i. e. $\mathcal{R}_1$ is not changed by algebraic manipulations of the ϕ_τ.

We also need a geometric way to deal with local functions $f : I \to X$ defined on an interval $I \subset T$. This is achieved by considering their graphs, the point set[1] $f = \{(t, x_i) \in T \times X \,|\, t \in I, x_i = f_i(t)\}$. The first prolongation of a function f is

[1]For simplicity, we denote the graph by the same letter as the function.

defined as the point set $j_1(f) = \{(t, x_i, \dot{x}_i) \in \mathcal{J}_1(T, X) \mid t \in I, x_i = f_i(t), \dot{x}_i = \dot{f}_i(t)\}$. f is a solution of the differential equation, if and only if $j_1(f) \subset \mathcal{R}_1$.

In geometric approaches to autonomous systems the tangent bundle $\mathcal{T}X$ often serves as ambient space [1]. This is equivalent to the use of $\mathcal{J}_1(T, X)$, as we may also interpret $\dot{x}_i$ as coordinates of the tangent bundle. But the jet bundle language is more convenient for non-autonomous systems where it avoids somewhat unnatural constructions like the restricted tangent bundle [33]. Furthermore it allows for an easier generalization to partial differential equations without the need to consider infinite-dimensional manifolds.

Two important geometric operations with a differential equation $\mathcal{R}_1$ are its *prolongation* and its *projection*. The prolonged system $\mathcal{R}_2 \subset \mathcal{J}_2(T, X)$ is defined by the original equations $\phi_\tau(t, x_i, \dot{x}_i) = 0$ and their total derivatives, the second order equations $D_t\phi_\tau(t, x_i, \dot{x}_i, \ddot{x}_i) = \partial_t\phi_\tau + \sum_i(\partial_{x_i}\phi_\tau)\dot{x}_i + \sum_i(\partial_{\dot{x}_i}\phi_\tau)\ddot{x}_i = 0$. (One can also define it intrinsically without coordinates.)

The projected system $\mathcal{R}_0 \subset T \times X$ is defined with the help of the natural projection by $\mathcal{R}_0 = \pi_1(\mathcal{R}_1)$; thus it is an algebraic system. The actual construction of a local representation for it is in general a quite complicated problem in algebraic elimination theory. Fortunately, we will perform projections always *after* prolongations where it can be done with linear algebra. We can now express in a simple geometric way whether a given differential equation $\mathcal{R}_1$ can be written in a solved form $\dot{x}_j = \psi_j(t, x_i)$ or whether it is truly a differential algebraic equation. In the former case $\mathcal{R}_0 = T \times X$, whereas in the latter case $\mathcal{R}_0$ is a proper subset, namely the constraint manifold.

If we first prolong a differential equation $\mathcal{R}_1$ to $\mathcal{J}_2(T, X)$ and then project the obtained equation $\mathcal{R}_2$ back to $\mathcal{J}_1(T, X)$ using again the natural projection, we get $\mathcal{R}_1^{(1)} = \pi_2(\mathcal{R}_2)$. One might expect that this should always yield the original equation $\mathcal{R}_1$. However, in general $\mathcal{R}_1^{(1)}$ is only a proper subset of $\mathcal{R}_1$, as *integrability conditions* or *hidden constraints* may arise.

As a simple example consider the semi-explicit differential algebraic equation $\mathcal{R}_1$ defined by $\dot{x}_2 = f(t, x_1, x_2)$ and $g(t, x_1, x_2) = 0$ where we assume that $\partial_{x_1}g \neq 0$. Its prolongation $\mathcal{R}_2$ contains the additional equations $\ddot{x}_2 = D_tf$ and $D_tg = 0$. As the latter equation does not depend on any second order derivative, it survives the projection and $\mathcal{R}_1^{(1)}$ is defined by the two original equations plus this equation.

This example shows that to perform a prolongation and a subsequent projection of a semi-explicit system it suffices to prolong only the constraints. Prolonging the other equations leads to second order equations which drop out during the projection. Since the arising system is linear in the $\dot{x}_i$, it is trivial to obtain again a semi-explicit form for $\mathcal{R}_1^{(1)}$.

If we prolong in our example $\mathcal{R}_1^{(1)}$ to $\mathcal{J}_2(T, X)$, we get the system $\mathcal{R}_2^{(1)}$ which differs from $\mathcal{R}_2$ by the additional equation $D_{tt}g = 0$. As this equation depends on $\ddot{x}_1$, it drops out when we project back to $\mathcal{J}_1(T, X)$ to obtain $\mathcal{R}_1^{(2)} = \pi_2(\mathcal{R}_2^{(1)})$. Thus we find $\mathcal{R}_1^{(2)} = \mathcal{R}_1^{(1)}$.

Generally, we call a differential equation $\mathcal{R}_1 \subset \mathcal{J}_1(T, X)$ *formally integrable* or *involutive*, if a prolongation to $\mathcal{J}_2(T, X)$ and a subsequent projection back to $\mathcal{J}_1(T, X)$ yields again $\mathcal{R}_1$, i.e. $\mathcal{R}_1^{(1)} = \mathcal{R}_1$. This name stems from the fact that one can straightforwardly construct a formal power series solution for such a system, as no further integrability conditions or constraints are hidden. In our example $\mathcal{R}_1$

is not involutive, as there exists the integrability condition $D_t g = 0$. But $\mathcal{R}_1^{(1)}$ is involutive, since $\mathcal{R}_1^{(2)} = \mathcal{R}_1^{(1)}$.

Sometimes a formally integrable system $\mathcal{R}_1$ is called *locally solvable*. This has the following geometric meaning. We consider $\mathcal{R}_1$ as a submanifold of $\mathcal{J}_1(T, X)$. By definition, we have for any solution f that $j_1(f) \subset \mathcal{R}_1$. If we take the union of all prolonged solutions, we obtain in general only a proper subset of $\mathcal{R}_1$. But in the case of a formally integrable system we get (under some regularity assumptions) the whole submanifold $\mathcal{R}_1$. This implies that every point of $\mathcal{R}_1$ defines uniquely a solution (if $\mathcal{R}_1$ is not under-determined).

Let $\mathcal{R}_1$ be a given first order system. By repeated prolongations with subsequent projections we can generate a sequence of submanifolds $\mathcal{R}_1^{(s)} \subset \cdots \subset \mathcal{R}_1^{(1)} \subset \mathcal{R}_1$ where each submanifolds is of lower dimension than its successor. Obviously, the sequence terminates after at most $\dim \mathcal{R}_1$ steps, i.e. for some value $0 \leq s \leq \dim \mathcal{R}_1$ we find $\mathcal{R}_1^{(s+1)} = \mathcal{R}_1^{(s)}$. Thus $\mathcal{R}_1^{(s)}$ is involutive.

This process is called the *completion* of $\mathcal{R}_1$ to an involutive system. If we consider two systems of differential equations as equivalent, if they possess the same solution space, then $\mathcal{R}_1^{(s)}$ and $\mathcal{R}_1$ are equivalent, as the addition of integrability conditions does not affect the solution space. It only eliminates parts of $\mathcal{R}_1$, where no prolonged solutions lie.

This is a special case of the *Cartan-Kuranishi Theorem* that any consistent differential equation can be completed to an equivalent involutive system in a finite number of prolongations and projections. An ordinary differential equation is inconsistent, if at some step of the completion it is possible to deduce an equation of the form $\psi(t) = 0$, i.e. a condition on the independent variable. Geometrically this means that $\mathcal{R}_1^{(s)}$ is no longer a fibered submanifold.

In this brief outline we ignored some subtleties. Especially, we made the assumption that all considered systems $\mathcal{R}_1^{(k)}$ are submanifolds. This corresponds to a constant rank condition on their Jacobians. If this assumption is violated, we must make case distinctions, i.e. split the system into subsystems with constant rank and consider each of these subsystems separately. After each projection new case distinctions may arise. Thus we obtain in general a whole tree of disjoint subsystems.[2] We will also assume throughout this article that all functions involved are as often differentiable as necessary to perform the completion.

3. Constrained Hamiltonian Systems

The theory of constrained Hamiltonian systems was to a large part developed by Dirac [13, 14]. Although there exist other approaches we consider only the Dirac theory. General references for constrained dynamics are [19, 44, 45]. The application of the formal theory to constrained systems was studied in detail in [42].

Although we are concerned with Hamiltonian systems, we begin with a Lagrangian L, as this is the usual way to define a system. Let Q with local coordinates q_i be the n-dimensional configuration space. The Lagrangian is defined on the tangent bundle $\mathcal{T}Q$, thus $L = L(q_i, \dot{q}_i)$. Obviously, this covers only autonomous systems. The simplest way to include an explicit time dependency is to consider t as an additional variable and to take $T \times Q$ as configuration space.

[2] This signals the existence of so-called singular integrals [1, 20].

The equations of motion are given by the *Euler-Lagrange equations*

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0\,, \qquad i = 1, \dots, n\,. \tag{1}$$

If the Hessian $\partial^2 L/\partial\dot{q}_i\partial\dot{q}_j$ is singular, not all equations in (1) are of second order and the system is constrained. This effects especially the Legendre transformation to the Hamiltonian formalism where one introduces the canonically conjugate momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i}\,. \tag{2}$$

Geometrically, (q_i, p_i) are coordinates of the co-tangent bundle $\mathcal{T}^*Q$.

In the unconstrained case where the Hessian is regular, (2) can be solved for the velocities $\dot{q}_i$. In a constrained system (2) yields some *primary constraints*

$$\phi_\alpha(q_i, p_i) = 0\,, \qquad \alpha = 1, \dots, m \le n\,. \tag{3}$$

The *canonical Hamiltonian* of the system is given by[3]

$$H_c(q_i, p_i) = p_j\dot{q}_j - L(q_i, \dot{q}_i). \tag{4}$$

For an unconstrained system it is obvious that H_c can be considered as a function of (q_i, p_i) only, since the $\dot{q}_i$ can be eliminated using (2). One can show that because of the special form of the right hand side of (4) this is also true for constrained systems. But the resulting Hamiltonian H_c is uniquely defined only *on* the constraint manifold. Thus adding an arbitrary linear combination of the constraints has no effect on the formalism [19]. This leads to the *total Hamiltonian*

$$H_t = H_c + u_\alpha\phi_\alpha \tag{5}$$

where the multipliers u_α are yet arbitrary functions of (q_i, p_i).

Introducing the Poisson bracket of two phase space functions F, G

$$\{F, G\} = \frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial G}{\partial q_i}\frac{\partial F}{\partial p_i} \tag{6}$$

we can express the evolution of any observable $F(q_i, p_i)$ concisely as $\dot{F} = \{F, H_t\}$. This makes sense, as we recover the Hamiltonian equations of motion

$$\dot{q}_i = \frac{\partial H_t}{\partial p_i}\,, \qquad \dot{p}_i = -\frac{\partial H_t}{\partial q_i} \tag{7}$$

and thus $\{F, H_t\} = (\partial F/\partial q_i)\dot{q}_i + (\partial F/\partial p_i)\dot{p}_i$. (Alternatively, (7) can be derived with the help of a constrained variational principle [19].)

We require now that the constraints are preserved under the evolution of the system, i. e. if they are satisfied at some time t_0, they must hold at all times. This implies the conditions

$$\{\phi_\alpha, H_t\} \approx 0\,. \tag{8}$$

The $\approx$ signals a *weak equality*; it may hold only after taking the constraints into account. By a standard argument in differential geometry (see e. g. [19]) this implies that the Poisson bracket in (8) must be a linear combination of the constraints. There are three possibilities: (i) it yields modulo the constraints the equation $1 = 0$; (ii) it becomes $0 = 0$; (iii) we obtain a new equation $\psi(q_i, p_i) = 0$.

[3] We use the Einstein convention that a summation over repeated indices is always implied.

(i) means that the equations are inconsistent; they do not possess any solution. (ii) is the desired outcome. (iii) splits into two sub-cases. If ψ depends on some multipliers u_α, we consider it as an equation determining one of these. Otherwise we have found a *secondary constraint*. We must then check whether all secondary constraints are preserved by repeating the procedure until we either encounter case (i) or all constraints lead to case (ii). This is the *Dirac algorithm*.

To make contact with the formal theory, we consider the semi-explicit differential algebraic equation $\mathcal{R}_1 \subset \mathcal{J}_1(T, \mathcal{T}^*Q)$ comprising (7) and the primary constraints (3). The Dirac algorithm does nothing else than to complete $\mathcal{R}_1$ to an involutive system. Taking the Poisson bracket of a constraint with H_t is equivalent to prolonging it and for a semi-explicit system this suffices. If there are s generations of constraints (primary, secondary, etc), then $\mathcal{R}_1^{(s-1)}$ is involutive.

In systems arising from applications usually all multipliers u_α get determined during the completion. In the Dirac terminology this implies that all constraints are *second class*, i. e. if χ_α denotes all constraints (primary ones and those obtained with the Dirac algorithm), then the matrix $C_{\alpha\beta} = \{\chi_\alpha, \chi_\beta\}$ is regular.

First class constraints possess vanishing Poisson brackets with all constraints. They signal the existence of gauge symmetries and thus that the equations of motion are under-determined. Usually they only occur in infinite-dimensional systems and they can always be made second class by a gauge fixing. We will therefore study only systems without first class constraints.

Under this assumption there exists a simple geometric way of determining the number f of degrees of freedom of the system. If there are s generations of constraints, then $f = \frac{1}{2}\dim\mathcal{R}_1^{(s-1)}$. Classically one defines $f = n - m/2$ where m is the total number of constraints.[4] The equivalence of the two expressions can be easily seen. Since Q is n-dimensional, $\dim\mathcal{J}_1(T, \mathcal{T}^*Q) = 4n$. $\mathcal{R}_1^{(s-1)}$ comprises $2n$ differential equations and m constraints, thus $\dim\mathcal{R}_1^{(s-1)} = 2n - m$.

For applications the most important case of a constrained system is described by a regular Lagrangian L_0 and subject to m externally imposed holonomic constraints $\phi_\alpha(q) = 0$. In principle, this situation *cannot* be treated within the Dirac formalism, as it covers only singular Lagrangians. Therefore one introduces Lagrange multipliers λ_α and considers the Lagrangian $L = L_0 + \lambda_\alpha\phi_\alpha$. In contrast to the multipliers u_α in (5), the λ_α must be considered as additional dynamical variables and not as undetermined functions. Then L is singular, as it does not depend on the "velocities" $\dot{\lambda}_\alpha$.

To pass to the Hamiltonian formalism we must also introduce canonically conjugate momenta π_α for the λ_α. The primary constraints are simply $\pi_\alpha = 0$. If H_0 denotes the Hamiltonian of the regular system defined by L_0, the canonical Hamiltonian of the constrained system is $H_c = H_0 - \lambda_\alpha\phi_\alpha$; the total one $H_t = H_c + u_\alpha\pi_\alpha$. The Dirac algorithm yields the secondary constraints $\phi_\alpha = 0$ and the tertiary constraints $\psi_\alpha = \{\phi_\alpha, H_0\} = 0$. The next step gives equations for the λ_α

$$\{\psi_\alpha, H_0\} - \lambda_\beta\{\psi_\alpha, \phi_\beta\} = 0\,. \tag{9}$$

The fifth and last step yields $u_\alpha = 0$.

This rather long derivation can be shortened by *not* introducing the total Hamiltonian H_t and the momenta π_α. Starting with H_c and imposing $\phi_\alpha = 0$ as primary

[4] There is always an even number of second class constraints. This follows from the fact that the skew-symmetric matrix $C_{\alpha\beta}$ is regular.

constraints leads to equivalent results, as in the end $\pi_\alpha = u_\alpha = 0$. The standard approach is to take the Hamiltonian equations of motion for H_c and augment them by the constraints to get the following semi-explicit differential algebraic equation

$$\mathcal{R}_1 : \left\{ \dot{q}_i = \frac{\partial H_0}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H_0}{\partial q_i} + \lambda_\alpha \frac{\partial \phi_\alpha}{\partial q_i}, \quad \phi_\alpha(q) = 0 \, . \right. \tag{10}$$

$\mathcal{R}_1$ becomes involutive after three prolongations and subsequent projections. The first one adds the secondary constraints $\psi_\alpha = \{\phi_\alpha, H_0\} = 0$; the second one yields (9) determining the multipliers λ_α. In order to obtain an involutive system we must prolong once more to obtain equations for $\dot{\lambda}_\alpha$. All these equations together define the system $\mathcal{R}_1^{(3)}$.

There exist many equivalent ways to write the equations of motion $\mathcal{R}_1$ of a constrained system. If $\mathcal{R}_1^{(s)}$ is their involutive completion, only the final constraint manifold $\mathcal{R}_0^{(s+1)} = \pi_1(\mathcal{R}_1^{(s)}) \subset \mathcal{T}^*Q$ has a physical meaning. The ambient phase space $\mathcal{T}^*Q$ is an artifact of the modeling. We can modify the equations of motion at will, as long as they remain unchanged on the constraint manifold. Thus we can add arbitrary linear combinations of the constraints to them.

In the language of Dirac the different formalisms for constrained systems yield weakly equal equations of motion. Although they are physically equivalent, as they lead to identical trajectories, if the initial values lie on the constraint manifold, the numerical behavior of the various differential algebraic equations can be quite different. This will be discussed a bit more detailed in Section 5.

It might appear at first sight that our approach to constrained systems based on the formal theory consists merely of renaming the steps performed in the Dirac theory. This misses some important points. First of all we can conclude that the Dirac algorithm is not really a physical algorithm but a purely mathematical method to check the consistency of the equations of motion. Physics enters essentially only in the classification into first and second class constraints.

Once this fact is realized we see that we have got a constraint algorithm not only for Hamiltonian systems but for arbitrary systems. We could for example dispense with the Legendre transformation and directly complete the Euler-Lagrange equations to an involutive system (such a Lagrangian constraint algorithm can be found in [44]). We can also handle systems with higher order Lagrangian (i. e. depending on higher order derivatives of the q_i) or Newton-Euler equations or explicitly time-dependent systems. As soon as we have somehow obtained equations of motion, formal theory provides us with a constraint algorithm.

4. Differential Algebraic Equations

The numerical integration of differential algebraic equations has found much attention lately and several textbooks (e. g. [4, 16]) have meanwhile been written on this subject. An important topic is the *index* of a differential algebraic equation. Many different definitions have been proposed [6]; most of them belong to two groups, the differentiation and the perturbation indices, respectively.

Most indices belong the first group. In the language of Section 2 they are defined as the number of prolongations one must perform until the obtained system has some property. In the numerical literature this is often expressed with the derivative array [5]. The $(q+1)$-th derivative array for a differential algebraic equation $\mathcal{R}_1$ comprises the equations defining the q times prolonged system $\mathcal{R}_{q+1}$.

The mostly used index is “the” *differentiation index* and it can be defined as the smallest integer ν_d such that the Jacobian[5] $\partial\phi_\alpha/\partial\dot{x}_i$ of the system $\mathcal{R}_1^{(\nu_d)}$ has rank n where n is the number of dependent variables. This is equivalent to the formulation usually found in the numerical literature that the ν_d-th derivative array determines $\dot{x}_i$ uniquely as a function of t and x_i.

This implies that ν_d is finite, if and only if the system is not under-determined, as otherwise this rank condition will never be satisfied. For all other systems one finds from dimensional considerations the trivial upper bound $\nu_d \leq \dim\mathcal{R}_1$, as each prolongation and projection cycle reduces the dimension at least by one.

In [25, 29] it was claimed that the differentiation index was the smallest integer ν_f such that $\mathcal{R}_1^{(\nu_f)}$ is formally integrable. Although this holds for most differential algebraic equations in applications, it is not always true. In general, we have for any not under-determined system the inequality $\nu_f \geq \nu_d$. This can easily be demonstrated with the following class of over-determined systems

$$\mathcal{R}_1 : \begin{cases} \dot{x}_j = \phi_j(t, x_i)\,, & j = 1, \ldots, n\,, \\ \psi_k(t, x_i) = 0\,, & k = 1, \ldots, m \leq n\,. \end{cases} \tag{11}$$

Here $\nu_d = 0$, as all derivatives $\dot{x}_i$ are expressed as functions of t and x_i. But $\mathcal{R}_1$ is not necessarily formally integrable. Prolonging the constraints $\psi_k = 0$ may lead to further constraints. By definition of the differentiation index, $\mathcal{R}_1^{(\nu_d)}$ can after some algebraic manipulations always be written as a system of the form (11). Thus in order to check the consistency of a differential algebraic equation it does *not* suffice to prolong ν_d times. Since only the completion to a formally integrable systems unveils all hidden constraints, an existence and uniqueness theory can never be based on the differentiation index.

A better name for ν_d would be *determinacy index*, as it gives the number of prolongations necessary to obtain a determined system. We call ν_f the *(formal) integrability index*. For linear systems it has already been introduced under the name *strangeness index* [23, 24] (the codimension of the constraint manifold $\mathcal{R}_0^{(1)}$, i.e. the number m in (11), is sometimes called the strangeness of $\mathcal{R}_1$).

For many systems the integrability index ν_f is similar to the *uniform differentiation index* ν_{ud} introduced in [6, 7]. When the latter one is defined, it also ensures the existence and uniqueness of solutions. The fact that for its definition the systems $\mathcal{R}_{r+1}$ are used instead of $\mathcal{R}_1^{(r)}$ (i.e. no projections are performed) is not important, as it does not influence the obtained index values. Differences occur in two places. Condition (A4) of [6, 7] excludes the possibility of trivial integrability conditions, as they always occur in over-determined systems. Thus ν_{ud} is not defined for systems of the form (11).

The second important difference lies in the fact that in the formal theory all ranks are evaluated only *on* the submanifolds $\mathcal{R}_1^{(s)}$ (which may lead to some computational problems, see Section 6), whereas in the definition of ν_{ud} constant ranks are demanded in open neighborhoods of solutions. This can lead to very different index values for the same equation. Consider the following simple example taken

[5] In formal theory this matrix is called the *symbol* of the differential equation. The notion of 1-fullness [5] sometimes used in the theory of linear differential algebraic equations thus refers to an analysis of the symbol.

from [6]:

$$\sin(\dot{y})y + x = 0\,, \quad \sin(\dot{z})z + y = 0\,, \quad z = 0\,. \tag{12}$$

For the formal theory (12) is equivalent to the trivial system $x = y = z = 0$, as both sets of equations define the same submanifold $\mathcal{R}_1$ which becomes formally integrable after one prolongation. Thus $\nu_f = 1$. However, no algebraic manipulations of the equations are allowed in the determination of ν_{ud} and one finds $\nu_{ud} = 3$.

Any system of the form (11) defines a unique vector field on the constraint manifold $\mathcal{R}_0^{(1)}$. For any point $p \in \mathcal{R}_0^{(1)}$ the intersection of the fiber $\pi_1^{-1}(p)$ and $\mathcal{R}_1$ consists of exactly one point (under some suitable regularity assumptions) which can be interpreted as the value of a vector field at p. Reich [33] called it the *corresponding vector field* of the differential algebraic equation. Any solution of the original differential algebraic equation is an integral curve of it and vice versa.

The corresponding vector field should not be confused with an *underlying ordinary differential equation*. Given a system $\mathcal{R}_1$, another system $\tilde{\mathcal{R}}_1$ is called underlying, if $\mathcal{R}_1 \subset \tilde{\mathcal{R}}_1$ and $\tilde{\mathcal{R}}_0^{(1)} = T \times X$. The first condition implies that the solution space of $\mathcal{R}_1$ is a subset of that of $\tilde{\mathcal{R}}_1$. The second one geometrically expresses the absence of constraints, thus $\tilde{\mathcal{R}}_1$ is a pure differential equation.

Obviously, an underlying ordinary differential equation $\mathcal{R}_1$ defines a vector field, too. But whereas the corresponding vector field lives only on the constraint manifold $\mathcal{R}_0^{(1)} \subset T \times X$ and is unique, this vector field is defined on the whole manifold $T \times X$ and there exist many underlying equations to a given differential algebraic equation. All of them possess the same solutions for initial values on the constraint manifold, but for other values their solutions may differ.

Although the definition of the corresponding vector field is already possible with $\mathcal{R}_1^{(\nu_d)}$, it makes no real sense, if $\mathcal{R}_1^{(\nu_d)}$ is not formally integrable (actually Reich [33] defined it only for formally integrable systems). Otherwise the vector field is not everywhere tangent to the constraint manifold and at some points there might exist no integral curves lying in the manifold.

If we construct the corresponding vector field for a formally integrable system, we get a geometric version of the *state-space form* obtained by explicitly solving the constraints and eliminating the redundant coordinates. We can use this to derive existence and uniqueness theorems for differential algebraic equations, as now the standard theorems apply. This yields also a proof for the local solvability of a formally integrable system mentioned in Section 2.

We have so far seen the importance of the index for an existence and uniqueness theory of differential algebraic equations, but it has not become clear why it is often rather difficult to integrate them numerically. This can be better understood with the help of the *perturbation index* introduced by Hairer *et. al.* [15]. It measures the sensitivity against numerical errors, as it is based on an estimate for the difference between solutions of the given equation and of a perturbed one.

Let the differential algebraic equation $\mathcal{R}_1$ be defined by $\phi_\tau(t, x_i, \dot{x}_i) = 0$ and let $\xi_i(t)$ be a solution on an interval I for the initial condition $x_i(t_0) = \xi_i^{(0)}$. Denote by $||\cdot||$ the Euclidean norm on X and by $||\cdot||_\infty$ the supremum norm on I. Then $\mathcal{R}_1$ has along this solution the perturbation index ν_p, if for any solution $\hat{\xi}_i(t)$ of the perturbed equation $\phi_\tau(t, x_i, \dot{x}_i) = \delta_\tau(t)$ an estimate of the form

$$||\xi(t) - \hat{\xi}(t)|| \leq C\Big(||\xi^{(0)} - \hat{\xi}(t_0)|| + ||\delta||_\infty + ||\dot{\delta}||_\infty + \cdots + ||\delta^{(\nu_p - 1)}||_\infty\Big) \tag{13}$$

holds on the entire interval I whenever the right hand side is sufficiently small. The constant C depends on the interval I and the solution ξ.

Note that ν_p is defined for individual solutions and that we do not require that the perturbed solutions $\hat{\xi}(t)$ satisfy the same initial conditions. (13) implies that the initial value problem for differential algebraic equations is in principle an ill-posed problem, if $\nu_p > 1$, as derivatives of δ occur in the estimate. This explains the numerical difficulties in solving higher index equations. Classical methods like Runge-Kutta suffer a loss of order when applied to differential algebraic equations.

Note furthermore that in general the perturbed equation will not possess solutions $\hat{\xi}(t)$ for all possible choices of the perturbation $\delta(t)$. Especially, if the original system is over-determined, the functions $\delta_\tau(t)$ must generally satisfy compatibility conditions. A trivial example may demonstrate this effect. Take the system $\dot{x} = 0$, $x = 0$. The perturbed system $\dot{x} = \delta_1$, $x = \delta_2$ is inconsistent, if $\dot{\delta}_2 \neq \delta_1$.

We can summarize the situation as follows: the differentiation indices are (at least in principle) easier to determine; the perturbation indices are more important for the numerical integration of a differential algebraic equation. Therefore one is interested in relating the two classes of indices, e. g. by giving bounds for ν_p in terms of differentiation indices [6].

We propose here a solution of this problem based on the *parametrized* differential equation $\bar{\mathcal{R}}_1$ defined locally by the equations $\phi_\tau(t, x_i, \dot{x}_i) = \delta_\tau(t)$. Thus we consider the perturbations δ as parameters and not as additional dependent variables. Note that $\bar{\mathcal{R}}_1$ is not defined intrinsically but depends on the chosen local representation $\phi_\tau = 0$ of $\mathcal{R}_1$. Then we can compute the integrability index $\bar{\nu}_f$ of $\bar{\mathcal{R}}_1$.

It is easy to see that for any solution of $\mathcal{R}_1$ the estimate

$$\nu_p \leq \bar{\nu}_f + 1 \tag{14}$$

holds, as in $\bar{\mathcal{R}}_1^{(\bar{\nu}_f)}$ the highest occurring derivative of δ has order $\bar{\nu}_f$. During the completion one automatically determines the compatibility conditions δ must satisfy. If such conditions occur, a sharper bound than (14) may hold. Relevant for the bound is the highest δ derivative appearing in the corresponding vector field. If higher order derivatives appear only in the compatibility conditions, they do not effect the estimate (14).

The thus computed index $\bar{\nu}_f$ is very similar to the uniform differentiation index ν_{ud}, but the precise relationship is yet unclear. For the example (12) one obtains $\bar{\nu}_f = \nu_{ud} = 3$. This example also demonstrates why the δ_τ must be treated as parameters and not as additional dependent variables. Otherwise we would get again $\bar{\nu}_f = 1$ which is not what we want.

This approach also allows for a simple generalization of the perturbation index. The definition above is based on one of the simplest way to model numerical errors, namely including a perturbation on the right hand side. In some problems more special models might be available leading to a perturbed equation of the general form $\bar{\phi}_\tau(t, x_i, \dot{x}_i, \delta_\alpha) = 0$ where now the number of perturbations δ_α may differ from the number of equations $\bar{\phi}_\tau = 0$. Our formalism can handle this more general situation as easily as the standard one.

5. Numerical Analysis of Constrained Hamiltonian Systems

Constrained mechanical systems belong to the most important sources of differential algebraic equations. Usually, they are treated in the Lagrangian formalism.

But as most of the systems are of the form discussed at the end of Section 3 with the regular Lagrangian L_0 quadratic in the velocities, the transition of the first order form of the Euler-Lagrange equations to the Hamiltonian equations of motion corresponds to a simple linear transformation of the dependent variables.

The interest in the Hamiltonian formalism has grown with the development of symplectic integrators [36]. These are numerical methods preserving the symplectic structure of the phase space, i. e. the Poisson bracket (6). It has been shown that they retain much of the qualitative properties of the solution space and that they are often superior to conventional methods in long time integration.

Comparing the results of Section 3 and 4, we see that systems defined by a regular Lagrangian with externally imposed holonomic constraints have index 3 (system (10) needs three prolongations to become involutive). More generally, the integrability index of a constrained Hamiltonian system corresponds to the number of generations of constraints appearing in the Dirac algorithm ($\nu_f = s - 1$).

Although there exist meanwhile some methods for the direct numerical integration of higher index equations [10], currently available standard packages like DASSL [4] can reliably handle only systems with index 1 or 2. Thus one must either reduce the index or perform some form of stabilization.

Especially in multi-body dynamics various index reduced formulations of the equations of motion have been proposed (for an overview see [43]). The simplest approach consists of integrating one of the systems $\mathcal{R}_1^{(k)}$ for $1 \leq k \leq \nu_f$, as each prolongation and projection cycle reduces the index by one. However, empirical tests indicate that this approach can lead to numerical instabilities.

Thus additional stabilization by adding some terms vanishing on the constraint manifold is necessary. For general differential algebraic equations not much is known about how such terms can be found [3]. But for constrained Hamiltonian systems it is possible to derive stabilized forms of the equations of motion using physical arguments. Especially, it is possible to stabilize while maintaining the Hamiltonian character of the system.

One approach is based on the *extended Hamiltonian* H_e. Whereas only the primary constraints are used to define the total Hamiltonian H_t, H_e contains a linear combination of all constraints. The coefficients are determined by requiring that the Poisson bracket of H_e with any constraint vanishes. This yields a linear system for them.

The drawback of this approach is that already for the simple case of a regular Lagrangian with imposed constraints one needs third order derivatives of the constraints to set up the equations of motion. Thus these are in general rather complicated and expensive to derive. But numerical experiments and theoretical considerations demonstrate clearly the stabilizing effect of the extra terms [26].

An alternative approach consists of modifying the symplectic structure of the phase space instead of modifying the Hamiltonian, i. e. to use another definition for the Poisson brackets than (6). This has already been proposed by Dirac in form of the so-called Dirac brackets [13, 14]. One can show that the arising equations of motion, the Hamilton-Dirac equations, correspond to a simplification of the equations of motion derived with extended Hamiltonian H_e, namely to omitting the terms depending on the third order derivatives of the constraints [41].

The basic idea behind both approaches (and others like the Faddeev-Jackiw [40] or the impetus-striction formalism [12]) is to construct a *Hamiltonian* underlying ordinary differential equation. Thus one obtains unconstrained Hamiltonian systems and their solutions for initial values on the constraint manifold coincide with solutions of the original constrained system.

Although this allows us to use symplectic integrators for constrained Hamiltonian systems, too, all the approaches mentioned have some disadvantages. First of all, even if the original system was separable, this property will be destroyed. This excludes the use of explicit symplectic schemes. Thus more expensive methods like the implicit midpoint rule must be applied.

In the case of Dirac brackets the situation is even more difficult. Because of the modified symplectic structure it is unclear whether conventional symplectic integrators can be applied. However, the Dirac bracket is on the constraint manifold just the symplectic structure induced by the canonical Poisson bracket [19]. Thus as long as the constraints are preserved one deals in principle with the canonical structure. Preliminary numerical tests seem indeed to indicate that it makes sense to apply standard symplectic methods to the Hamilton-Dirac equations [41].

Nevertheless it appears that for regular systems with imposed holonomic constraints it is more efficient to include the constraints directly into the numerical methods instead of modifying the equations of motion. For these systems several types of symplectic integrators have meanwhile been developed [22, 34]. They do not suffer from a drift off the constraint manifold, as essentially at each step a projection is done. Stabilization can never achieve this (but it can significantly reduce the number of projections needed).

6. Computer Algebra Tools

There exist very few computer algebra packages for the Dirac algorithm or the determination of the index of a differential algebraic equation. But as we have seen these are just special cases of the general completion theory of differential equations and many completion packages have meanwhile been implemented in various computer algebra systems.

A Macsyma package for the Dirac algorithm was presented in [47]. It can handle only Lagrangians quadratic in the velocities, as otherwise there might be problems with solving (2) for them. The program is also able to classify the constraints into first and second class and to perform gauge fixings.

For linear differential algebraic equations with polynomial coefficients a Maple implementation of a “reduction” algorithm (which corresponds to what we call completion) was presented in [31]. The package does not require that the system satisfies a constant rank assumption.

Most implementations of completion algorithms are not based on the here used formal theory but on the Janet-Riquier theory [21, 35]. All of them are designed for partial differential equations, but they can of course also handle ordinary differential equations. Typically they have been developed in connection with the Lie symmetry theory for the analysis of determining systems.

The main difficulty of all completion algorithms is to decide the independence of equations. For general expressions this is an unsolved problem. Since prolonging a differential equation always yields quasi-linear equations, the construction of integrability conditions requires only linear algebra. But then it must be decided whether or not they are independent of the already present equations. This is not a problem in differential equations but in algebraic elimination theory.[6]

Therefore most packages are restricted to certain classes of differential equations. Rather simple is the theory of course for linear systems (like the determining equations in Lie theory) where Gaussian elimination suffices. The same holds in principle for quasi-linear systems. However, it is no guaranteed that a system remains quasi-linear during the completion process, as the occurring integrability conditions may be non-linear. Using Gröbner Bases one can theoretically handle any kind of polynomial nonlinearity. However, in practice the complexity of such computations is often too high.

Among the implementations based on Janet-Riquier theory the very efficient MAPLE package `standard_form` [35] is most notable. In many aspects similar are the so-called Differential Gröbner Bases [27] also implemented in MAPLE. There exists a REDUCE implementation of the Cartan-Kähler theory for exterior systems [17] which has also been used in connection with constrained dynamics [18]. We [38, 39] implemented in AXIOM an environment for the formal theory including a completion package. Currently, it is ported to MuPAD.

However, all these packages have made hardly any impact on the numerical analysis of differential algebraic equations (but see [7]). One can think of several reasons for this. The first one is a "psychological" one; many numerical analysts prefer methods like automatic differentiation to computer algebra, although this approach has problems, too [8]. Secondly, for large scale non-linear problems computer algebra systems are often still not sufficiently efficient. Furthermore the hidden constraints may be prohibitively large.

Finally, for many differential algebraic equations appearing in applications, one does not really need a complicated completion package. For example for the above considered class of regular systems with imposed holonomic constraints the completion steps are clear and well-known. Essentially, one needs only the Jacobian of the constraints. However, one might expect that computer algebra tools will become more important, as soon as there is more interest in the numerical analysis of general infinite-dimensional systems.

7. Conclusions

We showed in this article that the formal theory of differential equations provides a unifying theoretical framework for some aspects of constrained Hamiltonian systems as well as of the numerical analysis of differential algebraic equations. Actually, similar concepts also appear in control theory (relative degree) and probably in some other fields, too. It is somewhat surprising that although many approaches to the general completion problem like Janet-Riquier theory or Cartan-Kähler theory are not only older than the theory of differential algebraic equations but also than the Dirac theory, this connection has never been realized.

Less surprising is the fact that such rediscoveries have been made only for finite-dimensional systems governed by ordinary differential equations. Here it is rather straightforward to deal with the completion problem. A simple prolongation and

[6] Actually it is not really necessary to eliminate dependent equations. It suffices to determine the dimensions of the submanifolds $\mathcal{R}_1^{(s)}$. Jacobians are, however, not an efficient tool for that, as their rank must be evaluated *on* the submanifold.

projection loop suffices. The theory becomes more involved in the case of partial differential equations, as new phenomena appear requiring the introduction of further concepts like the symbol of a differential equation etc.

Formal integrability and involution are no longer identical concepts for partial differential equations. A formally integrable system must satisfy an additional condition to be involutive. It is of a more algebraic nature and connected with the symbol. Although it suffices for many purposes to complete a given system to a formally integrable one, no finite criterion for formal integrability is known. Only involution can be checked directly. The Cartan-Kuranishi Theorem states that any consistent system of partial differential equations can be completed in a finite number of steps to an equivalent involutive one. However, in general this system will be of higher order than the original one.

In [42] infinite-dimensional constrained systems were studied using the formal theory. It was shown that the direct extension of the Dirac algorithm used in the physical literature is in general not equivalent to the completion to an involutive system. As demonstrated at an explicit example this implies that in some cases the Dirac algorithm *cannot* decide the consistency of a field theory.

The extension of the results above on differential algebraic equations to infinite-dimensional systems is currently under investigation. The basic concept is that of a *normal* system or a system of *Cauchy-Kowalevsky form*. There a distinguished independent variable t exists, so that the system can be brought into the form

$$\partial_t u_\beta = \psi_\beta(t, z_i, u_\alpha, \partial_{z_i} u_\alpha) \tag{15}$$

where z_i denotes the remaining independent variables. Note that no t-derivatives appear on the right hand side of (15) and that the system comprises as many equations as there are dependent variables u_α.

In the case of ordinary differential equations where no variables z_i are present, normal means that the system can be solved for the derivatives. A non-normal system is a differential algebraic equation. A system of partial differential equations has more possibilities to be not normal, even if all equations are of the same order. One must now carefully analyze the *leading derivatives* of the system.

Formulating the various index concepts within the formal theory allows us to extend them rather easily to the infinite-dimensional case. For example, it is straightforward to define the integrability index ν_f for a general system of partial differential equations, whereas it is unclear how to generalize the uniform differentiation index ν_{ud}.[7] Our approach to consider the perturbation index as the integrability index of a perturbed system can similarly be extended without problems.

As already mentioned in the Introduction the purpose of this article was to provide a theoretical framework for the numerical analysis of constrained Hamiltonian systems. We did not study any specific method but showed connections to a well-established mathematical theory. That this is not just a game is shown by the work of Tuomela who used the formal theory to introduce a new approach to the numerical integration of general implicit ordinary differential equations [2, 49] and for an improved treatment of singularities including impasse points [48].

[7] See [9] for a discussion of some index concepts for infinite-dimensional systems.

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