# ON THE NUMERICAL SOLUTION OF INVOLUTIVE ORDINARY DIFFERENTIAL SYSTEMS

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Abstract. We propose a method for solving numerically ordinary differential systems. The system is considered geometrically as a submanifold in a jet space. The solutions are then certain integral manifolds which can be computed numerically, when the system has been transformed into involutive form.

## 1. Introduction

1.1. **Historical background.** We shall present a new approach to the computation of solutions of ordinary differential systems which is based on jet space techniques. The jets were introduced in the beginning of 50's by Ehresmann [15]. In spite of the fact that jets are already quite old, they have apparently remained outside the mainstream in differential geometry. Indeed, Spivak only mentions jets briefly in the final remarks of his five volume treatise under the heading 'miscellaneous', [51, vol. 5, p. 602]. However, he says (this was written in 1979) that jets

> ...are natural structures to consider in differential geometry, but they are only just beginning to be used in any serious way.

In recent years there has appeared (at least) two monographs on jet geometry [25], [48] and in the introduction to the former it is also argued that the jet theory is quite natural as well as fundamental in differential geometry. Be that as it may, the jet geometry found almost immediately two important applications outside the differential geometry properly speaking, namely the singularity theory and the theory of systems of partial differential equations. Thom used jets in the analysis and classification of singularities of differentiable maps [53], and this remains an active area of research even now [5].

We are interested in the other application. Now the study of rather general systems of PDEs is more than 100 years old. Riquier and Janet studied them from algebraic point of view [46], [22] and although their works were forgotten for some time, they influenced Ritt when he created the differential algebra [47]. There has been a renewed interest in these older works in recent years because of their connections to the Gröbner basis techniques. The geometric point of view was provided by Élie Cartan who formulated the problems in terms of differential forms [10], and his work was extended by Kähler [23].

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Then in the 50's and 60's Spencer, Kuranishi, Sternberg, Goldschmidt, Quillen and others studied arbitrary systems of PDEs using jet spaces, extending the above mentioned classical results [50], [29], [16]. We shall try to explain some of these developments below, in particular the notion of the involutivity (or formal integrability) which is important from the point of view of applications.

Apparently these results did not become well-known to a larger audience because Vinogradov remarks [59] (this is from his review of [38], written in 1981):

> Unfortunately, all these achievements have until now remained on the pages of difficult-to-read periodical literature (including the book of Spencer and Kumpera [28], which is also difficult to read) and in fact remained inaccessible to those for whom they were written, namely, for specialists in differential equations.

Nowadays on jets and PDEs there are already quite a few monographs [27], [38], [39], [40], [41], [52], see also surveys [14], [1], [50] and the collection of articles [31]. Also jets are used (among other techniques) in the analysis of the symmetries of differential equations [36] and in the problems of nonholonomic dynamical systems [57]. However, none of these works make an easy reading and require at least some background in differential geometry.

Now happily, though not unexpectedly, a lot of the complications disappear in the ODE case, so we do not have to introduce the whole framework in full generality below. In spite of that we need quite many notions from the differential geometry so this article cannot possibly be self-contained in this sense and we must refer to [51], [13] and [48] for more details and explanations on these basic matters. However, in section 2 we have tried to explain some basic ideas with minimum of technical details in order to motivate the introduction of the heavier machinery which is needed later on.

1.2. **Comparison to related work.** The main motivation of this article came from the theory of differential algebraic equations, but as the reader has remarked, this term does not appear in the title, and in fact we shall not need this concept at all. The reason is simple: from our point of view there is no difference between ODEs and DAEs. Hence we shall usually use the term differential system to remind the reader that this covers all the cases. Perhaps this sounds a bit surprising since in the traditional approach to DAEs it is always stressed that the ODEs and DAEs are basically different, see the well-known books [9], [18], [17] and the survey article [32], where extensive references to litterature are given. Intuitively, this (apparent) paradox can be explained as follows. From the jet point of view the differential systems are certain submanifolds of the jet space, and consequently one can speak of differential systems without actually writing down any particular equation. One might then say that the classical distinction of ODEs and DAEs is related to the representation of objects rather than to the objects themselves.

Since ODEs and DAEs are not distinguished, it is only natural that the notion of index is not needed either, see the above references for a discussion of this concept. In particular, the index is not related to any numerical difficulty of the problem when using our approach in the numerical solution. In a way, the index cannot even be defined in our context; we shall discuss briefly these matters at an appropriate place.

Let us further mention two interesting consequences of our point of view. The first one is that explicit methods can be used to solve general differential systems. In other words there is no intrinsic connection between DAEs and stiff systems. The second is that since the definition of the solution is not the usual one, some problems that are singular from traditional point of view become regular, hence easily computable, in our framework. This aspect is discussed in detail in [55], [56], so below we shall merely see some examples of this phenomenon.

In traditional methods one sometimes also talks about manifolds and projections to manifolds. Since both words are often used in the sequel, let us note that the manifolds in question are not the same as discussed below, nor are the projections the same.

Rabier, Rheinboldt and Reich have also studied DAEs from the differential geometric point of view, using the tangent bundle instead of jet spaces, [45], [42], [43], [44]. Some theorems and computations are seen to be (equivalent to) special cases of the more general results of Goldschmidt [16], see [26] for details.

Recently there has been quite much interest in applying geometric ideas to the numerical solution of differential systems. Iserles [19], [20] discusses in general how qualitative features of the solutions should be taken into account when designing numerical methods. For example nowadays Hamiltonian problems are usually treated with symplectic methods which preserve the underlying symplectic structure of the problem, see [49]. Also there are many papers dealing with flows on Lie groups and in general using Lie groups and Lie algebras in numerical methods. Since these works are not directly related to the present one (except for the fact that differential geometric ideas play an essential role in both cases), we will simply refer to following articles for further details, [11], [21], [33], [34], [35], [61], [62].

1.3. **Outline of the article.** In section 2 some motivating examples are given. By restricting the attention to simple equations, it is possible to explain some basic ideas relying on the geometrical intuition of the three dimensional space. In section 3 the jets are introduced and the important concept of involutivity is discussed. In section 4 there are some computations illustrating the notions introduced in previous sections. We also show that for quite a large class of systems, mechanical systems with holonomic constraints, it is possible to simplify the computations considerably by treating the Lagrange multiplier differently than other variables. Of course probably in all codes the multipliers receive special treatment, but because our formulation is not equivalent to traditional formulations, the role of multipliers is also different here.

In section 5 we first recall some notions of Riemannian geometry which are needed in the analysis of the local error. Then we formulate 3 different one step methods: explicit Euler, implicit Euler and midpoint rule. The analysis shows that the orders of these methods in our context are the same as their classical orders. In section 6 the actual numerical implementation is presented. It is seen that the subproblems arising in our algorithm can be treated with fairly standard techniques. In section 7 the numerical examples are given. We have chosen some representative problems which have appeared frequently in the litterature. Our methods work reliably, and the results show in particular that one can use explicit methods for these kind of problems, although in the litterature only implicit methods are considered. We conclude with section 8 where some directions of future work is indicated.

Essential parts of this article are based on reports [54], [7]. That jet spaces are useful for analysing differential-algebraic equations was first suggested in [58] and [37] (independently).

## 2. Differential equation as a surface

Let us start by explaining the basic ideas in a simple setting where we can visualize the situation in three dimensional space before formulating the general framework. Similar situation is considered in [4] and [12] where the emphasis is on the analysis of singularities. We will also say a few words about singularities in the examples, but do not insist on this aspect of the problem. While discussing the examples we also introduce some standard concepts of differential geometry. All maps and manifolds are assumed to be smooth, i.e. infinitely differentiable.

2.1. **Basic machinery.** Let us consider a single first order differential equation

$$f(x, y, y_1) = 0 \tag{2.1}$$

where $f$ is a smooth function and $y_1$ is the derivative of $y$.[1] Now forgetting for the moment about derivatives we can interprete $(x, y, y_1)$ as coordinates of $\mathbb{R}^3$. Hence the zero set of (2.1) is a subset of $\mathbb{R}^3$, denoted by $\mathcal{R}_1 = f^{-1}(0) \subset \mathbb{R}^3$. If zero is a regular value of $f$, i.e. if the gradient of $f$ never vanishes on $\mathcal{R}_1$, then $\mathcal{R}_1$ is a smooth two-dimensional manifold.

Now what are the solutions of (2.1)? Classically the solutions are defined as (smooth) curves $c : \mathbb{R} \to \mathbb{R}$ such that (2.1) is identically satisfied. Here we shall take another, more geometrical as well as more general, point of view. Having defined $\mathcal{R}_1$ one could perhaps consider defining solutions as certain curves $c : \mathbb{R} \to \mathcal{R}_1$. However, it is only the image of the curve which is important, the parametrization of it is irrelevant. Hence the solutions should be defined directly as certain one-dimensional submanifolds of $\mathcal{R}_1$ without any reference to parametrizations. So let $S$ be a smooth one-dimensional submanifold of $\mathcal{R}_1$. When would it be meaningful to say that $S$ is a solution of (2.1)?

To proceed let us introduce some terminology. If $p \in \mathcal{R}_1$, the tangent plane of $\mathcal{R}_1$ at $p$ is denoted by $(T\mathcal{R}_1)_p$. Similarly $TS_p$ is the line tangent to $S$ at $p$, and it is evident that $TS_p \subset (T\mathcal{R}_1)_p$. Our next task is to add to this framework some extra structure in such a way that we can say that $\mathcal{R}_1$ is a differential equation. Consider $\mathbb{R}^3$ with coordinates $(x, y, y_1)$; if $y_1$ is really the derivative of $y$ with respect to $x$, then in infinitesimal notation we should have $dy - y_1 dx = 0$. To make sense of this we must define what is meant by $dy$ and $dx$. In Spivak's words [51, vol. 1, p. 153] symbols like $dx$

> ...metamorphosed into functions, and it became clear that they must be distinguished from tangent vectors. Once this realization came, it was only a matter of making new definitions, which preserved the old notation, and waiting for everybody to catch up.

So $dx$, $dy$ and $dy_1$ are linear functions on the tangent space $(T\mathbb{R}^3)_p$, hence elements of the dual space of $(T\mathbb{R}^3)_p$. This dual space is called the cotangent space and denoted by $(T^*\mathbb{R}^3)_p$. Let us then define $\alpha = dy - y_1 dx$; at each point of $\mathbb{R}^3$, $\alpha$ is then a linear function on $(T\mathbb{R}^3)_p$. Now we can define a subspace of $(T\mathbb{R}^3)_p$ as follows

$$\mathcal{C}_p = \left\{ v \in (T\mathbb{R}^3)_p \,|\, \alpha(v) = 0 \right\}$$

All these $\mathcal{C}_p$'s together is called a *contact distribution*, denoted by $\mathcal{C}$. In general let us define:

[1] Later $y_1$ is called a jet coordinate.

**Definition 2.1.** *A* distribution *on a manifold $M$ is a map which to each point of $p \in M$ associates a certain subspace of the tangent space $TM_p$.*

In the present case $\mathcal{C}$ is then a two-dimensional distribution on $\mathbb{R}^3$. One may think of distributions as generalisations of vector fields. Now a vector field may be interpreted as a differential equation, and hence the integral curves of the vector field are said to be solutions of the corresponding differential equation. A generalisation of this idea leads to the notion of an integral manifold.

**Definition 2.2.** *Let $S$ be a submanifold of $M$ and $\mathcal{D}$ a distribution on $M$. $S$ is an* integral manifold *of $\mathcal{D}$ if $TS_p = \mathcal{D}_p$ at each $p \in S$.*[2]

Let us go back to our differential equation (2.1). Since $(T\mathcal{R}_1)_p$ can also be interpreted as a subspace of $(T\mathbb{R}^3)_p$, we can define an intersection $\mathcal{D}_p = (T\mathcal{R}_1)_p \cap \mathcal{C}_p$. Hence $\mathcal{D}$ is in general one-dimensional. Of course at some points tangent and contact planes may coincide; we will discuss this event and its consequences in the examples below. Ignoring these exceptional points for the moment leads to

**Definition 2.3.** *Solutions of* (2.1) *are integral manifolds of $\mathcal{D}$.*[3]

Since one-dimensional distributions always have integral manifolds, see [51, vol. 1, p. 245], we get

**Theorem 2.1.** *Given $p \in \mathcal{R}_1$ such that $\mathcal{D}$ is one-dimensional in a neighborhood of $p$, there exists a solution $S$ of* (2.1) *such that $p \in S$.*

Note that this kind of existence theorem is not valid for many dimensional distributions. For example it is readily checked that the contact distribution does not admit any integral manifolds, even locally. Incidentally, this implies that tangent and contact planes cannot coincide in an open set of $\mathcal{R}_1$. Since we are interested only in one-dimensional distributions, i.e. ordinary differential equations, we will not consider these matters further and refer to [51, vol. 1, chapter 6] for more information.

2.2. **Comparison to classical solutions.** Consider again the problem (2.1) and let $p \in \mathcal{R}_1$ be a regular point, i.e. $\partial f/\partial y_1 \neq 0$ at $p$. Then by the implicit function theorem there is a map $\varphi : \mathbb{R}^2 \to \mathbb{R}$ such that in a neighborhood of $p$, $\mathcal{R}_1$ can be represented by the equation $y_1 + \varphi(x, y) = 0$. The solutions of this equation can be defined in the usual way and one thinks of them either as curves $\mathbb{R} \to \mathbb{R}$ or as (one-dimensional) submanifolds of $\mathbb{R}^2$. Let us take the latter point of view. Let us define a projection $\pi : \mathbb{R}^3 \to \mathbb{R}^2$ by $(x, y, y_1) \mapsto (x, y)$ and let $S$ be a solution of (2.1) in the sense of Definition 2.3. Now if $p \in S$ is regular, then one can show that $\pi(S)$ is the classical solution in some neighborhood of $\pi(p)$.

Hence around regular points there is bijective correspondence between solutions in the sense of Definition 2.3 and classical solutions. However, because the implicit function theorem is not constructive, the reduction to the standard form is not in general possible in practice. Note also that Definition 2.3 provides more smooth solutions than the classical setting since tangent and contact planes need not (and in general do not) coincide even if $\partial f/\partial y_1 = 0$. We shall see shortly examples of this phenomenon.

[2]Sometimes another terminology is used, for example in [12]. If $\mathcal{D}$ has constant dimension on $M$, then it determines a foliation of $M$ and each integral manifold is called a leaf of this foliation.

[3]In [12] this way of defining solutions is called 'méthode de Lie'.

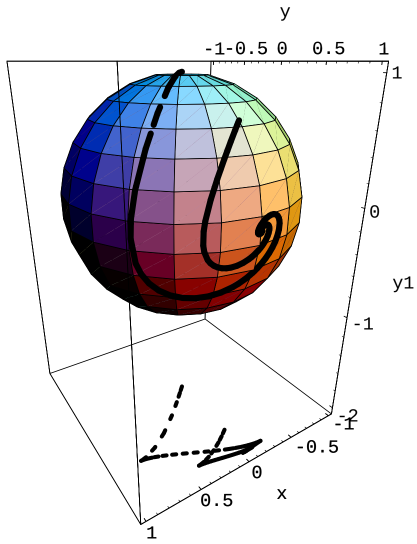



FIGURE 2.1. Some solution curves of the equation (2.2) and their projections.

**Remark 2.1.** This property of having more smooth solutions than in the classical case is quite interesting from the numerical point of view. Indeed, it is possible to use general methods for a larger class of problems than the classical framework allows.

## 2.3. Examples.

2.3.1. *Sphere.* Consider the problem

$$f(x, y, y_1) = (y_1)^2 + y^2 + x^2 - 1 = 0 \tag{2.2}$$

Hence $\mathcal{R}_1 = f^{-1}(0)$ is the unit sphere and at each point $p \in \mathcal{R}_1$, $\mathcal{D}_p$ is given by the nullspace of

$$A = \begin{pmatrix} -y_1 & 1 & 0 \\ x & y & y_1 \end{pmatrix}$$

One observes that $\dim(N(A)) = 1$, except at $(0, \pm 1, 0)$. So only at these two points tangent and contact planes coincide; in the classical sense all the points of the equator are singular. In figure 2.1 there are some solutions as well as their projections. When the solution crosses the equator, there is a cusp in the projected solution, which in convenient coordinates can be represented by the equation $u^2 = v^3$. The singularities at exceptional points $(0, \pm 1, 0)$ are called folded focuses [6, p. 34].

2.3.2. *Asymptotic curves.* Let us consider the following problem of classical differential geometry. Let $N \subset \mathbb{R}^3$ be a surface defined by the equation

$$\tfrac{1}{4}\left(x^4 + y^4\right) - 3xy - z = 0 \tag{2.3}$$

We want to compute some asymptotic curves on this surface. There are several characterizations of these curves, see [51, vol. 3] or any book on classical differential geometry. The one which is convenient for our purposes is the following: the tangent of an asymptotic curve makes the second fundamental form vanish. Asymptotic curves exist only in those parts of the surface where Gaussian curvature is negative or zero, in the

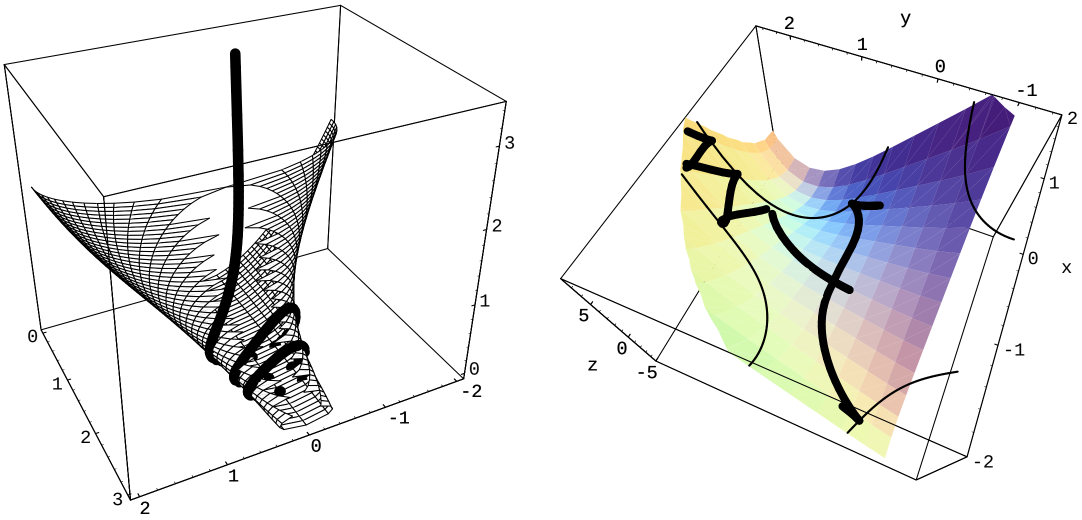



FIGURE 2.2. A solution of equation (2.4) (left) and some asymptotic curves on surface (2.3) (right). Thin lines are the sets of parabolic points.

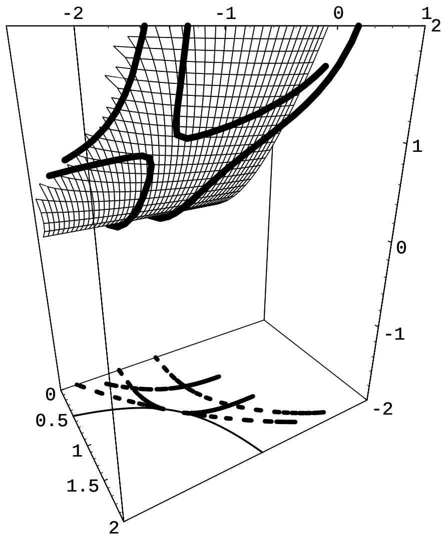


FIGURE 2.3. Some solution curves of the equation (2.4) and their projections.

present case in the region where $x^2y^2 \leq 1$. The curves can be computed by solving the differential equation

$$f(x, y, y_1) = y^2(y_1)^2 - 2y_1 + x^2 = 0 \tag{2.4}$$

The distribution is everywhere one-dimensional on $\mathcal{R}_1 = f^{-1}(0)$, except at $(1, -1, 1)$ and $(-1, 1, 1)$. Now the problem can be solved by computing the solution in $\mathcal{R}_1$, projecting it to $\mathbb{R}^2$ and finally lifting it to $N$. Note that the solutions (2.4) are smooth in the sense of Definition 2.3, although the corresponding asymptotic curves on surface $N$ have familiar cusps at $x^2y^2 = 1$, see figure 2.2. The singularities at exceptional points $(1, -1, 1)$ and $(-1, 1, 1)$ are called folded saddles, see [6, p. 34] and figure 2.3 where there are some solutions and their projections around $(1, -1, 1)$.

2.3.3. *Distributions and their singularities.* Distributions are perhaps less intuitive and less familiar objects than vector fields, so let us see an example where distributions come directly from the problem. In fact the previous example is such a case. The condition defining the asymptotic directions clearly defines a subspace of the tangent space, hence a distribution. In this way we arrived directly at distributions without passing by differential equations. In the previous example we have not used this distribution. Also the condition defining the lines of curvature of a surface leads directly to distributions. In this case the distribution is determined by the eigenspaces of the differential of the Gauss map.

Let us then show that singularities of distributions are more general than singularities, i.e. zeros, of vector fields. Consider any smooth surface $N \subset \mathbb{R}^3$ and let us suppose that distribution $\mathcal{D}$ is one-dimensional except at some isolated points which are called singular points of $\mathcal{D}$. Recall that around a regular point $p$ there is a vector field $V$ such that $0 \neq V_a \in \mathcal{D}_a$ for all $a$ in some neighborhood of $p$ and conversely every such $V$ spans a certain distribution. However, around a singular point such a vector field may not exist. Let us see an example of this phenomenon. Consider the problem

$$f(x, y, y_1) = x(y_1)^2 - 2yy_1 - x = 0 \tag{2.5}$$

It is easily checked that this is a regular problem, and in fact the classical solutions are seen to be a family of parabolas, see figure 2.4 Now clearly there is no vector field in the neighborhood of the origin whose integral curves were the parabolas. Incidentally, the pattern of parabolas is the same as the pattern of the lines of curvature around an umbilic on an ellipsoid, see [51, vol. 3, p. 288]. In other words the index of the singularity is the same, namely 1/2 in both cases, see [51, vol. 3, p. 324]. Note also that if one transforms the above problem into a classical problem using square roots, the correct solution is obtained only if one jumps from one branch of the square root to the other when crossing $x = 0$.

## 3. Differential systems and jet bundles

Lychagin describes the importance of jets in the analysis of differential equations as follows [31, p. ix].

> Thus, whereas connection between linear differential equations and differential geometry were few and far between, as were the connections between analytic geometry (in the elementary sense of the term) and geometry in the sense of Felix Klein, in contrast the theory of nonlinear differential equations is clearly a geometric theory, based on the special geometry of jet spaces.

Hence to proceed we must introduce more ideas from differential geometry and in particular jets. For more details on jet geometry we refer to [48]. In all that follows various maps are required to be defined only in some convenient open set of the relevant manifold. For notational simplicity this set is not indicated.

### 3.1. Jet bundles.

Let us consider two maps $y, z : \mathbb{R}^s \to \mathbb{R}^n$, let $\nu \in \mathbb{N}^s$ be a multi-index and $|\nu| = \nu_1 + \cdots + \nu_s$.

**Definition 3.1.** *The maps $y$ and $z$ are $q$–equivalent at $x$, if*

$$\frac{\partial^{|\nu|} y}{\partial x^\nu}(x) = \frac{\partial^{|\nu|} z}{\partial x^\nu}(x)$$

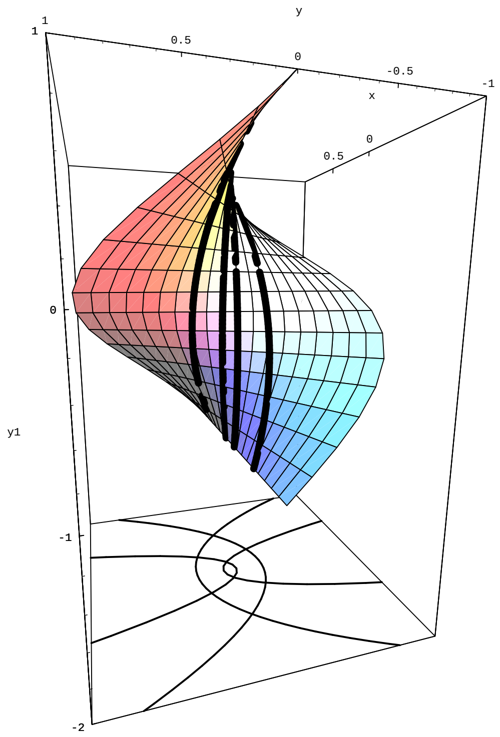



FIGURE 2.4. Some solution curves of the equation (2.5) and their projections.

*for all* $0 \leq |\nu| \leq q$.

The equivalence thus defined is clearly an equivalence relation so we can further define

**Definition 3.2.** *The $q$–jet of $y$ at $x$, denoted by $j^q_x(y)$, is the equivalence class of the above equivalence relation. The $q$–jet of $y$, denoted by $j^q(y)$, is the map $x \mapsto j^q_x(y)$.*

Intuitively the $q$–jet of $y$ at $x$ is its Taylor expansion up to order $q$. Since all these considerations are local, the previous definitions make also sense when $\mathbb{R}^s$ and $\mathbb{R}^n$ are replaced by manifolds. However, in the jet theory one usually prefers to talk about sections rather than maps. So let us introduce

**Definition 3.3.** *A* fibered manifold *is a triple $(\mathcal{E}, \pi, \mathcal{B})$ where $\mathcal{E}$ and $\mathcal{B}$ are manifolds and $\pi : \mathcal{E} \to \mathcal{B}$ is a surjective submersion. $\mathcal{E}$ is called the* total space*, $\mathcal{B}$ the* base space *and $\pi$ the* projection*. For each $p \in \mathcal{B}$, the set $\pi^{-1}(p)$ is called the* fiber *over $p$.*

We adopt the terminology used in [48]. Note that for example in [41] a fibered manifold is defined to be what we shall call a bundle.

**Definition 3.4.** *A fibered manifold is a* bundle*, if every fiber is diffeomorphic to each other.*

We shall usually refer to a bundle by the total space, although this might be confusing in some situations; indeed in jet theory there are frequently situations where the same total space is considered with different base spaces and projections. However, in our context this kind of confusion is not likely to occur.

**Definition 3.5.** *A* section *of a fibered manifold* $(\mathcal{E}, \pi, \mathcal{B})$ *is a map* $y : \mathcal{B} \to \mathcal{E}$ *such that* $\pi \circ y = \text{identity}$. *The set of all sections of* $\mathcal{E}$ *is denoted by* $\Gamma(\mathcal{E})$.

Note that if $\mathcal{E} = \mathcal{B} \times \mathcal{F}$, then a section of $\mathcal{E}$ is simply the graph of a map $\mathcal{B} \to \mathcal{F}$. A bundle need not be a cartesian product globally; however, for any $p \in \mathcal{B}$, there is a neighborhood $U \subset \mathcal{B}$ such that $\pi^{-1}(U) \simeq U \times \mathcal{F}$. Hence working with bundles and sections is a little more general than working with cartesian products and maps. In local coordinates one may then define jets for sections in the same way as above for maps. Putting all the local information together gives

**Definition 3.6.** *Let* $(\mathcal{E}, \pi, \mathcal{B})$ *be a bundle. The set of all q-jets of its sections is a bundle* $(J_q(\mathcal{E}), \pi^q, \mathcal{B})$, *the q'th jet bundle of* $(\mathcal{E}, \pi, \mathcal{B})$.

For example if $\mathcal{E} = \mathbb{R} \times \mathbb{R}$, then $\mathbb{R}^3$ in the previous section is denoted by $J_1(\mathcal{E})$. If $y$ is a section of $\mathcal{E}$, then $j^1(y)$ is a section of $J_1(\mathcal{E})$ defined by $x \mapsto (x, y(x), y'(x))$. Note that not every section of $J_1(\mathcal{E})$ is a 1-jet of a section of $\mathcal{E}$. We are now ready to define a differential equation.

**Definition 3.7.** *Let* $\mathcal{E}$ *be a bundle. A (partial)* differential system *(or equation) of order* $q$ *on* $\mathcal{E}$ *is a subbundle* $\mathcal{R}_q$ *of* $J_q(\mathcal{E})$.

Requiring that $\mathcal{R}_q$ is a bundle is rather excessive in practice; in the problems we have in mind it is enough that $\mathcal{R}_q$ is a submanifold. The present definition, however, is convenient for the general discussion in the next subsection. This formulation also allows the definition of the solutions in a natural way.

**Definition 3.8.** *Let* $\mathcal{R}_q \subset J_q(\mathcal{E})$ *be a differential system and* $y$ *a section of* $\mathcal{E}$. *Then* $y$ *is a solution of* $\mathcal{R}_q$, *if* $j^q(y)$ *is a section of* $\mathcal{R}_q$.

This is not how we defined the solutions in the previous section. In fact the idea presented there generalises in a straightforward way only in the ODE case. Before restricting our attention to the ODE case, let us make some general remarks.

3.2. **On the formal theory of PDEs.** We will only very briefly describe some ideas and refer for more information to [50], [16], [27], [29], [38], [39], [40], [41], [52], [14], [1]. Spencer defines the formal theory as follows [50]:

> The first step in the study of overdetermined systems is obviously the investigation of the formal properties of the given complex and the finding of criteria in order that the complex be formally exact. This we call the *formal theory*.

The word formal is used for the following reason. When Riquier and others started studying fairly arbitrary systems of PDEs at the end of 19th century, they had in mind a generalization of Cauchy–Kovalevaskaia theorem and this involved two steps: first to construct the solution as a *formal* power series, and then to show that it converges. Now Riquier realized that given an arbitrary system, it was not possible to obtain the formal power series without first transforming the initial system to a 'canonical' form, or in modern terms formally integrable or involutive form. This is in essence what Spencer says: one should be able to recognize when the system is indeed formally integrable, and if it is not, one should find ways to transform a given system into a formally integrable system which has the same solutions as the initial system.

The second step is then to prove the convergence of the power series in the analytical case, or in modern terms to show that the complex is also differentiably exact. This is rather easy in the ODE case: it is simply Theorem 2.1. However, in the PDE case it is an open problem in this generality.

Now is it always possible to find the involutive form? Perhaps already Riquier and Cartan thought that this must be the case for a 'generic' system, and the result was proved in full generality by Goldschmidt [16], based on the work of Spencer. It is beyond the scope of the present article to state precisely this theorem, but we shall try to explain the main ideas. We will not define one crucial concept, namely the symbol of the differential system, because it is not needed in the ODE case. However, in the PDE case the analysis of the symbol is absolutely essential.

To formulate the criteria Spencer talks about, we must introduce two basic operations: prolongation and projection. The latter is rather straightforward. Given a bundle $\mathcal{E}$, we can define for all $q$ and $r$ the projections $\pi_q^{q+r} : J_{q+r}(\mathcal{E}) \to J_q(\mathcal{E})$ which in coordinates are simply the maps which 'forget' highest order derivatives. Then given a differential system, we can naturally restrict these maps to the relevant submanifolds, and hence we can speak about projections of differential systems. The definition of prolongation is more involved.

**Definition 3.9.** *Let $\mathcal{R}_q \subset J_q(\mathcal{E})$ be a differential system. The $r$-prolongation of $\mathcal{R}_q$, denoted by $\rho_r(\mathcal{R}_q)$, is*

$$\rho_r(\mathcal{R}_q) = J_r(\mathcal{R}_q) \cap J_{q+r}(\mathcal{E}) \subset J_r(J_q(\mathcal{E}))$$

Perhaps it seems a bit strange to 'operate' on $\mathcal{R}_q$ with $J_r$, since $\mathcal{R}_q$ is already a subset of a jet bundle. However, $\mathcal{R}_q$ can be considered as a bundle in its own right, so $J_r(\mathcal{R}_q)$ is certainly well-defined. On the other hand we do not want to 'forget' that $\mathcal{R}_q$ is indeed already a submanifold of a jet bundle which explains why we have to take the intersection with $J_{q+r}(\mathcal{E})$. This intersection is in turn well-defined since both sets are in a natural way subsets of $J_r(J_q(\mathcal{E}))$.

When there is no risk of confusion we shall denote the prolongations simply by $\mathcal{R}_{q+r} = \rho_r(\mathcal{R}_q)$ and it is also convenient to use the notation $\mathcal{R}_{q+r}^{(s)} = \pi_{q+r}^{q+r+s}(\rho_{r+s}(\mathcal{R}_q))$. Note that we always have $\mathcal{R}_{q+r}^{(s)} \subset \mathcal{R}_{q+r}$, so the restricted maps $\pi_q^{q+r} : \mathcal{R}_{q+r} \to \mathcal{R}_q$ are well-defined. In the above Definition, $\rho_r(\mathcal{R}_q)$ is just a well-defined subset, which in general need not be a bundle. For further discussion it is convenient to restrict our attention to systems which remain bundles in prolongations and projections.

**Definition 3.10.** *A system $\mathcal{R}_q \subset J_q(\mathcal{E})$ is* regular, *if $\mathcal{R}_{q+r}^{(s)}$ is a bundle for all $r$, $s \geq 0$.*

Then we are in a position to define the formal integrability.

**Definition 3.11.** *A system $\mathcal{R}_q \subset J_q(\mathcal{E})$ is* formally integrable, *if it is regular and $\mathcal{R}_{q+r}^{(s)} = \mathcal{R}_{q+r}$ for all $r$, $s \geq 0$.*

In other words, it is required that the maps $\pi_{q+r}^{q+r+s} : \mathcal{R}_{q+r+s} \to \mathcal{R}_{q+r}$ are surjective. Of course this is not very useful in practice, since there is an infinite number of conditions. However, Goldschmidt was able to prove that one can constructively test formal integrability, hence he provided the criteria Spencer desired.

**Theorem 3.1.** *Let $\mathcal{R}_q \subset J_q(\mathcal{E})$ be a differential system and suppose that $\mathcal{R}_{q+1} \subset J_{q+1}(\mathcal{E})$ is a bundle. If $\pi_q^{q+1} : \mathcal{R}_{q+1} \to \mathcal{R}_q$ is surjective and the symbol of $\mathcal{R}_q$ is 2-acyclic, then $\mathcal{R}_q$ is formally integrable.*

We shall not define the symbol or 2-acyclicity for two reasons: in the first place this would require a lenghty discussion and secondly these notions are not really needed in the ODE case which mainly interests us. The important point is that now we really have criteria which can be constructively applied in a given situation. We have also used the word involutive, so let us give

**Definition 3.12.** *A system $\mathcal{R}_q \subset J_q(\mathcal{E})$ is* involutive*, if it is formally integrable and its symbol is m-acyclic, where $m = dim(\mathcal{B})$. Also the symbol is said to be involutive, if it is m-acyclic.*

Now it happens that any symbol is 1-acyclic and on the other hand the condition of 2-acyclicity is equivalent to 1-acyclicity in the ODE case. Hence formally integrable and involutive is equivalent in this case. The importance of involutivity comes from the fact that $m$-acyclicity implies 2-acyclicity, if $m > 2$, and that there are algorithms to test $m$-acyclicity while it is apparently not known how to test directly 2-acyclicity. Anyway in the ODE case we can write the Goldschmidt's theorem as follows.

**Theorem 3.2.** *Let $\mathcal{R}_q \subset J_q(\mathcal{E})$ be an ordinary differential system and suppose that $\mathcal{R}_{q+1} \subset J_{q+1}(\mathcal{E})$ is a bundle. If $\pi_q^{q+1} : \mathcal{R}_{q+1} \to \mathcal{R}_q$ is surjective, then $\mathcal{R}_q$ is formally integrable (involutive).*

Now if our initial system $\mathcal{R}_q$ is not formally integrable, what should be done? Recall that we have only two operations available, namely projections and prolongations. Hence one could hope that $\mathcal{R}_{q+r}^{(s)}$ were formally integrable for some $r$ and $s$. To justify these manipulations we need

**Theorem 3.3.** *The solution sets of $\mathcal{R}_q$ and $\mathcal{R}_{q+r}^{(s)}$ are same for all $r$, $s \geq 0$.*

Here solutions are understood as in Definition 3.8. The existence of involutive or formally integrable system follows, if we assume some more regularity of the initial system.

**Definition 3.13.** *A system $\mathcal{R}_q \subset J_q(\mathcal{E})$ is* strongly regular*, if it is regular and the symbol of $\mathcal{R}_{q+r}^{(s)}$ is induced from a vector bundle over $\mathcal{B}$ for all $r$, $s \geq 0$.*

Again this simplifies considerably in the ODE case, since the relevant symbols are same (or can be identified) for all $r$, $s \geq 0$.

**Theorem 3.4.** *If $\mathcal{R}_q \subset J_q(\mathcal{E})$ is a strongly regular differential system, there are integers $r$, $s \geq 0$ such that $\mathcal{R}_{q+r}^{(s)}$ is formally integrable (involutive).*

This is again constructive: at each stage one can test if various criteria are fulfilled or not. Some upper bounds are known for a sufficient number of prolongations required to produce an involutive symbol. However, these bounds are so absurdly high that they are not useful in practice.

3.3. **Ordinary differential systems.** We have defined a differential equation as a submanifold, without mentioning any equations. To be able to write down the equations in this framework we still need some general concepts.

**Definition 3.14.** *Let $(\mathcal{E}, \pi, \mathcal{B})$ and $(\tilde{\mathcal{E}}, \tilde{\pi}, \tilde{\mathcal{B}})$ be bundles. A pair of maps $f : \mathcal{E} \to \tilde{\mathcal{E}}$, $\bar{f} : \mathcal{B} \to \tilde{\mathcal{B}}$ is called a bundle morphism, if $\tilde{\pi} \circ f = \bar{f} \circ \pi$. If $\mathcal{B} = \tilde{\mathcal{B}}$ and $\bar{f} =$* identity*, we shall in this case say that $f$ is a morphism.*

In fact $\bar{f}$ is uniquely determined by $f$. Note also that $f$ maps fibers of $\mathcal{E}$ to fibers of $\tilde{\mathcal{E}}$. If $\bar{f}$ is a diffeomorphism, a bundle morphism induces a map $\Gamma(\mathcal{E}) \to \Gamma(\tilde{\mathcal{E}})$. In particular this is the case when $f$ is a morphism. Now $j^q$ can be considered as a morphism $\mathcal{E} \to J_q(\mathcal{E})$ and hence as a map $\Gamma(\mathcal{E}) \to \Gamma(J_q(\mathcal{E}))$. This leads to

**Definition 3.15.** *Let $f : J_q(\mathcal{E}) \to \tilde{\mathcal{E}}$ be a morphism. The $q$'th order differential operator determined by $f$ is $D_f = f \circ j^q : \Gamma(\mathcal{E}) \to \Gamma(\tilde{\mathcal{E}})$.*

Let us then relate these definitions to the elementary examples in the beginning. Consider the problem (2.1). When we want to define $\mathcal{R}_1$ as a zero set, we think of $f$ on the left-hand side as a morphism $J_1(\mathcal{E}) \to \mathcal{E}$, where $\mathcal{E} = \mathbb{R} \times \mathbb{R}$. One the other hand, when we think about the solutions as in Definition 3.8, we really interprete the left-hand side as a map $\Gamma(\mathcal{E}) \to \Gamma(\mathcal{E})$. It may appear strange that $f$ is a morphism whose target $\mathcal{E}$ is two-dimensional while we have only one scalar equation. However, even classically on the right-hand side there is really a zero *function*, i.e. the zero section of $\mathcal{E}$. So when writing an equation we suppress the base manifold and describe only the action of the morphism on the fibers. Of course this is convenient and we shall always do so in the sequel.

Let us then finally take up the ODE case and describe the morphism $f : J_q(\mathcal{E}) \to \tilde{\mathcal{E}}$ with coordinates. Let $\mathcal{E} = \mathbb{R} \times \mathbb{R}^n$, $\tilde{\mathcal{E}} = \mathbb{R} \times \mathbb{R}^k$ and let us denote the coordinates of $J_q(\mathcal{E})$ by $(x, y^1, \ldots, y^n, y^1_1, \ldots, y^n_q)$; they are called *jet coordinates*. Hence superscripts denote the components of the vector and subscripts correspond to jets (or derivatives) of different order. Let us write the equation

$$f(x, y, y_1, \ldots, y_q) = 0 \tag{3.1}$$

where strictly speaking on the right-hand side there is a zero section, but from the point of view of inverse images we can consider this as a map $J_q(\mathcal{E}) \simeq \mathbb{R}^{(q+1)n+1} \to \mathbb{R}^k$. Hence let $\mathcal{R}_q = f^{-1}(0) \subset J_q(\mathcal{E})$.

Before we can formulate the concept of solution which is convenient for the numerical computation, we must still introduce some terminology. We denote the tangent (resp. cotangent) bundle of a manifold $M$ by $TM$ (resp. $T^*M$), and the tangent (resp. cotangent) space at $p \in M$ by $TM_p$ (resp. $T^*M_p$). The sections of $TM$ are vector fields and the sections of $T^*M$ are one-forms.[4] In the introductory examples $\alpha$ was a section of $T^*J_1(\mathbb{R} \times \mathbb{R})$ and now we must formulate this idea in the general case.

Let us then consider the system (3.1) and let us define the one-forms on $J_q(\mathcal{E})$ by

$$\alpha^i_j = dy^i_{j-1} - y^i_j dx \qquad i = 1, \ldots, n \qquad j = 1, \ldots, q \tag{3.2}$$

With these forms one can formulate the appropriate generalisation of the contact plane and contact distribution. Let $p \in J_q(\mathcal{E})$ and define

$$\mathcal{C}_p = \left\{ v_p \in (TJ_q(\mathcal{E}))_p \,\middle|\, \alpha^i_j(v_p) = 0 \right\}$$

This defines a distribution $\mathcal{C}$ on $J_q(\mathcal{E})$, which is called a Cartan distribution, and it is easily checked that $\dim(\mathcal{C}) = n + 1$.[5] Let us see that this distribution captures the 'infinitesimal' idea expressed in the notation of the one-forms. Let $y$ (resp. $z$) be a

[4] Incidentally, distributions can also be considered as sections: one-dimensional distributions are then sections of the projective bundle and many dimensional distributions are sections of an appropriate Grassmann bundle.

[5] The Cartan distribution defines a contact structure on $J_q(\mathcal{E})$ only in the case $n = q = 1$.

section of $\mathcal{E}$ (resp. $J_q(\mathcal{E})$). Identifying sections and their images we may consider $j^q(y)$ and $z$ as submanifolds of $J_q(\mathcal{E})$. Then for all $p \in j^q(y)$, $(Tj^q(y))_p \subset \mathcal{C}_p$ and conversely if for all $p \in z$, $(Tz)_p \subset \mathcal{C}_p$, then $z = j^q(y)$ for some $y$.

Let $\mathcal{R}_q = f^{-1}(0) \subset J_q(\mathcal{E})$ where $f$ is given in (3.1) and supposing that zero is a regular value of $f$, $\mathcal{R}_q$ is a smooth manifold. Now as in the simple examples in the beginning we can define a distribution $\mathcal{D}$ at each point of $p \in \mathcal{R}_q$ by

$$\mathcal{D}_p = (T\mathcal{R}_q)_p \cap \mathcal{C}_p$$

**Definition 3.16.** *Supposing that $\mathcal{R}_q$ is involutive and $\mathcal{D}$ is one-dimensional, the solutions of* (3.1) *are integral manifolds of $\mathcal{D}$.*

Note that here it is sufficient to assume that $\mathcal{R}_q$ is a submanifold, it need not be a bundle. Now Theorem 2.1 generalizes as such to the present situation, so we conclude that there always exist a unique solution through $p \in \mathcal{R}_q$, if $\mathcal{D}$ is one-dimensional in some neighborhood of $p$.

**Remark 3.1.** Is $\mathcal{D}$ really one-dimensional? The dimensions of $\mathcal{C}_p$, $(T\mathcal{R}_q)_p$ and $(TJ_q(\mathcal{E}))_p$ are $n+1$, $qn+n-k+1$ and $qn+n+1$ which implies that $\mathcal{D}_p$ is at least $n-k+1$ dimensional. Consequently for $k < n$ (i.e. underdetermined systems) $\mathcal{D}$ cannot be one-dimensional. Note that in this case the solutions can still be defined as in Definition 3.8, although evidently there is no unique solution through a given point. In some problems it may be interesting to analyse the space of solutions of underdetermined systems, but we will not consider these below. An interesting example of an underdetermined system is $y^1_1 - (y^2_2)^2 = 0$. Hilbert gave it as an example where the general solution cannot be expressed in terms of an arbitrary function and a finite number of its derivatives, see [3].

For $k = n$ one would expect that $\mathcal{D}$ is 'generically' one-dimensional, and in fact this is always the case if $f$ is in the standard form

$$f(x, y, y_1, \ldots, y_q) = y_q + \tilde{f}(x, y, y_1, \ldots, y_{q-1})$$

More generally, the transversal intersection of $(T\mathcal{R}_q)_p$ and the Cartan distribution is one-dimensional.

Finally if $k > n$, then for $f$ taken 'at random' one would expect that $\mathcal{D}$ is zero-dimensional. However, systems arising in practice have additional structure which 'allows' $\mathcal{D}$ to be one-dimensional.

**Remark 3.2.** Why should the system be involutive? Consider the following systems in $J_1(\mathbb{R} \times \mathbb{R}^2) \simeq \mathbb{R}^5$.

$$\mathcal{R}_1 \ : \quad \begin{cases} y^1 + 1 = 0 \\ y^2_1 + 1 = 0 \end{cases} \qquad\qquad \mathcal{R}^{(1)}_1 \ : \quad \begin{cases} y^1 + 1 = 0 \\ y^1_1 = 0 \\ y^2_1 + 1 = 0 \end{cases}$$

$\mathcal{R}^{(1)}_1$ is involutive form of $\mathcal{R}_1$. Recall that the solution sets, in the sense of Definition 3.8, are same for $\mathcal{R}_1$ and $\mathcal{R}^{(1)}_1$ by Theorem 3.3. Now the distribution on $\mathcal{R}_1$ is one-dimensional, *except* when $y^1_1 = 0$, and hence if the initial point is *not* on $\mathcal{R}^{(1)}_1$ we get a well defined integral manifold. However, this is not really what we want since the equation $y^1_1 = 0$ should also be satisfied. For the involutive system $\mathcal{R}^{(1)}_1$ one verifies that the corresponding distribution is everywhere one-dimensional. This is typical:

noninvolutive systems can contain open sets where there are no solutions at all, and in spite of that the distribution can be one-dimensional in such a set. On the other hand, the dimension of the distribution of a noninvolutive system can be greater than one in an open set where there are unique solutions.

**Remark 3.3.** Note that it is unnecessary to transform the system into a first order system before the numerical solution. In fact it is better not to transform since the dimension of the ambient space is bigger for the first order system. Let $q > 1$, $\mathcal{R}_q \subset J_q(\mathcal{E})$ and let the corresponding first order system be $\mathcal{R}_1 \subset J_1(\mathbb{R} \times \mathbb{R}^{qn})$; then $\dim(J_1(\mathbb{R}\times\mathbb{R}^{qn})) = 2qn+1 > (q+1)n+1 = \dim(J_q(\mathcal{E}))$. Of course $\dim(\mathcal{R}_q) = \dim(\mathcal{R}_1)$. For the same reason it does not pay to transform a nonautonomous system into autonomous form.

**Remark 3.4.** It is interesting that when one computes the solution, one obtains automatically approximations to derivatives up to order $q$.

**Remark 3.5.** Note that there is no natural way to extend the distribution $\mathcal{D}$ outside $\mathcal{R}_q$, even in the neighborhood of $\mathcal{R}_q$. Such an extension would mean relaxing some of the 'tangent conditions' (the curve would not be tangent to $\mathcal{R}_q$) and/or 'Cartan conditions' (the jet coordinates would not correspond to derivatives). Evidently choosing this relaxation is quite arbitrary. Of course in some special situations there can be an easily constructed extension, which might prove useful in the computations.

3.4. **Preliminary conclusions.** Having defined our basic framework we pause to make a few comments before moving on to the numerical part of the article. Since the basic objects of study, i.e. differential equations and solutions of differential equations, have been redefined, it is perhaps not so surprising that this approach opens up new points of view for many aspects of analysis of differential systems. First of all, on the purely conceptual level, it is quite nice to be able to discuss such a large class of systems in a unified way; recall that no special property is required of the map $f$ in (3.1).

The important concept which emerges from this framework is involutivity, and because of Theorem 3.1 one might from the theoretical point of view restrict one's attention to involutive systems. However, in practice the systems are usually not involutive initially and hence they must first be transformed to an involutive form before actual numerical computations. Now this transformation involves usually some symbolic manipulation of the given system, and consequently can be rather time consuming. Of course the algorithms for symbolic manipulation are progressing all the time, so perhaps this is not such a severe problem. Moreover, it is not quite clear how much symbolic computation is really required: in some situations a mixture of numerical and symbolic techniques could be sufficient.

However, the transformation to involutive form should also be seen as an analysis (of singularities) of the system. Recall that in Theorems 3.1, 3.2 and 3.4 there are some regularity assumptions. One may think that in general these conditions are satisfied in some open set of the relevant manifold. Now the set where these conditions fail indicate some sort of singularity of the system: the manifold is perhaps not smooth everywhere, or perhaps it can be factored to several subsystems. Obviously it is impossible to analyse the situation using only the original, i.e. non-involutive, system. Also it is quite interesting to locate the sets where the distribution fails to be one-dimensional, because this gives essential information about the solutions. Again these sets cannot be known in general, if the system is not involutive.

This leads yet to another aspect, namely genericity. When analysing singularities of the solutions for example, it is well-known that certain singularities are typical while others disappear when the system is perturbed a little [5]. Of course this kind of analysis is important in applications, where usually models and the coefficients are only known approximatively. Without pursuing this matter further let us just mention one interesting fact. Now the points where the distribution fails to be one-dimensional are evidently the generalizations of the singularities (i.e. zeros) of vector fields. It is known that generically singularities of vector fields appear only at isolated points. This is not true for distributions. In fact one expects that generically the singularities of distributions appear in the sets of codimension two, see [5], [55] and [56] for more information.

Finally there is the numerical aspect which is the main topic of the present article. Below we will show how to use jet spaces in numerical computations. Here also the new point of view leads to different conclusions than the classical approach. This will be discussed in more detail below.

## 4. Examples and simplifications

Since a lot of problems arising in practice are of the type mechanical systems with constraints it seems worthwhile to discuss explictly some problems in this class. Moreover, the computations that follow are also useful as illustrations of the concepts and definitions introduced above.

### 4.1. **Pendulum.**

Consider the simple pendulum which in the classical notation is given by

$$\begin{cases} x'' + \lambda x = 0 \\ y'' + \lambda y + 1 = 0 \\ x^2 + y^2 - 1 = 0 \end{cases} \tag{4.1}$$

Here $x$ and $y$ are the cartesian coordinates and $\lambda$ is the tension in the string (or Lagrange multiplier). Let us introduce the jet coordinates:

$$x \longleftrightarrow y^1 \qquad y \longleftrightarrow y^2 \qquad \lambda \longleftrightarrow y^3$$

The system is not involutive, but prolonging and projecting (i.e. differentiating and eliminating) 4 times produces the following involutive form:[6]

$$
\begin{cases}
y^1_2 + y^1 y^3 = 0 \\
y^2_2 + y^2 y^3 + 1 = 0 \\
y^3_2 + 3y^2_2 = 0 \\
y^1 y^1_1 + y^2 y^2_1 = 0 \\
(y^1_1)^2 + (y^2_1)^2 - y^2 - y^3 = 0 \\
3y^2_1 + y^3_1 = 0 \\
(y^1)^2 + (y^2)^2 - 1 = 0
\end{cases}
\tag{4.2}
$$

Let $\mathcal{E} = \mathbb{R}\times\mathbb{R}^3$ and denote the above equations by $f(x, y, y_1, y_2) = 0$ and $\mathcal{R}_2 = f^{-1}(0) \subset J_2(\mathcal{E})$. Evidently $\dim(\mathcal{R}_2) = 3$. Note that by Theorem 3.3 the original system and the involutive system have the same set of solutions in the sense of Definition 3.8, but Definition 3.16 makes sense only for the involutive form. Now the relevant distribution can be computed from the nullspace on the following matrix.

$$
A = \begin{pmatrix}
-y^1_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-y^2_1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-y^3_1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-y^1_2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
-y^2_2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
-y^3_2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & y^3 & 0 & y^1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & y^3 & y^2 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 1 \\
0 & y^1_1 & y^2_1 & 0 & y^1 & y^2 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & 2y^1_1 & 2y^2_1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 3 & 1 & 0 & 0 & 0 \\
0 & y^1 & y^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

It is easily checked that $\dim(N(A)) = 1$ everywhere on $\mathcal{R}_2$, though $A$ is usually of full rank outside $\mathcal{R}_2$. Hence the problem is regular and through every initial point there exist a unique solution. Of course in this simple problem one sees immediately that one could drop the last 4 rows of the matrix in actual computations. However, in general one must use the full matrix and hence to treat an overdetermined system of linear equations.

The problem is quite simple and one could use the above formulation in the numerical computations. However, the number of equations can be reduced, or more geometrically, the manifold and the distribution can be projected to a lower dimensional ambient space. Since this projection can also be done for quite a large class of problems (see below), let us see how this can be achieved.

Recall that if one has a system of the form $y_1 + \varphi(x, y) = 0$, this always induces a distribution or vector field on $\mathcal{E}$, because in this case $\mathcal{R}_1$ is simply the graph of $\varphi$.

[6] We have to differentiate 4 times, although the system is said to be of (differential) index 3...

Hence the projection $(x, y, y_1) \mapsto (x, y)$ induces a diffeomorphism between $\mathcal{R}_1$ and $\mathcal{E}$, and the differential of the projection transports the distribution from $\mathcal{R}_1$ to $\mathcal{E}$. Note that the graph cannot be vertical, so that the distribution remains one-dimensional.

Now looking at the system (4.2) we see that it is 'graph like' with respect to $y_2$, so in this case we could project the system from $J_2(\mathcal{E})$ to $J_1(\mathcal{E})$ with the natural map $\pi_1^2 : (x, y, y_1, y_2) \mapsto (x, y, y_1)$. This gives

$$\begin{cases} y^1 y_1^1 + y^2 y_1^2 = 0 \\ (y_1^1)^2 + (y_1^2)^2 - y^2 - y^3 = 0 \\ 3y_1^2 + y_1^3 = 0 \\ (y^1)^2 + (y^2)^2 - 1 = 0 \end{cases} \tag{4.3}$$

and the distribution is given by the nullspace of

$$\tilde{A} = \begin{pmatrix} -y_1^1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -y_1^2 & 0 & 1 & 0 & 0 & 0 & 0 \\ -y_1^3 & 0 & 0 & 1 & 0 & 0 & 0 \\ y^1 y^3 & 0 & 0 & 0 & 1 & 0 & 0 \\ y^2 y^3 + 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ -3y^2 y^3 - 3 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & y_1^1 & y_1^2 & 0 & y^1 & y^2 & 0 \\ 0 & 0 & -1 & -1 & 2y_1^1 & 2y_1^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 1 \\ 0 & y^1 & y^2 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Denote the system (4.3) by $\mathcal{R}_1 = \tilde{f}^{-1}(0) \subset J_1(\mathcal{E})$. Again it is immediate that $\dim(\mathcal{R}_1) = 3$, $\dim(N(\tilde{A})) = 1$ on $\mathcal{R}_1$, and that $\pi_1^2 : \mathcal{R}_2 \to \mathcal{R}_1$ is a diffeomorphism. Hence there is a bijective correspondence between the solutions of (4.2) and (4.3).

However, one can do another reduction. Recall that $\lambda$ in the original equations (4.1) was 'only' a Lagrange multiplier, so one suspects that perhaps it is not necessary to treat it and other variables in the same way. Let us try to get a formulation where we can use the special features of $\lambda$ in the problem. So let us introduce

$$x \longleftrightarrow y^1 \qquad\qquad y \longleftrightarrow y^2$$

Hence here $y = (y^1, y^2)$ and $\mathcal{E} = \mathbb{R} \times \mathbb{R}^2$. Now differentiating twice the constraint in (4.1), we get

$$\begin{cases} y_2^1 + y^1 \lambda = 0 \\ y_2^2 + y^2 \lambda + 1 = 0 \\ \langle y, y_1 \rangle = 0 \\ |y_1|^2 + \langle y, y_2 \rangle = 0 \\ |y|^2 - 1 = 0 \end{cases} \tag{4.4}$$

Consequently $y_2$ and $\lambda$ can be solved from the equations

$$\begin{pmatrix} 1 & 0 & y^1 \\ 0 & 1 & y^2 \\ y^1 & y^2 & 0 \end{pmatrix} \begin{pmatrix} y_2^1 \\ y_2^2 \\ \lambda \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ |y_1|^2 \end{pmatrix} = 0 \tag{4.5}$$

Note that the matrix cannot be singular since $y^1$ and $y^2$ cannot be both zero. Now we can regard $y_2$ and $\lambda$ simply as parameters which have to be (numerically!) computed, and this leads to a simple problem in $J_1(\mathcal{E})$. First let us consider the system (4.4) in $J_2(\mathcal{E})$ and denote the manifold by $\mathcal{R}_2$. Now of course $\mathcal{R}_2$ depends on $\lambda$, but obviously $\mathcal{R}_1 = \pi_1^2(\mathcal{R}_2)$ does not; in fact $\mathcal{R}_1$ is given by the system

$$\begin{cases} |y|^2 - 1 = 0 \\ \langle y, y_1 \rangle = 0 \end{cases}$$

Hence we can solve the problem in $\mathcal{R}_1 \subset J_1(\mathcal{E})$, provided we can compute the distribution on $\mathcal{R}_1$. This is done with (4.5). The projected distribution is the nullspace of

$$A = \begin{pmatrix} -y_1^1 & 1 & 0 & 0 & 0 \\ -y_1^2 & 0 & 1 & 0 & 0 \\ -y_2^1 & 0 & 0 & 1 & 0 \\ -y_2^2 & 0 & 0 & 0 & 1 \\ 0 & y_1^1 & y_1^2 & y^1 & y^2 \\ 0 & y^1 & y^2 & 0 & 0 \end{pmatrix}$$

where $y_2^1$ and $y_2^2$ are computed from (4.5). Again it is seen that the last two rows can be dropped, and we can immediately write down a vector which spans the nullspace: $(1, y_1^1, y_1^2, y_2^1, y_2^2)$, or more briefly and conveniently $(1, y_1, y_2)$. Hence the final form of the problem is:

$$\begin{cases} |y|^2 - 1 = 0 \\ \langle y, y_1 \rangle = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \big(1, y_1, y_2\big) \\ \begin{pmatrix} 1 & 0 & y^1 \\ 0 & 1 & y^2 \\ y^1 & y^2 & 0 \end{pmatrix} \begin{pmatrix} y_2^1 \\ y_2^2 \\ \lambda \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ |y_1|^2 \end{pmatrix} = 0 \end{cases} \tag{4.6}$$

In the next section we generalize the above reduction argument.

4.2. **Mechanical systems with holonomic constraints.** Let $f : \mathbb{R}^m \to \mathbb{R}^k$ be a smooth map. The first (resp. second) differential of $f$, denoted by $df$ (resp. $d^2 f$), is a map $\mathbb{R}^m \to L(\mathbb{R}^m, \mathbb{R}^k)$ (resp. $\mathbb{R}^m \to L(\mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^k)$) where $L(\mathbb{R}^m, \mathbb{R}^k)$ (resp. $L(\mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^k)$) denotes the space of linear (resp. bilinear) maps. The value of $df$ (resp. $d^2 f$) at $p$ is denoted by $df_p$ (resp. $d^2 f_p$).

Following class of systems occurs often in applications

$$
\begin{cases} B(x,y,y_1)y_2 + f(x,y,y_1) + (dg)^t\lambda = 0 \\ g(y) = 0 \end{cases} \tag{4.7}
$$

where $B$ is invertible, $dg$ has a full rank and $\lambda$ is Lagrange multiplier. Note that the pendulum system (4.1) is of this form and that the rank conditions need to be satisfied only on the zero set of $g$. Now proceeding as in the pendulum case we differentiate twice the constraint and get the system

$$
\begin{pmatrix} B & (dg)^t \\ dg & 0 \end{pmatrix} \begin{pmatrix} y_2 \\ \lambda \end{pmatrix} + \begin{pmatrix} f \\ d^2g\,(y_1, y_1) \end{pmatrix} = 0
$$

This linear system has a solution under the present hypothesis. Hence projecting the system from $J_2(\mathcal{E})$ to $J_1(\mathcal{E})$ leads to

$$
\begin{cases} g(y) = 0 \\ dg\, y_1 = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \big(1, y_1, y_2\big) \\ \begin{pmatrix} B & (dg)^t \\ dg & 0 \end{pmatrix} \begin{pmatrix} y_2 \\ \lambda \end{pmatrix} + \begin{pmatrix} f \\ d^2g\,(y_1, y_1) \end{pmatrix} = 0 \end{cases} \tag{4.8}
$$

Note that the overdetermined character of the system has disappeared and that the solution of the linear system can be computed numerically. If the system is big, the symbolic computation of $d^2g$ may be rather time consuming. Fortunately this is not necessary: automatic differentiation permits a very accurate and efficient numerical evaluation of the required quantities. However, discussion of these techniques is outside the scope of the present article and we refer to [8] for more information on this subject.

4.3. **On the index.** Before discussing the actual numerical methods, let us say a few words about index. There are many definitions of the index, see [9], [18], [17], [32], and this notion (or these notions) has been used to characterize the numerical difficulty of the problem. One of the definitions, the differential index, is rather close in spirit to the following definition: index is the number of prolongation and projection steps needed to transform the given system into an involutive system. Hence one may interprete the index as measuring the lack of information in the original system, and so it is quite natural that higher index problems are numerically more difficult, *if one uses the original system in the numerical computations.* We use the involutive form, and therefore the index plays no role in our framework.

Indeed, from the point of view of the involutive system one cannot even define the index. This is because one cannot do the projection/prolongation steps 'backwards', i.e. there is no unique initial system where the involutive system 'comes from'. Let us elaborate on this point using some concepts of differential algebra, [24], [47]. Let the original system be given by a system of differential polynomials. The set of solutions is characterized by the radical differential ideal generated by the system. Now prolonging, projecting and factoring we may look for the prime decomposition of the system: according to a theorem of Ritt, any radical differential ideal is a finite intersection of prime ideals. This process creates a tree structure: if the systems factors, i.e. it is not prime as an algebraic ideal, the system splits into subsystems, and we look for the involutive form of each of them. Hence we get a tree where the root is the original system and the leaves are the involutive systems corresponding to the prime decomposition.

Now the differential index is intuitively the length of the path from the root to the given leaf. Of course these numbers can be different for different leaves, so that in a way even for the root the index cannot be defined, at least as an integer. This phenomenon is well-known: it has been expressed by saying that the index depends on the solution. Of course one need not know the solution, it is sufficient to know the corresponding prime ideal. Again, imagining the tree structure one sees that it is impossible to define the index of a leaf: clearly any leaf could be a part of a rather arbitrary tree, and hence the length of the path from the leaf to the root can be arbitrary.

The traditional methods can handle only problems with as many equations as unknowns; the numerical analysis is done on the root. Since jet bunbles allow us to treat overdetermined systems in a numerically stable way, we can do our numerics on the leaves.

## 5. Computation of one-dimensional integral manifolds

5.1. **Preliminary remarks.** We have seen above that the computation of the solutions of a differential system reduces to the following:

> Given a manifold $M$, a point $p \in M$ and one-dimensional distribution $\mathcal{D}$ on $M$, compute the integral manifold of $\mathcal{D}$ through $p$.

By Theorem 2.1 there exists a unique solution to this problem. Now in practice $M$ is given as a zero set of some map as in (3.1), but usually $\mathcal{D}$ is not explicitly known. However, given a point $p \in M$ we can numerically evaluate $\mathcal{D}_p$ and this is sufficient in applications. The standard ODE codes work in the same way: it is not necessary to know a formula for the vector field, it is enough to be able to evaluate it at a given point.

Recall that around a regular point $p$ one can find a vector field $V$ such that $0 \neq V_a \in \mathcal{D}_a$ for all $a$ in some neighborhood of $p$ and we can also normalize by requiring $|V_a| = 1$. Such a $V$ is called a vector field associated to $\mathcal{D}$. Note that $V$ may not exist globally, as our example in section 2 showed. Finally let us remark that $V$ is not needed in actual computations, but it is useful in the analysis of numerical methods.

Let us also remark that there is no reason why the problem should be always stiff, so there is no need to restrict one's attention to implicit methods. Of course our formulation includes all the classical stiff systems: simply take $M$ to be some Euclidean space and $V$ to be a vector field which defines a stiff system. However, the point is that overdetermined systems (or DAEs) are not intrinsically stiff.

To proceed in our construction and analysis of numerical methods to the above problem we must pause to introduce some terminology.

5.2. **Some notions of Riemannian geometry.** For more details on Riemannian geometry we refer to [51, vol. 2 and vol. 4] or [13]. Let $M$ be a smooth submanifold of $\mathbb{R}^m$. Then its normal space at $p$ is denoted by $NM_p$. In these circumstances $NM_p$ is the orthogonal complement of $TM_p$ in $(T\mathbb{R}^m)_p$. Let us give $M$ the Riemannian metric induced by the standard metric in $\mathbb{R}^m$ and denote by $\nabla$ the (unique) symmetric connection which is compatible with this metric.

Let $X$ and $Y$ be vector fields on $M$; denoting their extensions to $\mathbb{R}^m$ by the same letter we have

$$dY(X_p) = \nabla_{X_p} Y + S(X_p, Y_p) \tag{5.1}$$

where $dY(X_p)$ is the standard directional derivative, $\nabla_{X_p} Y$ is the covariant derivative and $S$ is the second fundamental tensor. Note that $\left(\nabla_{X_p} Y\right)_p \in TM_p$ and that at each point $p$, $S$ is a symmetric bilinear map $TM_p \times TM_p \to NM_p$.

Note that the covariant derivative is intrinsic to $M$ while the second fundamental tensor depends on how $M$ is embedded in $\mathbb{R}^m$. Let $V$ be a vector field on $M$ and $c$ be an integral curve of $V$. If $|V_p| = 1$ for all $p$, i.e. if $c$ is parametrized by arclength, then $\left|\nabla_{V_p} V\right|$ is called the geodesic curvature and $|S(V_p, V_p)|$ is called the normal curvature $c$ at $p$.

5.3. **Analysis of local error for some methods.** Let $k < m$ and $f : \mathbb{R}^m \to \mathbb{R}^k$ be a smooth map and let zero be a regular value of $f$. We think of $f$ as in (3.1), but for the present discussion it is convenient to regard $J_q(\mathcal{E})$ simply as a big Euclidean space $\mathbb{R}^m$ where $m = (q+1)n + 1$. Hence $M := f^{-1}(0) \subset \mathbb{R}^m$ is a smooth manifold of dimension $m - k$. Let us give $M$ the Riemannian metric induced by the standard metric in $\mathbb{R}^m$. When it is convenient the objects defined on $M$ will also be considered as defined on $\mathbb{R}^m$ without writing explicitly the inclusion map. Let $\mathcal{D}$ be a smooth one-dimensional distribution on $M$ and let $V$ be the vector field associated to it. We would like to compute some integral manifolds of $\mathcal{D}$.[7]

Let $p \in M$ be the current point and $c : \mathbb{R} \to M$ be the integral curve of the associated vector field with $c(0) = p$ and $c'(0) = V_p$. The arclength parameter is denoted by $s$. Let us compute an approximation of $c(h)$ for small $h$. The simplest possibility is to use Euler's method in the following form.

1. Choose the step-size $h$ and take an 'Euler step' along the tangent space; this gives a point $p + V_p h$.
2. Since $p + V_p h \notin M$ in general we project it orthogonally back to $M$. This projection is well defined for $h$ sufficiently small by the tubular neighborhood theorem [51, vol. 1, p. 466].

Hence an approximation $q$ of $c(h)$ is obtained by solving

$$\begin{cases} q + (df_q)^t \mu = p + V_p h \\ f(q) = 0 \end{cases} \tag{5.2}$$

where $\mu \in \mathbb{R}^k$. It can easily be verified that this system has a solution for small $h$. To get error estimates we compute first few terms in the expansions

$$q = q^0 + q^1 h + q^2 h^2 + \cdots$$
$$\mu = \mu^0 + \mu^1 h + \mu^2 h^2 + \cdots$$

This leads to

[7] In the limiting case where $m = k + 1$ and hence the integral manifold is $M$ itself, this problem has been studied quite extensively, see [2].

**Proposition 5.1.**

$$q = p + V_p h - (df_p)^t \mu^2 h^2 + O(h^3)$$

$$\mu = \tfrac{1}{2}\left(df_p(df_p)^t\right)^{-1} d^2 f_p(V_p, V_p) h^2 + O(h^3)$$

*Proof.* Obviously $q^0 = p$ and $\mu^0 = 0$. For linear terms we get the equations

$$q^1 + (df_p)^t \mu^1 = V_p$$
$$df_p q^1 = 0$$

This implies that $q^1 = V_p$ and $\mu^1 = 0$. Then the quadratic terms give

$$q^2 + (df_p)^t \mu^2 = 0$$
$$2 df_p q^2 + d^2 f_p(V_p, V_p) = 0$$

from which the result follows. □

**Proposition 5.2.**

$$q^2 = \tfrac{1}{2} S(V_p, V_p)$$

*Proof.* Let $c : \mathbb{R} \to M$ be any curve (parametrized by arclength) such that $c(0) = p$ and $c'(0) = V_p$. Recall that $(T\mathbb{R}^m)_p = TM_p \oplus NM_p$ and denote by $\pi$ the orthogonal projection $\pi : \mathbb{R}^m \to NM_p$. Now it is known that $\pi(c''(0)) = S(V_p, V_p)$, see [51, vol. 3, p. 5]. On the other hand differentiating twice the identity $f \circ c = 0$ we obtain

$$df_p c''(0) + d^2 f_p(V_p, V_p) = 0$$

Now $c''(0) = v + \pi(c''(0)) = v + (df_p)^t a$ for some $v \in TM_p$ and some $a \in \mathbb{R}^k$. Since $df_p v = 0$ we can use the above equation to compute $a$ which then gives the required result. □

Let us then compare the approximation to exact value. Using (5.1) we obtain

$$c(h) = p + V_p h + \tfrac{1}{2}\Big((\nabla_{V_p} V)_p + S(V_p, V_p)\Big) h^2 + O(h^3)$$

Subtracting the expansions we get immediately

**Corollary 5.1.**

$$c(h) - q = \tfrac{1}{2}\left(\nabla_{V_p} V\right)_p h^2 + O(h^3)$$

Hence our simple method (5.2) is of first order (i.e. local error is $O(h^2)$). Note that the main error term is rather natural: it reduces to standard directional derivative of the classical case when $M$ is an Euclidean space.

Let us then consider some simple implicit methods. One can formulate the implicit Euler method in two ways.

$$(5.3) \qquad \begin{cases} p + (df_p)^t \mu = q - V_q h \\ f(q) = 0 \end{cases} \qquad \begin{cases} q + (df_q)^t \mu = p + V_q h \\ f(q) = 0 \end{cases}$$

In either case we obtain

**Proposition 5.3.** *Let $q$ solve either of the systems* (5.3)*; then*

$$c(h) - q = -\tfrac{1}{2}\left(\nabla_{V_p} V\right)_p h^2 + O(h^3)$$

*Proof.* Expanding as before $q = p + q^1 h + q^2 h^2 + \dots$, we immediately get $q^1 = V_p$ and $\mu^1 = 0$. Expanding the second system in (5.3) we get

$$\begin{aligned} & q^2 + (df_p)^t \mu^2 = dV\, V_p \\ & df_p q^2 + \tfrac{1}{2}\, d^2 f_p(V_p, V_p) = 0 \end{aligned}$$

Hence $\left(df_p (df_p)^t\right)\mu^2 = \frac{1}{2}\, df_p\, S(V_p, V_p)$ and $q^2 = \nabla_{V_p} V + \frac{1}{2}\, S(V_p, V_p)$. Expanding the first system produces same $q^2$, but $\mu^2$ changes sign. ☐

The implicit mid-point rule can be formulated as follows.

$$\begin{cases} q + (df_q)^t \mu = p + V_r h \\ f(q) = 0 \\ r + (df_r)^t \nu = \frac{1}{2}(p+q) \\ f(r) = 0 \end{cases} \tag{5.4}$$

**Proposition 5.4.** *Let $q$ solve the above system; then*

$$c(h) - q = O(h^3)$$

*Proof.* Evidently $q^0 = r^0 = p$, $q^1 = V_p$, $r^1 = V_p/2$, $\mu^0 = \mu^1 = \nu^0 = \nu^1 = 0$. For second order terms we get

$$\begin{aligned} & q^2 + (df_p)^t \mu^2 = \tfrac{1}{2}\, dV\, V \\ & df\, q^2 + \tfrac{1}{2}\, d^2 f(V, V) = 0 \end{aligned}$$

Hence $\mu^2 = 0$ and $q^2 = \frac{1}{2}\, dV\, V$ from which the result follows. ☐

We have seen that it is rather straightforward to formulate low order schemes in the present context. Moreover their error terms are what one expects by the classical theory. The analysis of higher order schemes is more involved and will be treated elsewhere. Note that the methods (5.2), (5.3) and (5.4) are one-step methods whose local errors are of order 2, 2 and 3. By standard theorems we can then conclude that the global errors for sufficiently small $h$ are 1, 1 and 2.

## 6. Numerical implementation

We have actually implemented the explicit Euler method (5.2) and the midpoint rule (5.4). Implicit Euler (5.3) is only used for step size control as explained below. There are three basic tasks in our methods.

1. Given a point $p \in M$, compute the distribution $\mathcal{D}_p$.
2. Step size control.
3. Solving the nonlinear system (5.2), (5.3) or (5.4).

All these subproblems reduce to fairly standard numerical problems so we will say just a few words of them. All computations were done with *Mathematica*, [60]. Of course this is not as efficient as using standard languages like Fortran or C. However, at this stage we found *Mathematica* to be more convenient than the traditional languages, so the implementation in Fortran or C has to wait future versions of our code.

6.1. **Computing the distribution.** As we have seen in the examples, the $\mathcal{D}_p$ can easily be represented as a nullspace of some matrix $A$. Now this problem is (mildly) ill-posed numerically since we have in general an overdetermined system of linear equations and hence because of the round-off errors the nullspace would be trivial. To circumvent this difficulty, we use the standard singular value decomposition

$$A = U\Sigma V^t$$

where $U$ and $V$ are orthogonal and $\Sigma$ contains the singular values in descending order in its diagonal. The last singular value should be very close to zero, and hence the last column of $V$ should give a good approximation of the required direction. Of course we must check that there is only one singular value which is much smaller than the others; if this is not the case, this would indicate some singularity of the solution. We did not encounter any problems of this sort in the examples below.

Of course using the full singular value decomposition is rather excessive, and consequently this step could be done more efficiently. One possibility is to use QR decomposition. Also $A$ has a special structure: recall that the representation of the Cartan distribution in $A$ is the same for all points of $M$. Hence it could be advantageous to preprocess $A$ in some way which take into account this fact and yield a more rapid computation of the nullspace. These possibilities will be discussed in the future versions.

Note also that for mechanical systems with holonomic constraints, i.e. problems of the form (4.7), the distribution can be computed from the regular linear system.

6.2. **Step size.**

6.2.1. *Explicit Euler.* For step size control we used the standard technique: take one big step of size $2h$ achieving point $b$ and two smaller ones of size $h$, thus achieving points $a_1$ and $a_2$. Then we computed $|a_2 - b|$ in the ambient space and accepted the step if the difference was smaller than given tolerance. If the step was rejected we halved the step-size because then 'old' $a_1$ could be used as a 'new' $b$.

6.2.2. *Midpoint rule.* Here it was convenient to use the auxiliary point $r$ in (5.4) which has to be computed anyway. One can easily check that the local error of $r$ is of order 2. Hence we can take an implicit Euler step from $r$ with the step $h/2$ and compare this value to the value $q$ obtained by the midpoint rule.

6.3. **Projection.** We used Newton's method to solve the systems (5.2), (5.3) and (5.4). The values $q := p$ and $\mu := 0$ were used as initial guesses. The Jacobian was computed symbolically, and it was evaluated at every third step during the iteration of one point. However, usually two iterations were enough. In test problems we typically used $10^{-2} \ldots 10^{-8}$ as an error tolerance for the Newton iteration. For example, in Hénon-Heiles case the error tolerance of the iteration was 0.01 and the distance of the point from $M$ was of the order $10^{-5}$.

Again here we could improve the efficiency. Instead of doing the full Newton iteration, one could try pseudoinverses which would result in a smaller system to be solved. Since we are close to the manifold, one would expect that this kind of iteration would also converge quite rapidly. However, the projection would not be orthogonal anymore, and it is not clear how this would affect the accuracy.

## 7. Numerical examples

7.1. **Pendulum.** The pendulum system is of the form (4.7) with $y \in \mathbb{R}^2$, $\lambda \in \mathbb{R}$, $g(y) = (|y|^2 - 1)/2$, $f = (0,1)$ and $B = I$. The resulting simplified system was given in (4.6). In figure 7.1 there is a solution of (4.6) with quite a large tolerance and with initial value $(x, y, y_1) = (0,1,0,0,0)$. The solution is not very satisfactory since the energy deviates quite rapidly from the correct value and in particular the computed solution goes above the $y^1$–axis although the correct solution would stay all the time below it. This is not surprising because our method is of the first order, so one expects that the energy is also only 'first order correct'. However, one can easily impose the conservation of the energy. It is sufficient to add the energy equation to system (4.6) which yields

$$
\begin{cases}
|y|^2 - 1 = 0 \\
\langle y, y_1 \rangle = 0 \\
\frac{1}{2}|y_1|^2 + y^2 - a = 0 \\
\mathcal{D} = \operatorname{span}(V) \\
V = \big(1, y_1, y_2\big) \\
\begin{pmatrix} 1 & 0 & y^1 \\ 0 & 1 & y^2 \\ y^1 & y^2 & 0 \end{pmatrix} \begin{pmatrix} y_2^1 \\ y_2^2 \\ \lambda \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ |y_1|^2 \end{pmatrix} = 0
\end{cases}
\tag{7.1}
$$

where $a$ is the constant energy. Note that the distribution restricts to the appropriate submanifold. In figure 7.1 there is also a solution of (7.1) with same initial values and same tolerance that were used without the conservation of energy.

In figure 7.2 we show the evolution of the energy in various cases. It is seen that with midpoint method the energy deviates quite slowly from the correct value. Recall that the classical midpoint method is symplectic, so it is perhaps not so surprising that our version of it behaves well with respect conservation of energy. Note that in case of variable step size, the step sizes were between 0.05 and 1, so the case $h = 0.5$ represents a kind of average step size. Anyway let us repeat that adding the energy constraint does not make the system more difficult to solve.

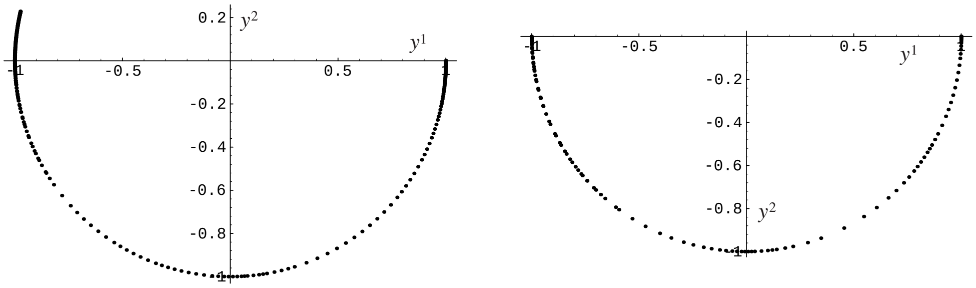



FIGURE 7.1. A solution of system (4.6) and the system (7.1), $0 \leq x \leq 5.1$.

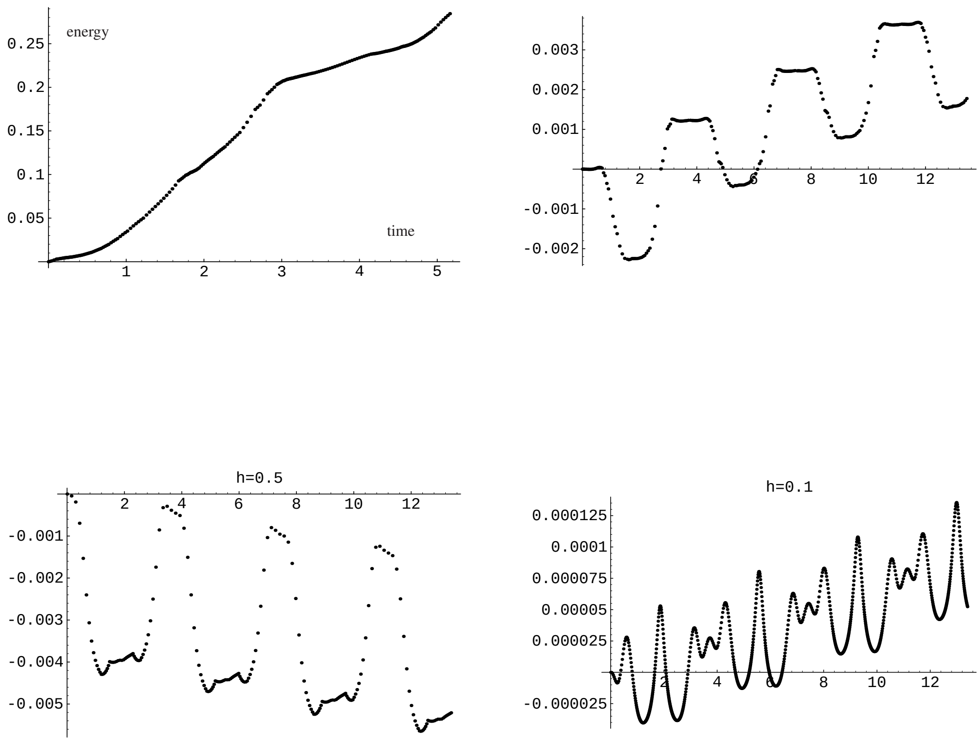



FIGURE 7.2. Evolution of the energy: first with Euler method, then midpoint method using variable stepsize, and midpoint method using step sizes $h = 0.5$ and $h = 0.1$.

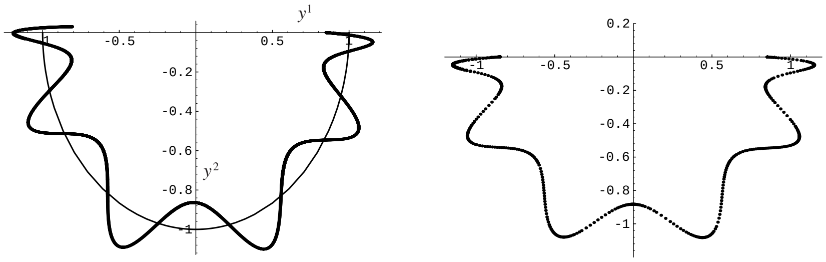



FIGURE 7.3. A solution of system (7.2), $0 \leq x \leq 1.7$, $\varepsilon = 0.1$. Euler method on the left and midpoint method on the right.

7.2. **Stiff pendulum.** Let us then consider the stiff pendulum [17, p. 119] whose involutive form is

$$\begin{cases} y^1_2 + y^1 y^3 = 0 \\ y^2_2 + y^2 y^3 + 1 = 0 \\ \big((y^1)^2 + (y^2)^2\big)\big(\varepsilon^2 y^3 - 1\big)^2 - 1 = 0 \\ \varepsilon^2 y^3_1 + \big(y^1 y^1_1 + y^2 y^2_1\big)\big(\varepsilon^2 y^3 - 1\big)^3 = 0 \\ \big(\varepsilon^2 y^3 - 1\big)\varepsilon^2 y^3_2 - 3\varepsilon^4 (y^3_1)^2 + \big((y^1_1)^2 + (y^2_1)^2 - y^2\big)\big(\varepsilon^2 y^3 - 1\big)^4 - y^3\big(\varepsilon^2 y^3 - 1\big)^2 = 0 \end{cases}$$

Now $y^3$ cannot be solved without introducing square roots, and we want to avoid this. However, we can still do the projection $J_2 \to J_1$. In addition, $y^3_1$ is 'graph-like', so one can get rid of it as well. The simplified system can be written as

$$\begin{cases} \big((y^1)^2 + (y^2)^2\big)\big(\varepsilon^2 y^3 - 1\big)^2 - 1 = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \big(1, y^1_1, y^2_1, -\big(y^1 y^1_1 + y^2 y^2_1\big)\big(\varepsilon^2 y^3 - 1\big)^3/\varepsilon^2, -y^1 y^3, -y^2 y^3 - 1\big) \end{cases} \tag{7.2}$$

Here $V$ is given in symbolic form just for the purposes of illustration. This form is not needed, but if a symbolic form is available, it could be given to the program. This would somewhat speed up the computation.

Let us take $\varepsilon = 0.1$ and compute the solution in the interval $0 \leq x \leq 1.7$ using the initial value $(x, y^1, y^2, y^3, y^1_1, y^2_1) = (0, .85, 0, -17.65, 0, 0)$. In figure 7.3 we show the results obtained with Euler method and the midpoint method. In the former case we needed about 4700 points and in the latter about 500 points. Then in figure 7.4 we computed the solution using the midpoint method with $\varepsilon = 0.01$ and the initial value $(x, y^1, y^2, y^3, y^1_1, y^2_1) = (0, 1, 0, -17.65, 0.016, 0)$. Of course even in the implicit case the step size has to be quite small, because of the rapid oscillations.

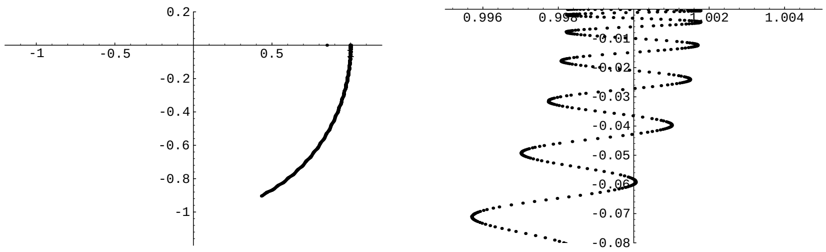



FIGURE 7.4. A solution of system (7.2), $\varepsilon = 0.01$, midpoint method. On the right we have magnified a part of the picture on the left.

7.3. **Discharge pressure control problem.** Let us consider the discharge pressure flow problem given in [17, p. 116], whose involutive form is

$$
\begin{cases}
20y_1^1 + y^1 - y^2 = 0 \\
75y_1^2 + 5y_1^3 + y^3 - c_1 = 0 \\
20y_1^4 + y^5 - f = 0 \\
c_2 y^4 (y^5)^2 - c_3 y^4 y^5 + c_4 y^4 - y^3 = 0 \\
(y^1)^2 (y^4)^2 - c_5 (y^1)^2 + c_6 f^2 = 0 \\
(40 c_2 y^4 y^5 - 20 c_3 y^4) y_1^5 - 20 y_1^3 - c_2 (y^5)^3 + g_1 (y^5)^2 - g_2 y^5 + c_4 f = 0 \\
y^1 y^2 (y^4)^2 - (y^1)^2 y^4 y^5 + f (y^1)^2 y^4 - c_5 y^1 y^2 + c_6 g_3 = 0 \\
20 y^1 \big( (y^4)^2 - c_5 \big) y_1^2 - 20 (y^1)^2 y^4 y_1^5 + (y^2)^2 (y^4)^2 + (y^1)^2 y^4 y^5 - \\
4 y^1 y^2 y^4 y^5 + (y^1)^2 (y^5)^2 - f (y^1)^2 y^4 - 2 f (y^1)^2 y^5 + 4 f y^1 y^2 y^4 + \\
20 f' (y^1)^2 y^4 + f^2 (y^1)^2 - c_5 (y^2)^2 + c_6 g_4 = 0
\end{cases}
\tag{7.3}
$$

where

$$
\begin{array}{lll}
c_1 = 99.1 & c_2 = 0.001 & c_3 = 0.075 \\
c_4 = 3.35 & c_5 = 2458.18 & c_6 = 1/1.44
\end{array}
$$

and

$$
\begin{array}{ll}
f = 5 \tanh(x - 10) + 15 & g_1 = c_2 f + c_3 \\
g_2 = c_3 f + c_4 & g_3 = f^2 + 20 f f' \\
g_4 = f^2 + 60 f f' + 400 (f')^2 + 400 f f'' &
\end{array}
$$

The values of the parameters are as given in [17, p. 116]. We computed the solution with initial value

$$
\begin{aligned}
(x, y, y_1) = (&0, 0.25, 0.25, 99.1, 36.7, 9.998, \\
&0, -8.45 \cdot 10^{-7}, 1.27 \cdot 10^{-5}, 8.5 \cdot 10^{-5}, 1.1 \cdot 10^{-4}).
\end{aligned}
\tag{7.4}
$$

The solution curves obtained with Euler scheme are in figure 7.5 and those obtained with midpoint scheme are in figure 7.6. In [17] only $y^5$ (output) is given and the solution obtained is qualitatively the same as here.

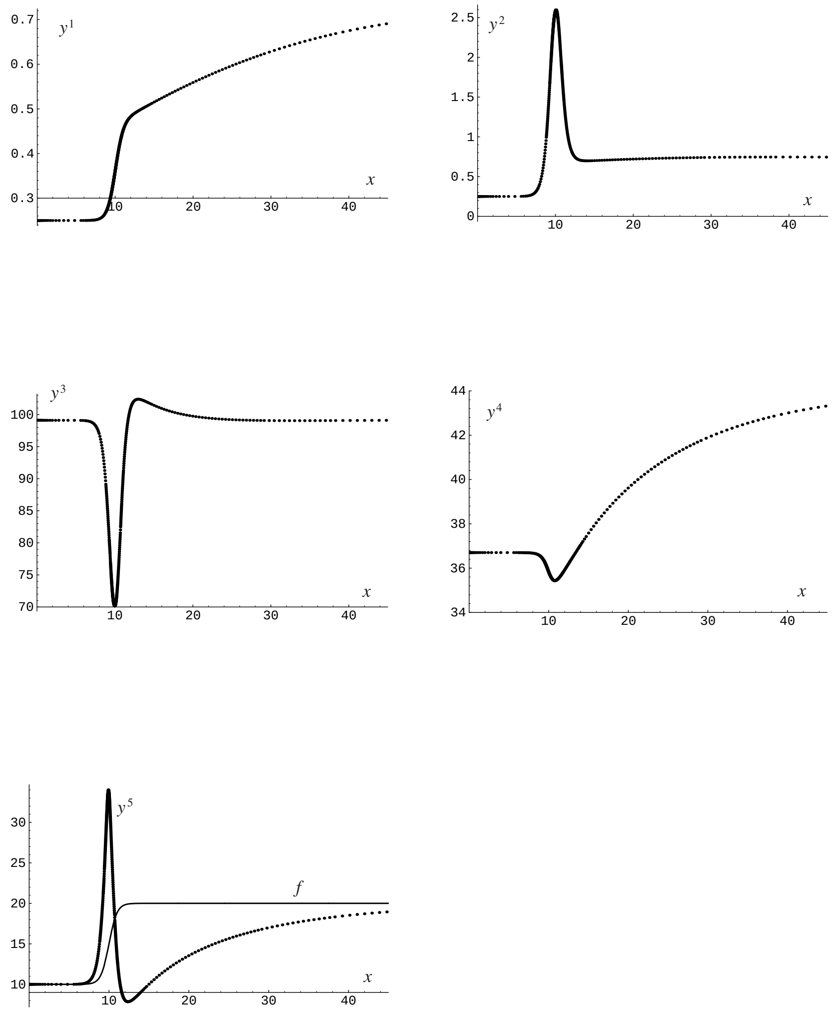



FIGURE 7.5. A solution of system (7.3) with $f = 5\tanh(x-10)+15$ using explicit Euler.

7.4. **Hamiltonian systems.** Let $H : \mathbb{R}^{2n} \to \mathbb{R}$ and let $M = H^{-1}(0)$; then the Hamiltonian system on $\mathbb{R}\times M$ is given by the vector field

$$V = \big(1, \frac{\partial H}{\partial y^{n+1}}, \dots, \frac{\partial H}{\partial y^{2n}}, -\frac{\partial H}{\partial y^{1}}, \dots, -\frac{\partial H}{\partial y^{n}}\big)$$

which defines a distribution on $\mathbb{R}\times M$. If the given system has more invariants (or integrals) then we restrict $V$ to appropriate submanifold of $\mathbb{R}\times M$. Now in many cases (in particular in the examples that follow), the momenta and first order jets are identified, so it is convenient to identify $\mathbb{R}\times\mathbb{R}^{2n}$ and $J_1(\mathbb{R}\times\mathbb{R}^n)$. Hence the system is $\mathcal{R}_1 = \mathbb{R}\times M$. Note that $V$ induces a symplectic flow on $\mathbb{R}^{2n}$. However, the flow restricted to $M$ or $\mathcal{R}_1$ is not symplectic.

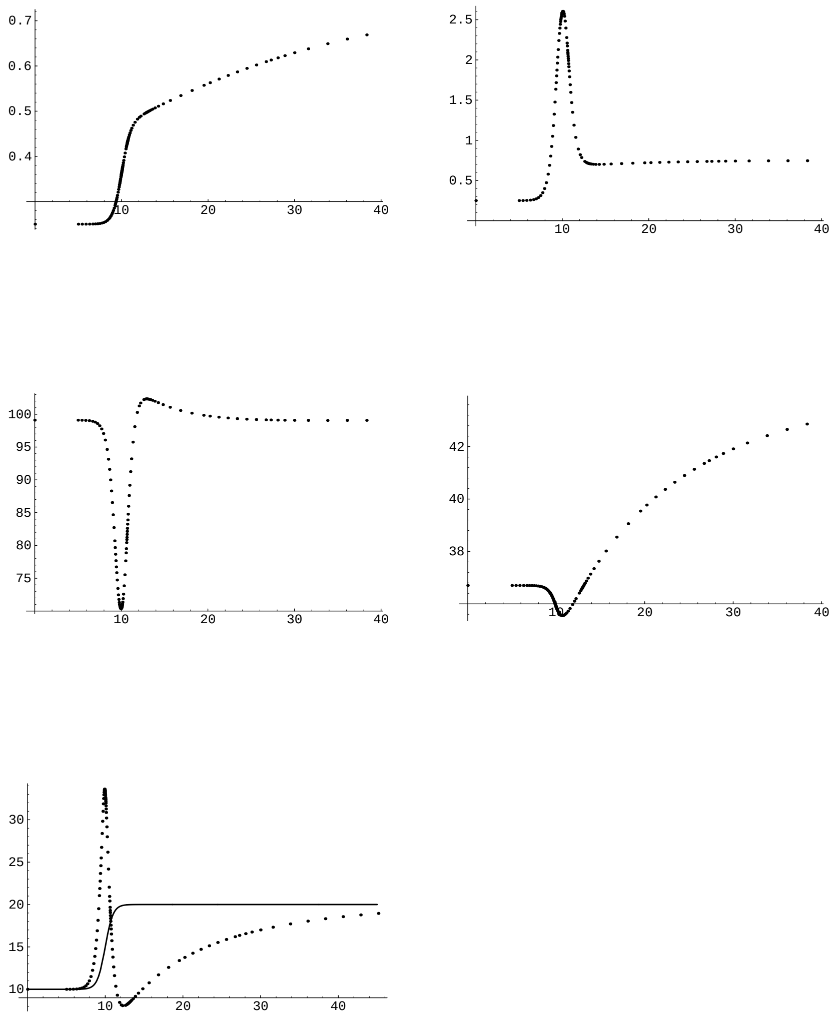



FIGURE 7.6. A solution of system (7.3) with $f = 5\tanh(x-10)+15$ using midpoint method.

Consider the following Kepler problem [49, p. 6]

$$
\begin{cases}
\frac{1}{2}\left|y_1\right|^2 - \dfrac{1}{|y|} - a = 0 \\
y^1 y_1^2 - y^2 y_1^1 - b = 0 \\
\mathcal{D} = \operatorname{span}(V) \\
V = \left(1, y_1^1, y_1^2, -y^1/\left|y\right|^3, -y^2/\left|y\right|^3\right)
\end{cases}
\tag{7.5}
$$

where $a$ and $b$ are constants (energy and angular momentum). The analytic solution is periodic with period $2\pi$. In figure 7.7 we show two solutions with same initial values, $(x, y, y_1) = (0, 0.5, 0, 0, 1.73)$; on the left with the Euler method and on the right with the midpoint method. The tolerances were chosen such that qualitatively the solutions were similar. The solutions were computed for $0 \leq x \leq 100$ and with the Euler method about 8000 points was needed while for the midpoint method about 900 points was sufficient.

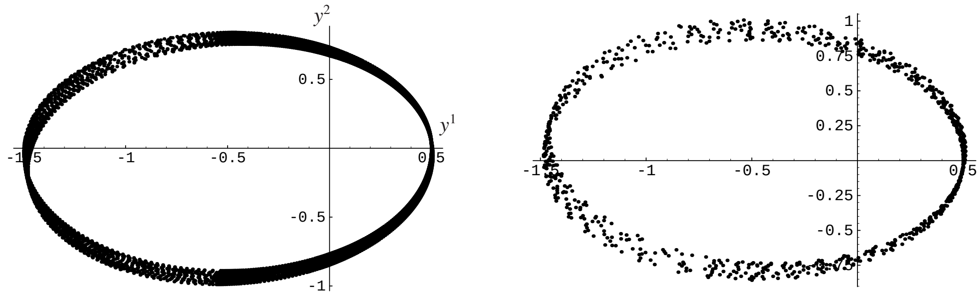



FIGURE 7.7. A solution of the Kepler problem (7.5) with Euler and midpoint methods.

Next we take Hénon-Heiles system [49, p. 13]

$$
\begin{cases} \frac{1}{2}\left|y_1\right|^2 + \frac{1}{2}\left|y\right|^2 + (y^1)^2 y^2 - \frac{1}{3}(y^2)^3 - a = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \left(1, y_1^1, y_1^2, y^1 + 2y^1 y^2, y^2 + (y^1)^2 - (y^2)^2\right) \end{cases} \tag{7.6}
$$

where $a$ is again the (constant) energy. For this system we took as an initial value $(x, y, y_1) = (0, 0.12, 0.12, 0.12, 0.12)$, which yields quasiperiodic solutions. We computed the solution with both methods, $0 \leq x \leq 303$. In figure 7.8 we have plotted the values of the solution in the $(y^2, y_1^2)$–plane when the hyperplane $y^1 = 0$ was crossed. On the left there is the solution with Euler method (101 points) and on the right the solution with the midpoint method (141 points). With the Euler method, 5000 points had to be computed and with the midpoint method 2500. The plots should yield closed curves rather than the spirals that can be seen in the pictures. However, the results are quite satisfactory, taking into account the fact that tolerances were not particularly strict and methods are of low order.

7.5. **Mechanical system.** As a final example we consider the system given in [30]. It is of the form (4.7) with $y \in \mathbb{R}^{12}$, $\lambda \in \mathbb{R}^5$, $B = I_{12}$, $f = \nabla F$, where $F = 5/2\langle y, Ky\rangle$ and $K$ and $g$ are given by

$$
K = \begin{pmatrix} I_2 & 0 & -I_2 & 0 & 0 & 0 \\ 0 & I_2 & 0 & -I_2 & 0 & 0 \\ -I_2 & 0 & 2I_2 & 0 & -I_2 & 0 \\ 0 & -I_2 & 0 & 2I_2 & 0 & -I_2 \\ 0 & 0 & -I_2 & 0 & I_2 & 0 \\ 0 & 0 & 0 & -I_2 & 0 & I_2 \end{pmatrix} \qquad g(y) = \frac{1}{2}\begin{pmatrix} (y^1 - y^3)^2 + (y^2 - y^4)^2 - 1 \\ (y^3 - y^5)^2 + (y^4 - y^6)^2 - 1 \\ (y^5 - y^7)^2 + (y^6 - y^8)^2 - 1 \\ (y^7 - y^9)^2 + (y^8 - y^{10})^2 - 1 \\ (y^9 - y^{11})^2 + (y^{10} - y^{12})^2 - 1 \end{pmatrix}
$$

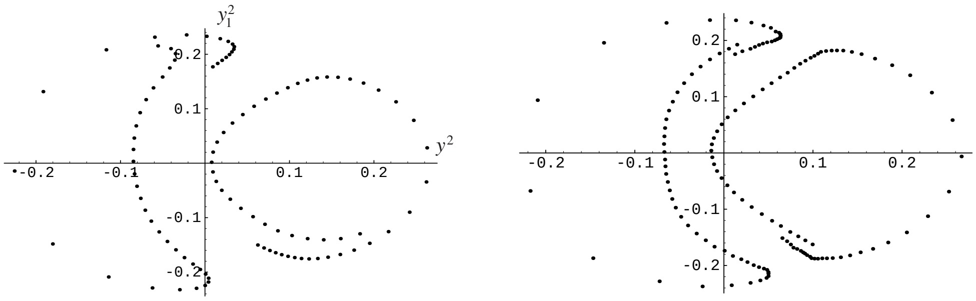



FIGURE 7.8. The Poincaré sections for Hénon-Heiles system 7.6 with Euler method on the left and midpoint method on the right.

Variables $y^1, \ldots, y^{12}$ are coordinates of six points in the plane. In this case the system (4.8) can be written as

$$\mathcal{R}_1 \; : \; \begin{cases} g(y) = 0 \\ dg\, y_1 = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \big(1, y_1, -(dg)^t\lambda - 5Ky\big) \\ dg(dg)^t\lambda + 5\, dg\, Ky - d^2g\,(y_1, y_1) = 0 \end{cases} \tag{7.7}$$

So the final problem is in $J_1(\mathbb{R}\times\mathbb{R}^{12}) \simeq \mathbb{R}^{25}$ and $\dim(\mathcal{R}_1) = 15$. It can readily be verified that treating Lagrange multipliers like other variables and transforming the system into involutive form produces a 15-dimensional system in 52-dimensional ambient space.

The energy of the system is

$$E = \frac{1}{2}\,|y_1|^2 + \frac{5}{2}\langle y, Ky\rangle$$

In figure 7.9 we show the evolution of energy for the Euler and midpoint methods, and like in the pendulum case, the midpoint method remains quite close to the correct manifold. In figure 7.10 we show the time evolution of the configuration of the system (7.7) with initial value

$$\begin{aligned}(x, y, y_1) = (&0, 0, 0, 0.5, 0.866, 1, 0, 1.5, 0.866, 2, 0, 2.5, 0.866,\\ &1, -5.77, -1, -4.62, 1, -3.464, -1, -2.31, 1, -1.155, -1, 0).\end{aligned}$$

For small values of $x$, the solutions with both methods are very similar so we have plotted only one figure. For bigger values of $x$, the energy in the Euler case starts to grow quite fast, so the results also soon become quite different in the two cases.

Now adding the energy equation gives the system

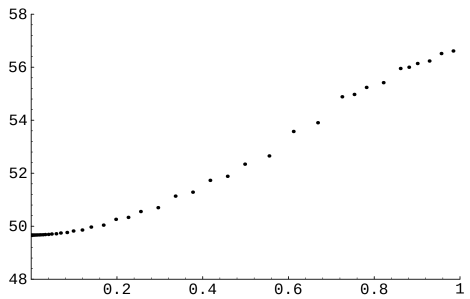
$$\begin{cases} g(y) = 0 \\ dg\, y_1 = 0 \\ \frac{1}{2}\,|y_1|^2 + \frac{5}{2}\langle y, Ky\rangle - a = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \big(1, y_1, -(dg)^t\lambda - 5Ky\big) \\ dg(dg)^t\lambda + 5dgKy - d^2g\,(y_1, y_1) = 0 \end{cases} \tag{7.8}$$

where $a$ is the constant energy. Solution of the system (7.8) is given in figure 7.11 where the configurations are given at same time instants as in figure 7.10. The same initial values and same tolerance were used as for system (7.7). Again there was practically no difference between the solutions obtained with Euler and midpoint methods, so only one plot is given. However, comparing the results obtained with conservation of energy to those obtained without conservation of energy, it is seen that the results become quite different very rapidly. This is surprising because the midpoint method remains rather close to the energy surface even without explicit conservation of energy. The same phenomenon was also observed with other initial values.

## 8. Conclusion

We have introduced a new framework to treat arbitrary systems of ODEs and DAEs. The main notion which emerges is the involutivity of the system, and we have seen that using involutive form in the computations (and analysis) leads to rather different conclusions than the traditional treatment of such systems. To sum up, let us list a few of them.

- We have not defined DAEs. This is simply because geometrically there is no difference between ODEs and DAEs.
- It is possible to obtain reliable results even with low order explicit methods. Hence DAEs are not intrinsically stiff.



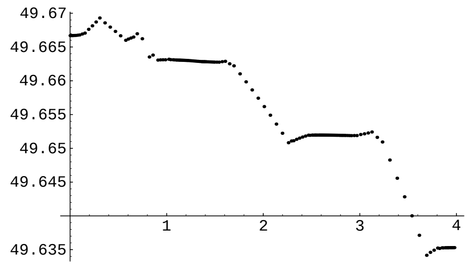




FIGURE 7.9. Evolution of the energy.

- The concept of index is not needed. Hence the index is not related to the numerical difficulty of solving an *involutive* system.
- Because the notion of the solution is more general than the traditional one we obtain more smooth solutions and hence encounter less singularities than in the traditional setting.

This work can be extended in many directions. The most immediate tasks are analysis of higher order methods, and optimizing various subproblems in the implementation. An interesting aspect is also the question of genericity of the system and analysis of the system with respect to perturbations. Also this geometric framework gives tools to analyse various singularities of the system, and in particular discuss the generic singularities of the solutions.

## References

[1] D. V. Alekseevskij, A. M. Vinogradov, and V. V. Lychagin, *Basic ideas and concepts of differential geometry*, Geometry I (R. V. Gamkrelidze, ed.), Encyclopaedia of Mathematical Sciences, vol. 28, Springer, 1991.

[2] E. Allgower and K. Georg, *Numerical continuation methods*, Springer series in computational mathematics, vol. 13, Springer, 1990.

[3] I. Anderson, N. Kamran, and P. J. Olver, *Internal symmetries of differential equations*, Modern group analysis: Advanced analytical and computational methods in mathematical physics (N. H. Ibragimov, M. Torrisi, and A. Valenti, eds.), Kluwer, 1993, pp. 7–21.

[4] V. Arnold, *Geometrical methods in the theory of ordinary differential equations*, Grundlehren, vol. 250, Springer, 1983.

[5] V. I. Arnold, S. M. Gussein-Zade, and A. N. Varchenko, *Singularities of differentiable maps, vol. I*, Birkhäuser, 1985.

[6] V. I. Arnold and Yu. S. Ilyashenko, *Ordinary differential equations*, Dynamical systems I (D. V. Anosov and V. I. Arnold, eds.), Encyclopaedia of Mathematical Sciences, vol. 1, Springer, 1988, pp. 1–148.

[7] T. Arponen and J. Tuomela, *On the numerical solution of involutive ordinary differential systems: Numerical results*, Research Report A370, Helsinki University of Technology, 1996.

[8] M. Berz, C. Bischof, G. Corliss, and A. Griewank (eds.), *Computational differentiation*, SIAM, 1996.

[9] K. Brenan, S. Campbell, and L. Petzold, *Numerical solution of initial-value problems in differential-algebraic equations*, North-Holland, 1989.

[10] É. Cartan, *Les systèmes différentiels extérieurs et leurs applications géométriques*, Hermann, 1945.

[11] P. Crouch and R. Grossman, *Numerical integration of ordinary differential equations on manifolds*, Nonlinear Science **3** (1993), 1–33.

[12] L. Dara, *Singularités génériques des équations différentielles multiformes*, Bol. Soc. Bras. Mat. **6** (1975), 95–128.

[13] M. do Carmo, *Riemannian geometry*, Birkhäuser, 1992.

[14] P. I. Dudnikov and S. N. Samborski, *Linear overdetermined systems of partial differential equations*, Partial differential equations VIII (M. A. Shubin, ed.), Encyclopaedia of Mathematical Sciences, vol. 65, Springer, 1996, pp. 1–86.

[15] C. Ehresmann, *Les prolongements d'une variété différentielle I: Calcul des jets, prolongement principal*, C. R. Acad. Sc. Paris **233** (1951), 598–600.

[16] H. Goldschmidt, *Integrability criteria for systems of non-linear partial differential equations*, J. Diff. Geom. **1** (1967), 269–307.

[17] E. Hairer, C. Lubich, and M. Roche, *The numerical solution of differential-algebraic systems by Runge-Kutta methods*, Lecture notes in mathematics, vol. 1409, Springer, 1989.

[18] E. Hairer and G. Wanner, *Solving ordinary differential equations II, Stiff and differential-algebraic problems*, Springer series in comp. math., vol. 14, Springer, 1991.

[19] A. Iserles, *Beyond the classical theory of computational ordinary differential equations*, State of the Art in Numerical Analysis (I.S. Duff and G.A. Watson, eds.), Oxford University Press, 1996.
[20] ______, *Numerical methods on (and off) manifolds*, Foundations of Computational Mathematics (F. Cucker, ed.), Springer-Verlag, 1997, pp. 180–189.
[21] A. Iserles and S. Nørsett, *On the solution of linear differential equations in Lie groups*, Technical Report 1997/NA3, DAMTP, University of Cambridge, 1997.
[22] M. Janet, *Leçons sur les systèmes d'équations aux dérivées partielles*, Gauthier-Villars, 1929.
[23] E. Kähler, *Einführung in die Theorie der Systeme von Differentialgleichungen*, Chelsea, 1949.
[24] I. Kaplansky, *An introduction to differential algebra*, Hermann, 1957.
[25] I. Kolář, P. Michor, and J. Slovák, *Natural operations in differential geometry*, Springer, 1993.
[26] T. Korvola, *On the formal integrability of differential algebraic systems*, Research Report A381, Helsinki University of Technology, 1997.
[27] I. S. Krasilshchik, V. V. Lychagin, and A. M. Vinogradov, *Geometry of jet spaces and nonlinear partial differential equations*, Advanced studies in contemporary mathematics, vol. 1, Gordon & Breach, 1986.
[28] A. Kumpera and D. Spencer, *Lie equations, volume 1 : General theory*, Annals of mathematics studies vol 73, Princeton university press, 1972.
[29] M. Kuranishi, *Lectures on involutive systems of partial differential equations*, Publicações da sociedade de matemática de São Paulo, 1967.
[30] B. Leimkuhler and R. Skeel, *Symplectic numerical integrators in constrained Hamiltonian systems*, J. Comp. Phys. **112** (1994), 117–125.
[31] V. V. Lychagin (ed.), *The interplay between differential geometry and differential equations*, Amer. Math. Soc. Translations, vol. 167, Amer. Math. Soc., 1995.
[32] R. März, *Numerical methods for differential-algebraic equations*, Acta numerica **1** (1992), 141–198.
[33] H. Munthe-Kaas, *Lie-Butcher theory for Runge-Kutta methods*, BIT **35** (1995), 572–587.
[34] ______, *High order Runge-Kutta methods on manifolds*, Technical Report 1997/NA14, DAMTP, University of Cambridge, 1997.
[35] H. Munthe-Kaas and A. Zanna, *Numerical integration of differential equations on homogeneous manifolds*, Foundations of Computational Mathematics (F. Cucker, ed.), Springer Verlag, 1997, pp. 305–315.
[36] P. J. Olver, *Equivalence, invariants, and symmetry*, Cambridge university press, 1995.
[37] O.-P. Piirilä and J. Tuomela, *Differential-algebraic systems and formal integrability*, Research Report A326, Helsinki University of Technology, Institute of Mathematics, 1993.
[38] J. F. Pommaret, *Systems of partial differential equations and Lie pseudogroups*, Mathematics and its applications, vol. 14, Gordon and Breach Science Publishers, 1978.
[39] ______, *Differential Galois theory*, Mathematics and its applications, vol. 15, Gordon and Breach Science Publishers, 1983.
[40] ______, *Lie pseudogroups and mechanics*, Mathematics and its applications, vol. 16, Gordon and Breach Science Publishers, 1988.
[41] ______, *Partial differential equations and group theory*, Kluwer, 1994.
[42] P. Rabier and W. Rheinboldt, *A general existence and uniqueness theory for implicit differential-algebraic equations*, Diff. Int. Eqns. **4** (1991), 563–582.
[43] ______, *A geometric treatment of implicit differential-algebraic equations*, J. Diff. Eqns. **109** (1994), 110–146.
[44] S. Reich, *On an existence and uniqueness theory for nonlinear differential-algebraic equations*, Circuits, systems and signal proc. **10** (1991), 343–359.
[45] W. Rheinboldt, *Differential-algebraic systems as differential equations on manifolds*, Math. Comp **43** (1984), 473–482.
[46] C. Riquier, *Les systèmes d'équations aux dérivées partielles*, Gauthier-Villars, 1910.
[47] J. F. Ritt, *Differential algebra*, AMS Colloquium Publications, vol. 33, Am. Math. Soc., 1950, Dover, 1966.
[48] D. Saunders, *The geometry of jet bundles*, London Math. Soc. Lecture note series, vol. 142, Cambridge university press, 1989.
[49] J. M. Sanz Serna and M. P. Calvo, *Numerical Hamiltonian problems*, Chapman & Hall, 1994.

[50] D. Spencer, *Overdetermined systems of linear partial differential equations*, Bull. Am. Math. Soc **75** (1969), 179–239.
[51] M. Spivak, *A comprehensive introduction to differential geometry, vol 1 - 5, 2nd ed.*, Publish or Perish, 1979.
[52] N. Tarkhanov, *Complexes of differential operators*, Kluwer, 1995.
[53] R. Thom, *Les singularités des applications différentiables*, Ann. Inst. Fourier **6** (1956), 43–87.
[54] J. Tuomela, *On the numerical solution of involutive ordinary differential systems*, Research Report A363, Helsinki University of Technology, 1996.
[55] ______, *On singular points of quasilinear differential and differential-algebraic equations*, BIT **37** (1997), 966–975.
[56] ______, *On the resolution of singularities of ordinary differential systems*, Research Report A388, Helsinki University of Technology, 1997.
[57] A. M. Vershik and V. Ya. Gershkovich, *Nonholonomic dynamical systems, geometry of distributions and variational problems*, Dynamical systems VII (V. I. Arnold and S. P. Novikov, eds.), Encyclopaedia of Mathematical Sciences, vol. 16, Springer, 1994, pp. 1–81.
[58] G. Le Vey, *Differential-algebraic equations: a new look at the index*, Research Report 808, IRISA, 1994.
[59] A. M. Vinogradov, Math. rev. 81 f:58046, 1981.
[60] S. Wolfram, *Mathematica: a system for doing mathematics by computer, 2nd ed.*, Addison-Wesley, 1991.
[61] A. Zanna, *Lie group methods for isospectral flows*, Technical Report 1997/NA2, DAMTP, University of Cambridge, 1997.
[62] A. Zanna and H. Munthe-Kaas, *Iterated commutators, Lie's reduction method and ordinary differential equations on matrix Lie groups*, Foundations of Computational Mathematics (F. Cucker, ed.), Springer-Verlag, 1997, pp. 434–441.

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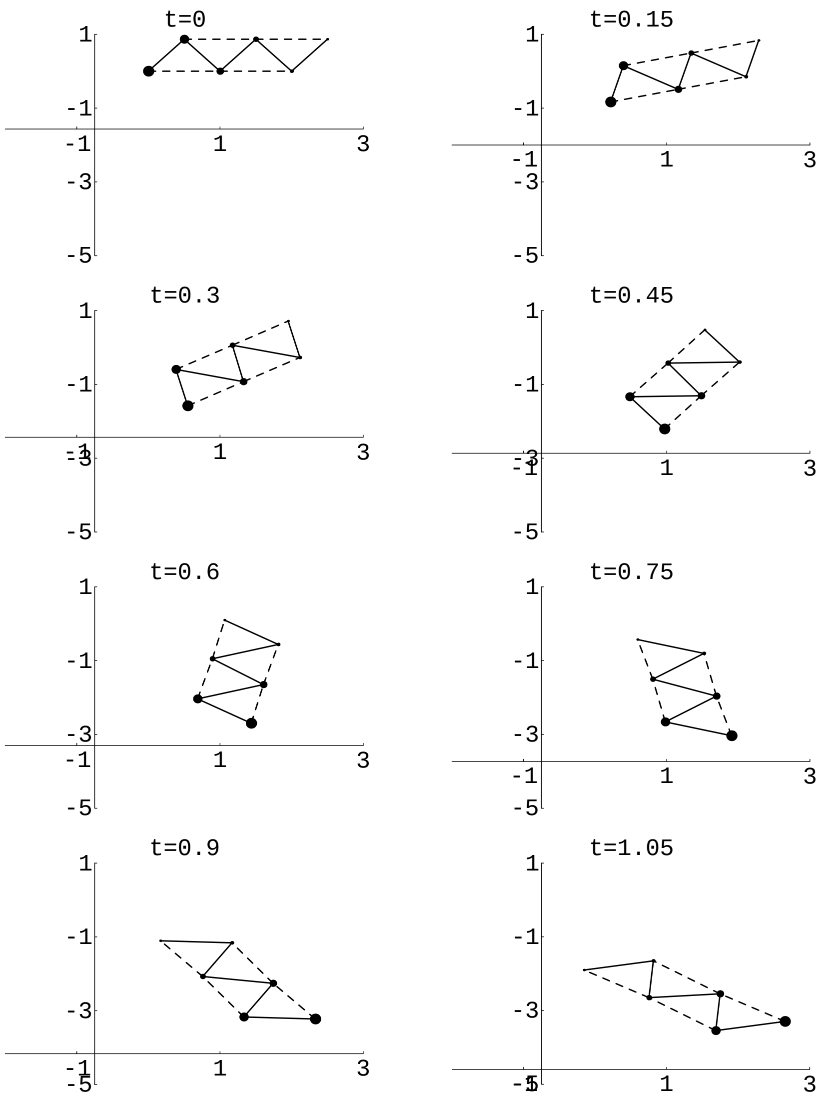


FIGURE 7.10. Evolution of the configuration of the system (7.7) without conservation of energy.

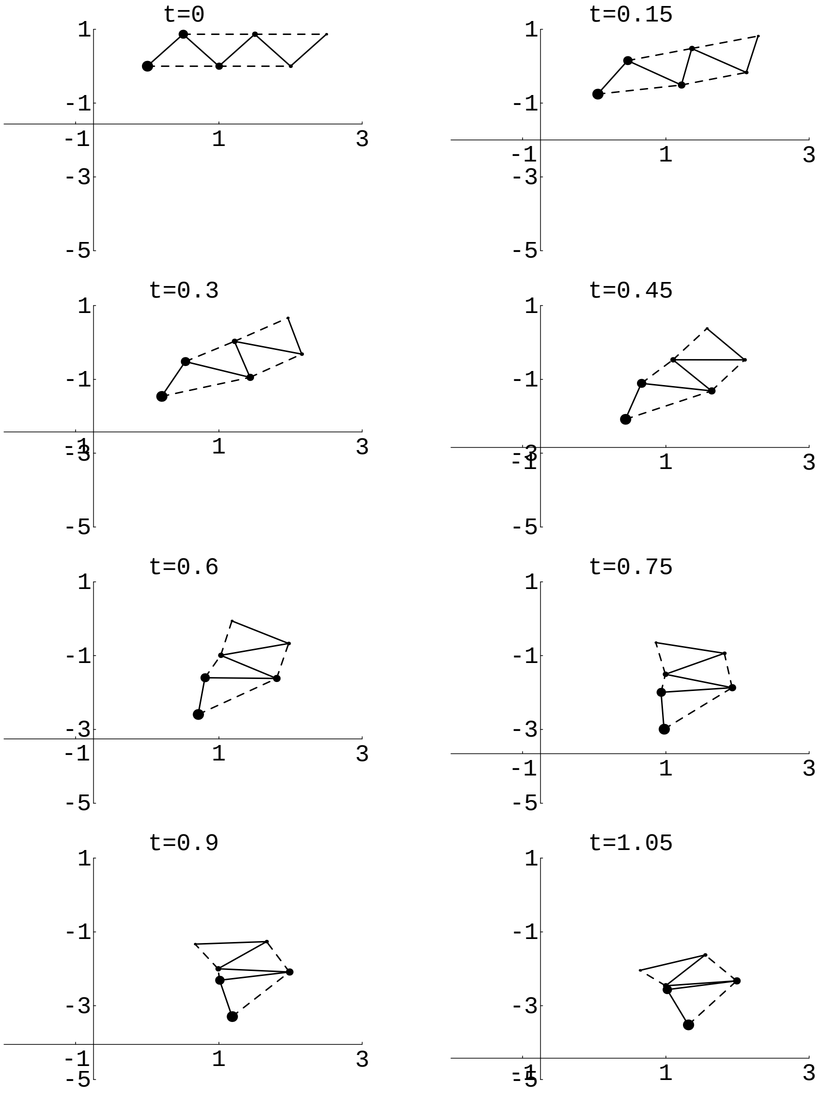


FIGURE 7.11. Evolution of the configuration of the system (7.8) with conservation of energy.