A Constructive Introduction to Involution*

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Abstract. We given a constructive introduction into the theory of involutive systems of algebraic or differential equations based on a unified combinatorial point of view. Concrete algorithms for the completion of arbitrary systems to involutive ones are presented. Some applications in the context of constrained mechanical systems and numerical analysis, resp., are discussed.

1 Introduction

Involution is a very general and fundamental concept with many different aspects and applications. Usually, it does not appear on its own but in connection with other ideas. So it is not so easy to say in a few words what involution means, especially as different people use it with different meanings. One may interpret it as a special kind of completeness and we will take this point of view here, as it also has the advantage of leading to concrete algorithms.

The concept of involution has its origin in the theory of differential equations, most notable in the works of Janet [20,21] and Riquier [30] or (in the language of exterior differential systems [4]) of Cartan [6] and Kähler [22]. Only in fairly recent times it has been applied in the context of polynomial equations, too, leading to the notion of an involutive basis, a special sort of (non-reduced) Gröbner bases [9]. A rather extensive introduction into this theory can be found in [37] which stresses combinatorial aspects and also presents some applications.

For general systems of algebraic or differential equations the first and immediate task of a completion to involution is to check the consistency of the equations and thus to decide the existence of (formal)

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solutions. The combinatorial nature of involution also allows us to make statements about the size of the solution space. However, involution is more than just these simple questions which could also be answered by other means.

The combinatorial decomposition implied by an involutive basis contains many important structural information. These allow us for example strong statements about the syzygy resolution or provides us with powerful tools for analysing the existence and uniqueness of solutions. In some recent works we have started to show that they are also very important for the numerical analysis of general systems of differential equations.

There exist a number of other approaches to general systems. For algebraic equations, this means mainly Gröbner bases [1,7]. As already mentioned above, involution leads to a specialisation of this theory. For differential equations, the classical theories by Janet-Riquier and Cartan-Kähler are still much studied and have been extended in various directions. Some important references are [4,12,23,29].

This article is organised as follows. The next section discusses the combinatorial approach to involution. In order not to have to distinguish all the time between algebraic and differential equations, we formulate this theory on the Abelian monoid of n-tuples with non-negative integers as entries. In Sect. 3 these n-tuples are interpreted as the exponent vectors of monomials and we are lead to involutive bases of polynomial ideals. In the following section they become multi indices of derivatives and thus we study differential equations. After a brief discussion of a few sample applications in Sect. 5, we finally give some conclusions.

2 Combinatorial Approach to Involution

In this article we take a combinatorial approach to involution. So we start with discussing the Abelian monoid $(\mathbb{N}^n, +)$. Its elements are ordered n-tuples $\mu = [\mu_1, \dots, \mu_n]$ where all entries μ_i are non-negative integers. We identify the n-tuples in a natural way with the vertices in an n-dimensional integer lattice. The addition is defined componentwise. We denote by N the set $N = \{1, \dots, n\}$ and by $\mathbb{N}_i = \{\mu \in \mathbb{N}^n \mid \mu_j = k\delta_{i,j},\ k \in \mathbb{N}\}$ the set of all n-tuples where all entries besides μ_i vanish.

Definition 1. An *involutive division* L is defined on $(\mathbb{N}^n, +)$, if a subset $N_{L,\mathcal{N}}(\nu) \subseteq N$ of *multiplicative indices* is associated to every n-tuple ν in a finite subset $\mathcal{N} \subset \mathbb{N}^n$ such that the following two conditions on the *involutive cones* $\mathcal{C}_{L,\mathcal{N}}(\nu) = \nu + \sum_{i \in N_{L,\mathcal{N}}(\nu)} \mathbb{N}_i \subset \mathbb{N}^n$ of the terms $\nu \in \mathcal{N}$ are satisfied.

1. If there exist two elements $\mu, \nu \in \mathcal{N}$ with $\mathcal{C}_{L,\mathcal{N}}(\mu) \cap \mathcal{C}_{L,\mathcal{N}}(\nu) \neq \emptyset$, either $\mathcal{C}_{L,\mathcal{N}}(\mu) \subset \mathcal{C}_{L,\mathcal{N}}(\nu)$ or $\mathcal{C}_{L,\mathcal{N}}(\nu) \subset \mathcal{C}_{L,\mathcal{N}}(\mu)$ holds.
2. If $\mathcal{N}' \subset \mathcal{N}$, then $N_{L,\mathcal{N}}(\nu) \subseteq N_{L,\mathcal{N}'}(\nu)$ for all $\nu \in \mathcal{N}'$.

The *non-multiplicative indices* form the complement of $N_{L,\mathcal{N}}(\nu)$ in N and are denoted by $\bar{N}_{L,\mathcal{N}}(\nu)$. An involutive division is *globally defined*, if the assignment of the multiplicative indices is independent of the set $\mathcal{N}$; in this case we write simply $N_L(\nu)$. □

This seemingly abstract definition has a simple geometric interpretation. An n-tuple ν generates the cone $\nu + \mathbb{N}^n$ in the lattice; the union of all cones generated by elements of a finite set $\mathcal{N}$ yields its *span* $\langle \mathcal{N} \rangle \subset \mathbb{N}^n$. An involutive division L defines lower dimensional restrictions of these cones — the involutive cones. Here we are allowed to proceed only in certain directions, namely those corresponding to the multiplicative indices (see Fig. 1 below). This leads to the *involutive span* of the set $\mathcal{N}$:

$$\langle \mathcal{N} \rangle_L = \bigcup_{\nu \in \mathcal{N}} \mathcal{C}_{L,\mathcal{N}}(\nu) \ . \tag{1}$$

An alternative interpretation which explains the terminology "involutive division" is the following. We say for n-tuples μ, ν that μ *divides* ν, if $\nu \in \mu + \mathbb{N}^n$ (i. e. $\mu_i \leq \nu_i$ for all i). Given an involutive division L and a set $\mathcal{N} \subset \mathbb{N}^n$ such that $\mu \in \mathcal{N}$, μ is an *involutive divisor* of ν (with respect to L and $\mathcal{N}$), if $\nu \in \mathcal{C}_{L,\mathcal{N}}(\mu)$. Thus an involutive division introduces a restricted divisibility relation on $\mathbb{N}^n$.

Example 2. One classical example of a globally defined involutive division is the *Pommaret division* P. It assigns the multiplicative indices according to the following simple rule: if $k \in N$ is the smallest index such that $\mu_k > 0$, then $N_P(\mu) = \{1, \ldots, k\}$.

Another important example is the *Janet division* J. In order to define it, we must introduce certain subsets of the given set $\mathcal{N} \subset \mathbb{N}^n$:

$$(d_k, \ldots, d_n) = \{ \mu \in \mathcal{N} \mid \mu_i = d_i \ , \ k \leq i \leq n \} \ . \tag{2}$$

Now the index n is multiplicative for a $\mu \in \mathcal{N}$, if $\mu_n = \max_{\nu\in\mathcal{N}} \{\nu_n\}$. The index $k < n$ is multiplicative for an n-tuple $\mu \in (d_{k+1}, \dots, d_n)$, if $\mu_k = \max_{\nu\in(d_{k+1},\dots,d_n)} \{\nu_k\}$. Obviously, the assignment of the multiplicative indices depends here on the set $\mathcal{N}$. □

Definition 3. The finite set $\mathcal{N} \subset \mathbb{N}^n$ is called *involutive* for the division L, if $\langle\mathcal{N}\rangle_L = \langle\mathcal{N}\rangle$. $\mathcal{N}$ is a *minimal involutive basis* of $\langle\mathcal{N}\rangle$, if the union in (1) is disjoint, i. e. there are no intersections between the involutive cones. We call any finite set $\mathcal{N} \subset \mathcal{N}' \subset \mathbb{N}^n$ such that $\langle\mathcal{N}'\rangle_L = \langle\mathcal{N}\rangle$ an *involutive completion* of $\mathcal{N}$. □

Minimal involutive bases yield a decomposition of the span of a set $\mathcal{N}$ into *disjoint* cones of varying dimensions. This is useful for many combinatorial applications. As a simple example we consider the following problem: determine the number $H(q)$ of n-tuples μ contained in $\langle\mathcal{N}\rangle$ with $|\mu| = \mu_1 + \cdots + \mu_n = q$ for some fixed integer $q \geq 0$. For an arbitrary set $\mathcal{N}$ this can be a rather complicated task.

Assume that we know a minimal involutive basis $\mathcal{N}'$ of $\langle\mathcal{N}\rangle$ for some involutive division L. If we denote $q_\nu = |\nu|$ and $k_\nu = |N_{L,\mathcal{N}'}(\nu)|$ (i. e. the number of multiplicative indices of ν), then for any $q \geq q_\nu$ the cone $\mathcal{C}_{L,\mathcal{N}'}(\nu)$ contains $\binom{q-q_\nu+k_\nu-1}{k_\nu-1}$ n-tuples of length q. As for a minimal involutive basis the union in (1) is disjoint, we obtain $H(q)$ by a simple summation over all elements $\nu \in \mathcal{N}'$.

Lemma 4. *If $\mathcal{N}$ is an involutive set, there exists a subset $\mathcal{N}' \subseteq \mathcal{N}$ such that $\mathcal{N}'$ is a minimal involutive basis of $\langle\mathcal{N}\rangle$.*

Proof. The proof represents a nice motivation for the two conditions in Def. 1 of an involutive division. If $\mathcal{N}$ is not yet a minimal involutive basis, the union in (1) cannot be disjoint. Thus there must exist involutive cones which intersect. By the first condition, this implies that some cones are contained in other ones; no other form of intersection is possible. If we eliminate the corresponding elements of $\mathcal{N}$, we get a subset $\mathcal{N}' \subset \mathcal{N}$ which has by the second condition the same involutive span, as the remaining elements may only gain additional multiplicative indices. Thus after a finite number of such eliminations we get a minimal involutive basis. □

Example 5. Figure 1 demonstrates the geometric interpretation of involutive divisions for $n = 2$. In both diagrams one can see the span of

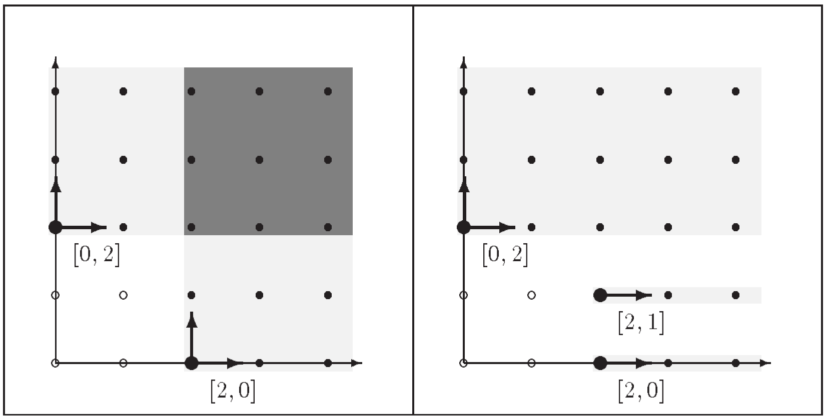

Fig. 1. *Left:* intersecting cones. *Right:* involutive cones.

the set $\mathcal{N} = \{[0,2],[2,0]\}$; the vertices belonging to it are marked by dark points. The arrows represent the multiplicative indices, i. e. the "allowed directions". Obviously the full cones of the two elements of $\mathcal{N}$ intersect in the dark shaded area. The right diagram shows a minimal involutive basis of $\langle \mathcal{N} \rangle$ for both the Janet and the Pommaret division. We must add to $\mathcal{N}$ the element $[2,1]$ and both for this element and for $[2,0]$ only the index 1 is multiplicative. One can clearly see how $\langle \mathcal{N} \rangle$ is decomposed into three disjoint cones: one of dimension 2, two of dimension 1. □

Under certain, rather technical conditions on the chosen involutive division L we can construct an involutive basis with the simple algorithm shown in Fig. 2 [9,37]. It requires a total order $\prec_s$ on $\mathbb{N}^n$ (compatible with the monoid structure) and proceeds as follows. For any n-tuple in the set $\mathcal{N}$ it studies all the n-tuples one gets if one increases the entry corresponding to one of the non-multiplicative indices. If some of these are not yet contained in the involutive span of $\mathcal{N}$, the minimal one with respect to $\prec_s$ is added to $\mathcal{N}$. One can show that if the input set is autoreduced, i. e. no element divides another one, the output is in fact a minimal involutive basis.

In Example 5 above, this algorithm needs precisely one iteration where it analyses the non-multiplicative index 2 for the tuple $[2,0]$. Obviously, the tuple $[2,1]$ does not lie in the involutive span $\langle \mathcal{N} \rangle_L$ and thus must be added. This yields the involutive completion shown in the right half of Fig. 1.

Algorithm: *Involutive completion*
Input: Finite subset $\mathcal{N} \subset \mathbb{N}^n$, involutive division L, order $\prec_s$
Output: Involutive basis of $\langle \mathcal{N} \rangle$

`repeat`
  $\mathcal{S} \leftarrow \{\nu + 1_i \mid \nu \in \mathcal{N},\, i \in \bar{N}_{L,\mathcal{N}}(\nu),\, \nu + 1_i \notin \langle \mathcal{N} \rangle_L\}$
  $\mathcal{N} \leftarrow \mathcal{N} \cup \{\min_{\prec_s} \mathcal{S}\}$
`until` $\mathcal{S} = \emptyset$
`return` $\mathcal{N}$

Fig. 2. Completion in $(\mathbb{N}^n, +)$

3 Involutive Systems of Algebraic Equations

Let $\mathcal{P} = \mathbb{K}[x_1, \dots, x_n]$ be a polynomial ring over the field $\mathbb{K}$. Then the set of all power products $\mathbb{T} = \{x^\mu = x_1^{\mu_1} \cdots x_n^{\mu_n} \mid \mu \in \mathbb{N}^n\}$ equipped with the usual multiplication is obviously isomorphic as an Abelian monoid to $(\mathbb{N}^n, +)$. So we can directly apply the theory developed in the last section to monomial ideals; especially we can use the algorithm in Fig. 2 to effectively compute involutive bases of such ideals. It is this application which has lead to the term "multiplicative" indices and where it becomes obvious why we speak of an involutive "division".

In order to define involutive bases for arbitrary polynomial ideals, we need besides an involutive division L one additional ingredient familiar from Gröbner bases [1,7]: a term order $\prec$, i. e. a total order on the set $\mathbb{T}$ such that 1 is the smallest element of $\mathbb{T}$ and that $x^\mu \prec x^\nu$ implies $x^{\mu+\rho} \prec x^{\nu+\rho}$ for all ρ.[1] Given an arbitrary polynomial $p \in \mathcal{P}$, its *initial term* $\mathrm{in}_\prec p$ is defined as its largest term with respect to the order $\prec$; for a set $\mathcal{F} \subset \mathcal{P}$ of polynomials we define $\mathrm{in}_\prec \mathcal{F} = \{\mathrm{in}_\prec p \mid p \in \mathcal{F}\}$. If $\mathcal{F}$ is finite, we can assign to each $p \in \mathcal{F}$ a set of *multiplicative variables* $X_{L,\prec,\mathcal{F}}(p) \subset \{x_1, \dots, x_n\}$: let $\mathcal{N} = \{\mu \in \mathbb{N}^n \mid x^\mu = \mathrm{in}_\prec p \text{ for some } p \in \mathcal{F}\}$; if $\mathrm{in}_\prec p = x^\mu$, then $X_{L,\prec,\mathcal{F}}(p) = \{x_i \mid i \in N_{L,\mathcal{N}}(\mu)\}$.

Definition 6. Let $I \subset \mathcal{P}$ be an ideal. An *involutive basis* of the ideal I for the involutive division L and the term order $\prec$ is a finite subset

[1] In other words the order must be compatible with the monoid structure of $\mathbb{T}$.

$\mathcal{H} = \{p_1, \dots, p_r\} \subset I$ such that

$$I = \sum_{\alpha=1}^{r} \mathbb{K}[X_{L,\prec,\mathcal{H}}(p_\alpha)] \cdot p_\alpha \,. \tag{3}$$

(Note that we do not require that the sum is direct.) □

One should remark that in the algorithm of Fig. 2 the selection order $\prec_s$ is only needed for technical reasons and that – perhaps surprisingly – its choice does not affect the final result. In Def. 6 the term order $\prec$ plays as important a role as for Gröbner bases and different term orders will in general yield different bases. This is demonstrated by Theorem 8 below.

Definition 7. A polynomial $p \in \mathcal{P}$ is in *involutive normal form* with respect to a finite set $\mathcal{F} \subset \mathcal{P}$, an involutive division L and a term order $\prec$, if no term contained in p lies in the involutive span $\langle\, \mathrm{in}_\prec \mathcal{F}\,\rangle_L$, i.e. no term in p can be obtained by multiplying one of the initial terms in $\mathcal{F}$ by multiplicative variables only. The set $\mathcal{F}$ is *involutively autoreduced*, if each polynomial $p \in \mathcal{F}$ is in involutive normal form with respect to $\mathcal{F} \setminus \{p\}$. The involutive basis $\mathcal{H}$ is called *minimal*, if it is involutively autoreduced and if $\mathrm{in}_\prec \mathcal{H}$ is a minimal involutive basis of the monomial ideal $\mathrm{in}_\prec I$. □

These definitions are completely analogous to the corresponding ones in Gröbner theory. The only difference is that the standard divisibility relation of monomials is replaced by the involutive division L. So we can use exactly the same algorithms as usual to compute a normal form; in general, they will, however, perform less reduction steps due to the restricted divisibility. For minimal involutive bases the sum in (3) is direct and thus every element in I possesses a unique involutive normal form.

Theorem 8. *A minimal involutive basis of an ideal I with respect to an arbitrary involutive division L and a term order $\prec$ is a (in general non-reduced) Gröbner basis of I for the order $\prec$.*

One can extend the algorithm in Fig. 2 so that it determines an involutive basis for arbitrary ideals and not just for monomial ones. Essentially, we follow precisely the same strategy: we check what happens if we multiply an element of our basis by one of its non-multiplicative variables. The decision whether the result lies in the involutive span of the basis requires now an involutive normal form computation.

In pseudocode this yields the algorithm depicted in Fig. 3. It requires two subalgorithms to determine involutive normal forms and for involutive autoreductions; because of their simplicity and analogy with the classical case we omit their precise form. Due to the consequent use of involutive autoreduction our algorithm even returns a *minimal* involutive basis of the ideal generated by $\mathcal{H}$.

Algorithm: *Polynomial Completion*
Input: Finite subset $\mathcal{H} \subset \mathcal{P}$, involutive division L, term orders $\prec$, $\prec_s$
Output: Minimal involutive basis of the ideal $\langle \mathcal{H} \rangle$

/1/ $\mathcal{H} \leftarrow \mathtt{InvAutoReduce}_{L,\prec}(\mathcal{H})$
/2/ `repeat`
/3/ $\quad \mathcal{S} \leftarrow \{x \cdot p \mid p \in \mathcal{H},\ x \in \bar{X}_{L,\mathcal{H}}(p)\}$
/4/ $\quad$ `repeat`
/5/ $\qquad \bar{q} \leftarrow \min_{\prec_s} \mathcal{S}$
/6/ $\qquad \mathcal{S} \leftarrow \mathcal{S} \setminus \{\bar{q}\}$
/7/ $\qquad q \leftarrow \mathtt{InvNormalForm}_{L,\prec}(\bar{q}, \mathcal{H})$
/8/ $\quad$ `until` $(q \neq 0)$ `or` $(\mathcal{S} = \emptyset)$
/9/ $\quad$ `if` $q \neq 0$ `then` $\mathcal{H} \leftarrow \mathtt{InvAutoReduce}_{L,\prec}(\mathcal{H} \cup \{q\})$
/10/ $\quad$ `else return` $\mathcal{H}$ `end_if`
/11/ `until` $FALSE$

Fig. 3. Completion for polynomial ideals

Note that two different term orders appear. The selection order $\prec_s$ is only used to choose the element $\bar{q}$ in line /5/; it has no further significance and can be chosen completely independent of the term order $\prec$ used to define the initial terms of the polynomials and thus strongly influencing the output.

Because of Theorem 8, this algorithm may be used as an alternative to the one by Buchberger for computing Gröbner bases. Experiments seem to indicate that it is in fact highly competitive and often faster. A heuristic explanation of this observation could be that one may consider the algorithm in Fig. 3 as a special sort of "Hilbert driven" completion which is known to be very efficient.

It follows from the considerations in the last section that one can trivially determine the *Hilbert function* of an ideal I as soon as one has got a minimal involutive basis of it, as this corresponds to the computation of the function $H(q)$ counting the number of monomials of degree q contained in the ideal $\mathrm{in}_\prec I$ [7]. Any involutively autoreduced basis of I provides us with a "guess" of the true Hilbert function, more precisely with a guess that is always less than or equal to the right answer. We have finished as soon as the guess is the right Hilbert function and our algorithm does nothing else than to check in each iteration whether there still exist some monomials in $\mathrm{in}_\prec I$ that are not contained in the involutive span $\langle \mathrm{in}_\prec \mathcal{H} \rangle_L$ and thus not counted by our trial Hilbert function.

Example 9. We demonstrate the algorithm of Fig. 3 with the simple ideal $I = \langle x_1 + \underline{x_2}, \underline{x_1 x_2} - 1 \rangle$ (the solutions are cyclic 2-roots). We want to compute an involutive basis of it for the Janet division J (see Example 2) and the degree reverse lexicographic order; the initial terms for this order are always underlined.

We first determine the multiplicative variables of each polynomial: $X_{J,\mathrm{in}_\prec I}(x_1 + x_2) = \{x_2\}$ and $X_{J,\mathrm{in}_\prec I}(x_1 x_2 - 1) = \{x_1, x_2\}$. Thus in the first iteration of the algorithm only one non-multiplicative product must be studied: $x_1 \cdot (x_1 + x_2) = x_1^2 + \underline{x_1 x_2}$. One (unique) involutive reduction yields the involutive normal form $\underline{x_1^2} + 1$; this polynomial must be added to our basis.

In this special case the sets of multiplicative variables for the original two polynomials in the basis do not change; for the new generator we obtain $X_{J,\mathrm{in}_\prec I}(\underline{x_1^2} + 1) = \{x_1\}$. Thus there arises only one new non-multiplicative product: $x_2 \cdot (x_1^2 + 1) = \underline{x_1^2 x_2} + x_2$. However, it is easy to see that this polynomial can be reduced to zero with two involutive reductions and the algorithm terminates with the involutive basis $\mathcal{H} = \{x_1 + \underline{x_2}, \underline{x_1 x_2} - 1, \underline{x_1^2} + 1\}$.

For the Pommaret division the situation is even simpler. An involutive autoreduction leads to the generators $x_1 + \underline{x_2}$ and $\underline{x_1^2} + 1$ which form already an involutive basis, as the involutive normal form of the only arising non-multiplicative product $\underline{x_1^2 x_2} + x_2$ is zero. □

If we drop the linear polynomial in this example and consider only the ideal generated by $x_1 x_2 - 1$, then it does not possess a finite Pommaret basis, i.e. our algorithm does not terminate. In contrast, the Janet division is *Noetherian* which means that the algorithm terminates for any finite input set $\mathcal{H}$. The non-termination for the Pommaret division is due to the use of "bad" coordinates x_1, x_2; this is the so-called problem of *δ-regularity* [37]. One can show that for generic coordinates, the algorithm will always terminate but that for certain singular coordinate systems no finite Pommaret basis exists. In our case one may use for example the coordinates $y_1 = x_1 + x_2$ and $y_2 = x_1 - x_2$.

4 Involutive Systems of Differential Equations

One straightforward way to apply the results of Sects. 2 and 3 to differential equations is to consider the ring $\mathcal{D}$ of linear differential operators over some function field $\mathbb{F}$ (for example, $\mathbb{F} = \mathbb{R}(x_1, \dots, x_n)$, the field of rational functions in the variables $x_1, \dots, x_n$ with real coefficients). We identify in a natural way the set $\mathbb{D} = \{\partial^\mu = \partial_{x_1}^{\mu_1} \cdots \partial_{x_n}^{\mu_n} \mid \mu \in \mathbb{N}^n\}$ with $\mathbb{N}^n$ as an *Abelian*[2] monoid and need only a term order $\prec$ on $\mathbb{D}$ to define involutive bases analogously to the algebraic case. We can even use the algorithm in Fig. 3 for determining the bases. In fact, this approach is possible not only for linear differential operators but for any Ore algebra which includes e. g. linear difference operators, too [37].

More general systems of differential equations can be treated within the so-called *formal theory*. It employs a geometric framework based on jet bundles [31] to study differential equations in an intrinsic, i. e. coordinate independent way. It is beyond the scope of this article to give an in-depth introduction to this theory; for details we must refer to the literature [26,33].

Let X, U be two manifolds (or simply open subsets of $\mathbb{R}^n$ and $\mathbb{R}^m$) with coordinates x_i $(1 \leq i \leq n)$ and u_α $(1 \leq \alpha \leq m)$, respectively. A jet is a truncated Taylor series of a function $f : X \to U$; the q-th order jet bundle $\mathcal{J}_q(X, U)$ consists of all series truncated at order q. So coordinates of the q-jet of such a function f are $(x_i; u_\alpha; p_{\alpha,\mu})$ with multi indices $\mu \in \mathbb{N}^n$ of length $|\mu| \leq q$. Here $x \in X$ denotes the expansion point of the series, $u = f(x) \in U$ the value of the function f at this point and $p_{\alpha,\mu} = \partial^{|\mu|} f_\alpha / \partial x_1^{\mu_1} \cdots \partial x_n^{\mu_n}(x)$ the value of the derivative corresponding to the multi index μ of the function f at the point x.

A differential equation of order q can be defined geometrically as a (fibred) submanifold $\mathcal{R}_q \subset \mathcal{J}_q(X, U)$. Locally, it is represented as the zero set of some functions $\phi_\tau : \mathcal{J}_q(X, U) \to \mathbb{R}$ $(\tau = 1, \dots, p)$; thus

[2] Of course the ring of linear differential operators is non-commutative; but the "monomial" operators contained in $\mathbb{D}$ commute.

we recover the familiar description $\phi_\tau(x_i, u_\alpha, p_{\alpha,\mu}) = 0$. There exist now two natural geometric operations with a differential equation $\mathcal{R}_q$: *projection* and *prolongation*.

From the definition of a jet bundle it is obvious that we have natural projections $\pi^{q+r}_q : \mathcal{J}_{q+r}(X,U) \to \mathcal{J}_q(X,U)$ which just "forget" the higher order Taylor coefficients. The projections can be restricted to submanifolds; however, a description in local coordinates is not so easy, as it requires a generally nonlinear elimination of the derivatives of order higher than q from the functions ϕ_τ.

Prolongation corresponds to taking total derivatives. If $\mathcal{R}_q$ is locally given by the equations $\phi_\tau = 0$, we can define the differential equation $\mathcal{R}_{q+1} \subset \mathcal{J}_{q+1}(X,U)$ locally given by the equations $\phi_\tau = 0$ and $D_i\phi_\tau = 0$ (for all $1 \leq i \leq n$) with the total derivative

$$D_i\phi_\tau = \frac{\partial \phi_\tau}{\partial x_i} + \sum_{\alpha=1}^{m} \frac{\partial \phi_\tau}{\partial u_\alpha} p_{\alpha,1_i} + \sum_{\alpha=1}^{m} \sum_{|\mu|\leq q} \frac{\partial \phi_\tau}{\partial p_{\alpha,\mu}} p_{\alpha,\mu+1_i} \,. \tag{4}$$

One might expect that first prolonging r times a differential equation $\mathcal{R}_q$ to obtain $\mathcal{R}_{q+r} \subset \mathcal{J}_{q+r}(X,U)$ and then projecting it back to its original order will recover $\mathcal{R}_q$. However, in general this is not true; instead one will obtain a submanifold $\mathcal{R}^{(r)}_q = \pi^{q+r}_q(\mathcal{R}_{q+r}) \subseteq \mathcal{R}_q$. This is the geometric version of integrability conditions!

The existence of such conditions presents a serious obstacle for the algorithmic construction of formal power series solutions. Only if at no order of prolongation any integrability condition appears, it is straightforward to build formal solutions order by order.

Definition 10. The differential equation $\mathcal{R}_q$ is *formally integrable*, if for all integers $r \geq 0$ the equality $\mathcal{R}^{(1)}_{q+r} = \mathcal{R}_{q+r}$ holds. □

For ordinary differential equations this concept completely suffices to tackle all formal problems with general systems. For partial differential equations we encounter the question of how to check formal integrability, as the condition in Def. 10 is infinite. Here involution enters the scene. But in order to be able to apply the theory of Sect. 2 we need first to introduce an algebraic structure.

Definition 11. Let the differential equation $\mathcal{R}_q \subset \mathcal{J}_q(X,U)$ be locally given by the equations $\phi_\tau(x,u,p) = 0$. The *symbol* $\mathcal{M}_q$ of $\mathcal{R}_q$ is defined as the solution space of the homogeneous linear system of equations

$$\mathcal{M}_q : \left\{ \sum_{\alpha=1}^{n} \sum_{\mu=q} \frac{\partial \phi_\tau}{\partial p_{\alpha,\mu}} v_{\alpha,\mu} = 0 \; , \qquad \tau = 1, \dots, p \right. \tag{5}$$

in the unknowns $v_{\alpha,\mu}$ with $\alpha = 1, \dots, m$ and multi indices $\mu \in \mathbb{N}^n$ with $|\mu| = q$ (i. e. one unknown for each derivative $p_{\alpha,\mu}$ of maximal order). The matrix of the linear system (5) is called *symbol matrix*. □

This definition is most easily understood for linear differential equations. Here (5) corresponds to taking the principal part of the equations only, i. e. to discarding all lower order derivatives. For nonlinear equations we linearise by differentiating ϕ_τ.

Now we perform a combinatorial analysis of the symbol matrix along the lines of Sect. 2. A rigorous mathematical formulation would require too much overhead, so we give here a more intuitive description. The role of terms are played by the unknowns $v_{\alpha,\mu}$. We must consider not only the symbol $\mathcal{M}_q$ of $\mathcal{R}_q$ but in fact the symbols $\mathcal{M}_{q+r}$ of all prolonged differential equations $\mathcal{R}_{q+r}$. These are defined as the solution spaces of the linear systems

$$\mathcal{M}_{q+r} : \left\{ \sum_{\alpha=1}^{n} \sum_{\mu=q} \frac{\partial \phi_\tau}{\partial p_{\alpha,\mu}} v_{\alpha,\mu+\nu} = 0 \; , \qquad \tau = 1, \dots, p \; , \; |\nu| = r \; . \right. \tag{6}$$

Obviously, the matrices of these systems grow rapidly. We can produce a row of the matrix of the symbol $\mathcal{M}_{q+1}$ by prolonging a row of the matrix of the symbol $\mathcal{M}_q$ with respect to a variable x_i which means nothing else than replacing any unknown $v_{\alpha,\mu}$ by $v_{\alpha,\mu+1_i}$. Iteration of this construction yields (6).

Def. 6 of an involutive basis required a term order. We define the *class* of an unknown $v_{\alpha,\mu}$ as the smallest integer k such that $\mu_k > 0$. A term order $\prec$ such that $v_{\alpha,\mu} \prec v_{\beta,\nu}$ whenever the class of $v_{\alpha,\mu}$ is less than the class of $v_{\beta,\nu}$, is called *class respecting*.

Definition 12. The symbol $\mathcal{M}_q$ is called *involutive*, if the rows of its matrix (possibly after some elementary row operations) form an involutive basis of the set generated by all rows of all prolonged symbol matrices with respect to a class respecting term order and the Pommaret division (cf. Example 2). □

One can show that it suffices for checking involution of a symbol to compare the matrices of $\mathcal{M}_q$ and $\mathcal{M}_{q+1}$ (such a "locality property" is also the basis of the algorithms presented in Figs. 2 and 3). In practice one proceeds as follows. One takes (5) and transforms the system with some linear operations in a row echelon form; the unknowns must remained ordered according to a class respecting term order during this transformation. Then we define the class of a row in the system as the class k of its pivot (or initial term) and assign the multiplicative variables $x_1, \dots, x_k$. $\mathcal{M}_q$ is now involutive, if we obtain all equations defining $\mathcal{M}_{q+1}$ by prolonging each row only with respect to its multiplicative variables.

Definition 13. The differential equation $\mathcal{R}_q$ is *involutive*, if it is formally integrable and if its symbol $\mathcal{M}_q$ is involutive. □

At first sight we have not gained much, as we still have no finite criterion for formal integrability and so it seems to be impossible to check algorithmically whether or not $\mathcal{R}_q$ is involutive. But this is not true. The combinatorial properties of an involutive basis are so strong that we obtain the following *finite* criterion for involution.

Theorem 14. *The differential equation $\mathcal{R}_q$ is involutive, if and only its symbol $\mathcal{M}_q$ is involutive and if $\mathcal{R}_q^{(1)} = \mathcal{R}_q$.*

This criterion requires only a comparison of the differential equations $\mathcal{R}_q$ and $\mathcal{R}_{q+1}$ plus their symbols. To test whether or not a symbol is involutive requires only linear algebra. To check algorithmically whether $\mathcal{R}_q^{(1)} = \mathcal{R}_q$ depends on how the equations are defined. If the functions ϕ_τ are, for example, polynomial in their arguments, the equality can be effectively checked with Gröbner techniques.

The *Cartan-Kuranishi theorem* asserts that any differential equation $\mathcal{R}_q$ can be completed in a finite number of steps to an equivalent involutive one of the form $\mathcal{R}_{q+r}^{(s)}$. The proof of the theorem even provides a constructive method for the completion shown in Fig. 4.

Fig. 4 contains more a sketch of an algorithm than really an algorithm. It is a very high level description and for some steps, most notably the evaluation of the equality in line /5/, it is not so clear how they can be performed effectively for arbitrary systems. For linear or polynomial systems it is comparatively straightforward to turn the sketch into a real algorithm.

Algorithm: *Cartan-Kuranishi completion*
Input: differential equation $\mathcal{R}_q$
Output: involutive differential equation $\mathcal{R}^{(s)}_{q+r}$

$r \leftarrow 0,\ s \leftarrow 0$
`repeat`
  `while` $\mathcal{M}^{(s)}_{q+r}$ is not involutive `do`
    $r \leftarrow r + 1$
  $\mathit{involutive} \leftarrow \left(\mathcal{R}^{(s+1)}_{q+r} = \mathcal{R}^{(s)}_{q+r}\right)$
  `if not(`*involutive*`) then` $s \leftarrow s + 1$
`until` *involutive*

Fig. 4. Cartan-Kuranishi completion of differential equations

Example 15. As an example for the Cartan-Kuranishi completion we consider the incompressible Navier-Stokes equations. They are a second order system in the independent variables t, x, y, z and the dependent variables $p, \boldsymbol{u} = (u, v, w)$ and take in vector notation the form

$$\mathcal{R}_2 : \begin{cases} \boldsymbol{u}_t + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} - \Delta \boldsymbol{u} + \boldsymbol{\nabla} p = 0 \,, \\ \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0 \,. \end{cases} \tag{7}$$

Obviously, we are dealing here with equations of differing order, as the incompressibility condition is only first order. The Navier-Stokes equations are in so far a simple example, as in every iteration of the outer loop we get an equation with involutive symbol, so that we can ignore the inner loop.

The first iteration leads to the equation $\mathcal{R}^{(1)}_2$ which is made up of all equations in (7) plus all prolongations of the first order equation, i. e. four additional equations. These represent in a certain sense trivial integrability conditions. In the next iteration we encounter a true integrability condition. Taking the divergence of the first (vector) equation in (7) yields a third order equation. Since $\boldsymbol{\nabla} \cdot \Delta \boldsymbol{u} = \Delta \boldsymbol{\nabla} \cdot \boldsymbol{u}$, the third order terms can be eliminated using the prolongations of the trivial integrability conditions of the last iteration. The term $\boldsymbol{\nabla} \cdot \boldsymbol{u}_t$ also vanishes as a consequence of these equations and we obtain the integrability condition

$$\Delta p + \boldsymbol{\nabla} \cdot (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = 0 \,. \tag{8}$$

A careful calculation shows that this is in fact the only arising new equation which must be added in order to obtain the involutive equation $\mathcal{R}_2^{(2)}$. □

5 Some Applications

The theory presented in the previous sections might appear rather abstract and difficult. However, simplified versions of it have been rediscovered many times in different fields of science. So actually the concepts seem to be rather natural. In this article we will briefly discuss only two applications concerning differential equations, namely *mechanical systems with constraints* [35,39] and the numerical analysis of *differential algebraic equations* [36,38]. For the algebraic side we recall that involutive bases are also Gröbner bases for which many important applications exists. Some further results specific to involutive bases can be found in [37].

Constrained dynamics is of central importance in physics and most engineering disciplines. The modeling of many systems leads to the appearance of constraints with the effect that the equations of motion (or field equations in the infinite-dimensional case) are no longer normal: in the case of ordinary differential equations some of the equations of motion might be algebraic; in the case of partial differential equations the field equations are no longer in Cauchy-Kowalevsky form. This in turn implies the possible existence of hidden constraints, namely integrability conditions.

In the literature, one can find many so-called constraint algorithms determining all these hidden constraints. In our language this is nothing else than a completion to involution. However, most algorithms found in the literature apply only to ordinary differential equations. This is easy to understand: for partial differential equations one needs the full theory developed in the previous sections; for ordinary differential equations the theory simplifies drastically.

The symbol of an ordinary differential equation is always involutive, as there exists only one independent variable. Thus we can skip the inner loop of the algorithm in Fig. 4. The outer loop can be brought into a simpler and more efficient version. This is due to the fact that for ordinary differential equations integrability conditions can only arise from the prolongation of lower order equations.

Instead of prolonging first and then projecting back, it is more efficient to reverse the order of operations and project first. This corresponds to effectively determining all lower order equations. Then these are prolonged and it must be checked whether the prolonged equations reduce to zero modulo the original equations. If not, an integrability condition has been found.

Example 16. As a simple example we consider (in Cartesian coordinates) a planar pendulum in a homogeneous gravitational field. It can be described by the Lagrangian

$$L(x, y, \dot{x}, \dot{y}) = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - mgy \tag{9}$$

for a free particle moving in the gravitational field plus the externally imposed constraint $\phi(x, y) = \frac{1}{2}(x^2 + y^2 - l^2) = 0$. Here m is the mass of the pendulum bob, g the gravitational acceleration and l the length of the pendulum.

Constrained variation yields the following Euler-Lagrange equations containing a Lagrangian multiplier λ (which can be interpreted as the amplitude of the constraint force needed to keep the pendulum bob on its circle)

$$\ddot{x} = \lambda x\,, \quad \ddot{y} = \lambda y - mg\,, \quad \frac{1}{2}(x^2 + y^2 - l^2) = 0\,. \tag{10}$$

This represents a differential equation $\mathcal{R}_2 \subset \mathcal{J}_2(X, U)$ where X is one-dimensional with the coordinate t and U is three-dimensional with coordinates x, y, λ. $\mathcal{R}_2$ is obviously not normal, as it contains equations of different orders, and we will now complete it to involution.

Projection yields an equation $\mathcal{R}_1^{(1)}$ defined by the last equation in (10). Prolonging it produces the new equation $x\dot{x} + y\dot{y} = 0$; thus $\mathcal{R}_2^{(1)}$ is made up of the original three equations plus this one. In the next projection-prolongation cycle we must do some eliminations: we obtain first $x\ddot{x} + y\ddot{y} + \dot{x}^2 + \dot{y}^2 = 0$, but the second order derivatives can be eliminated using (10): $\dot{x}^2 + \dot{y}^2 + \lambda(x^2 + y^2) - mgy = 0$. Adding this equation to $\mathcal{R}_2^{(1)}$ yields $\mathcal{R}_2^{(2)}$. One further such cycle shows that we have still not finished but that we must add $(x^2+y^2)(\dot{\lambda}+2\lambda) - mg(\dot{y}+2y) = 0$ to obtain finally the involutive equation $\mathcal{R}_2^{(3)}$. □

A practical implementation of similar ideas for the Dirac theory of constrained Hamiltonian system using Gröbner bases was presented in [10]. It should however be noted that there the differential completion is *not* done using involutive techniques; for this reason only finite-dimensional systems can be treated. The Gröbner bases are applied for deciding whether or not the prolonged equations can be reduced to zero. A full discussion of the Dirac theory in the context of involution can be found in [35,39].

Constrained mechanical systems are typical examples of what in numerical analysis is nowadays often called *differential algebraic equations* [3]: systems of ordinary differential equations of differing order. In applications one deals typically with first order equations and the lower order ones are then algebraic. From the involutive point of view this is just a slight generalisation of the situation above in that we make now no special assumptions about the form of the differential equations we treat.

A fundamental concept in the theory of differential algebraic equations is given by the *index*. It is used as a measure for the difficulties one has to expect in the numerical integration. In the literature one can find a large number of different indices; for an overview we refer to [5]. The so-called differentiation indices are closely related to the completion to involution. Basically they just count the number of prolongations needed for the completion [35,36].

The articles [27,28] present an intrinsic geometric approach to the differentiation index. They use the language of tangent bundles, whereas the formal theory is formulated in terms of jet bundles. But the translation of one formalism into the other one is trivial using the contact structure of jet bundles. It should, however, be noted that the theory presented in [27,28] applies only to ordinary differential equations, as it ignores the symbol and only considers formal integrability. We have seen above that a finite criterion for partial differential equations requires involution of the symbol.

In contrast, the approach presented in [36] based on the formal theory can be applied to arbitrary systems of partial differential equations. In fact, this work contains the first general definition of a differentiation index for partial differential equations that does not require either a semidiscretisation or an integral transform. Previous attempts to define indices in this general situation always relayed on a reduction to a differential algebraic equation and the result depended on the precise way the reduction was performed.

Example 17. We take again the incompressible Navier-Stokes equations of Example 15. We have seen above that the Cartan-Kuranishi completion needs two prolongations to obtain an involutive system. So we define the *involution index* of the incompressible Navier-Stokes equations as 2. According to a conjecture made in [38] this implies that any semidiscretisation of them will lead to a differential algebraic equation with an index of at least 2. For this special example this was in fact proven in [40]. □

6 Conclusions

Involution is unfortunately still a rather unknown concept despite its fundamental importance. For algebraic equations it provides not only an interesting alternative to Buchberger's algorithm for the construction of Gröbner bases, there also some applications like the determination of the Hilbert function or the syzygy theory where involutive bases seem to be clearly superior to classical Gröbner bases.

In the case of differential equations, most books and articles concentrate either on scalar equations or on normal systems satisfying the conditions of the Cauchy-Kowalevsky theorem. But there exist many important systems which are not normal; most notable examples are the Maxwell equations of electrodynamics or the incompressible Navier-Stokes equations in fluid dynamics. Similarly, many problems in differential geometry or control theory are described by overdetermined systems. Within computer algebra the main source of such systems are the determining systems in Lie symmetry theory [2,25].

Most application problems are not solved by a completion to involution; *but* such a completion will make the solution of most problems considerably easier. This is well-known in Commutative Algebra: once a Gröbner basis has been computed for a given ideal, most operations with the ideal are fairly straightforward. The concept of involution allows to extend this idea to differential equations.

An important aspect for concrete applications is the existence of reliable *implementations*. An Axiom implementation of the geometric completion theory of differential equations was presented in [32,34]. It was based on a direct translation of the algorithm in Fig. 4 and thus rather inefficient; it is no longer maintained.

Recently, we have developed within *MuPAD* [8,24] an object oriented environment for differential equations [14] that allows for an easy implementation of sophisticated application packages. Among the first applications is besides a Lie symmetry package [16] a completion package for linear and polynomial differential equations [15]. While also implementing the geometric theory, it is based on a new hybrid completion algorithm [13,17] that combines the algorithms of Figs. 3 and

4 into one efficient realisation of the Cartan-Kuranishi completion. All these packages and programs will be part of the next release 2.0 of *MuPAD*[3] due later this year.

Several implementations of involutive techniques are currently under way by different groups. Some results have been presented in [11,29]. Within the context of Lie symmetry there also exist a number of completion packages for differential equations on the basis of various mathematical theories. Some are mentioned in the review articles [18,19].

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