Chapter 1
Introduction

The dynamical behavior of physical processes is usually modeled via differential equations. But if the states of the physical system are in some ways constrained, like for example by conservation laws such as Kirchhoff's laws in electrical networks, or by position constraints such as the movement of mass points on a surface, then the mathematical model also contains algebraic equations to describe these constraints. Such systems, consisting of both differential and algebraic equations are called *differential-algebraic systems, algebro-differential systems*, *implicit differential equations* or *singular systems*.

The most general form of a differential-algebraic equation is

$$F(t, x, \dot{x}) = 0, \tag{1.1}$$

with $F\colon \mathbb{I} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}} \to \mathbb{C}^m$, where $\mathbb{I} \subseteq \mathbb{R}$ is a (compact) interval and $\mathbb{D}_x, \mathbb{D}_{\dot{x}} \subseteq \mathbb{C}^n$ are open, $m, n \in \mathbb{N}$. The meaning of the quantity $\dot{x}$ is ambiguous as in the case of ordinary differential equations. On one hand, it denotes the derivative of a differentiable function $x\colon \mathbb{I} \to \mathbb{C}^n$ with respect to its argument $t \in \mathbb{I}$. On the other hand, in the context of (1.1), it is used as an independent variable of F. The reason for this ambiguity is that we want F to determine a differentiable function x that solves (1.1) in the sense that $F(t, x(t), \dot{x}(t)) = 0$ for all $t \in \mathbb{I}$.

In connection with (1.1), we will discuss the question of existence of solutions. Uniqueness of solutions will be considered in the context of initial value problems, when we additionally require a solution to satisfy the condition

$$x(t_0) = x_0 \tag{1.2}$$

with given $t_0 \in \mathbb{I}$ and $x_0 \in \mathbb{C}^n$, and boundary value problems, where the solution is supposed to satisfy

$$b(x(\underline{t}\,), x(\,\overline{t}\,)) = 0 \tag{1.3}$$

with $b\colon \mathbb{D}_x \times \mathbb{D}_x \to \mathbb{C}^d$, $\mathbb{I} = [\,\underline{t}, \overline{t}\,]$ and some problem dependent integer d. It will turn out that the properties of differential-algebraic equations reflect the properties of differential equations as well as the properties of algebraic equations, but also that other phenomena occur which result from the mixture of these different types of equations.

Although the basic theory for linear differential-algebraic equations with constant coefficients

$$E\dot{x} = Ax + f(t), \tag{1.4}$$

where $E, A \in \mathbb{C}^{m,n}$ and $f : \mathbb{I} \to \mathbb{C}^m$, has already been established in the nineteenth century by the fundamental work of Weierstraß [223], [224] and Kronecker [121] on matrix pencils, it took until the pioneering work of Gear [90] for the scientific communities in mathematics, computer science, and engineering to realize the large potential of the theory of differential-algebraic equations in modeling dynamical systems. By this work and the subsequent developments in numerical methods for the solution of differential-algebraic equations, it became possible to use differential-algebraic equations in direct numerical simulation. Since then an explosion of the research in this area has taken place and has led to a wide acceptance of differential-algebraic equations in the modeling and simulation of dynamical systems. Despite the wide applicability and the great importance, only very few monographs and essentially no textbooks are so far devoted to this subject, see [29], [100], [105], [182]. Partially, differential-algebraic equations are also discussed in [11], [42], [43], [72], [79], [108], [181].

Until the work of Gear, implicit systems of the form (1.1) were usually transformed into ordinary differential equations

$$\dot{y} = g(t, y) \tag{1.5}$$

via analytical transformations. One way to achieve this is to explicitly solve the constraint equations analytically in order to reduce the given differential-algebraic equation to an ordinary differential equation in fewer variables. But this approach heavily relies on either transformations by hand or symbolic computation software which are both not feasible for medium or large scale systems.

Another possibility is to differentiate the algebraic constraints in order to get an ordinary differential equation in the same number of variables. Due to the necessary use of the implicit function theorem, this approach is often difficult to perform. Moreover, due to possible changes of bases, the resulting variables may have no physical meaning. In the context of numerical solution methods, it was observed in this approach that the numerical solution may drift off from the constraint manifold after a few integration steps. For this reason, in particular in the simulation of mechanical multibody systems, stabilization techniques were developed to address this difficulty. But it is in general preferable to develop methods that operate directly on the given differential-algebraic equation.

In view of the described difficulties, the development of numerical methods that can be directly applied to the differential-algebraic equation has been the subject of a large number of research projects in the last thirty years and many different directions have been taken. In particular, in combination with modern modeling tools (that automatically generate models for substructures and link them together via constraints), it is important to develop generally applicable numerical methods as well as methods that are tailored to a specific physical situation. It would be ideal if such an automatically generated model could be directly transferred to a numerical simulation package via an appropriate interface so that in practical design problems the engineer can optimize the design via a sequence of modeling and simulation steps. To obtain such a general solution package for differential-algebraic equations is an active area of current research that requires strong interdisciplinary cooperation between researchers working in modeling, the development of numerical methods, and the design of software. A major difficulty in this context is that still not all of the analytical and numerical properties of differential-algebraic systems are completely understood. In particular, the treatment of bifurcations or switches in nonlinear systems and the analysis and numerical solution of heterogeneous (coupled) systems combined of differential-algebraic equations and partial differential equations (sometimes called partial differential-algebraic equations) represent major research tasks.

It is the purpose of this textbook to give a coherent introduction to the theoretical analysis of differential-algebraic equations and to present some appropriate numerical methods for initial and boundary value problems. For the analysis of differential-algebraic equations, there are several paths that can be followed. A very general approach is given by the geometrical analysis initiated by Rheinboldt [190], see also [182], to study differential-algebraic equations as differential equations on manifolds. We will discuss this topic in Section 4.5. Our main approach, however, will be the algebraic path that leads from the theory of matrix pencils by Weierstraß and Kronecker via the fundamental work of Campbell on derivative arrays [44] to canonical forms for linear variable coefficient systems [123], [124] and their extensions to nonlinear systems in the work of the authors ([128], [129], [131], [132]).

This algebraic approach not only gives a systematic approach to the classical analysis of regular differential-algebraic equations, but it also allows the study of generalized solutions and the treatment of over- and underdetermined systems as well as control problems. At the same time, it leads to new discretization methods and new numerical software.

Unfortunately, the simultaneous development of the theory in many different research groups has led to a large number of slightly different existence and uniqueness results, particularly based on different concepts of the so-called index. The general idea of all these index concepts is to measure the degree of smoothness of the problem that is needed to obtain existence and uniqueness results. To set our presentation in perspective, we now briefly discuss the most common approaches.

1.1 Solvability concepts

In order to develop a theoretical analysis for system (1.1), one has to specify the kind of solution that one is interested in, i.e., the function space in which the solution should lie. In this textbook, we will mainly discuss two concepts, namely classical (continuously differentiable) solutions and weak (distributional) solutions, although other concepts have been studied in the literature, see, e.g., [148], [149].

For the classical case, we use the following solvability definition, the distributional case will be discussed in detail in Sections 2.4 and 3.5.

Definition 1.1. Let $C^k(\mathbb{I}, \mathbb{C}^n)$ denote the vector space of all k-times continuously differentiable functions from the real interval $\mathbb{I}$ into the complex vector space $\mathbb{C}^n$.

1. A function $x \in C^1(\mathbb{I}, \mathbb{C}^n)$ is called a *solution* of (1.1), if it satisfies (1.1) pointwise.
2. The function $x \in C^1(\mathbb{I}, \mathbb{C}^n)$ is called a *solution of the initial value problem* (1.1) with initial condition (1.2), if it furthermore satisfies (1.2).
3. An initial condition (1.2) is called *consistent* with F, if the associated initial value problem has at least one solution.

In the following, a problem is called *solvable* if it has at least one solution. This definition seems natural but it should be noted that in most of the previous literature, the term solvability is used only for systems which have a unique solution when consistent initial conditions are provided. For comparison with Definition 1.1, consider the solvability condition given in [29, Def. 2.2.1].

If the solution of the initial value problem is not unique which is, in particular, the case in the context of control problems, then further conditions have to be specified to single out specific desired solutions. We will discuss such conditions in Section 3.4 and in the context of control problems in Sections 2.5, 3.6, and 4.4.

1.2 Index concepts

In the analysis of linear differential-algebraic equations with constant coefficients (1.4), all properties of the system can be determined by computing the invariants of the associated matrix pair (E, A) under equivalence transformations. In particular, the size of the largest Jordan block to an infinite eigenvalue in the associated Kronecker canonical form [88], called *index*, plays a major role in the analysis and determines (at least in the case of so-called regular pairs) the smoothness that is needed for the inhomogeneity f in (1.4) to guarantee the existence of a classical solution. Motivated by this case, it was first tried to define an analogous index for linear time-varying systems and then for general implicit systems, see [95]. However, it was soon realized that a direct generalization by linearization and consideration of the local linearized constant coefficient system does not lead to a reasonable concept. The reason is that important invariants of constant coefficient systems are not even locally invariant under nonconstant equivalence transformations. This observation led to a multitude of different index concepts even for linear systems with variable coefficients, see [53]. Among the different approaches, the *differentiation index* and the *perturbation index* are currently the most widely used concepts in the literature. We will give formal definitions in Sections 3.3 and 3.4, respectively.

Loosely speaking, the differentiation index is the minimum number of times that all or part of (1.1) must be differentiated with respect to t in order to determine $\dot{x}$ as a continuous function of t and x. The motivation for this definition is historically based on the procedure to solve the algebraic equations (using their derivatives if necessary) by transforming the implicit system to an ordinary differential equation. Although the concept of the differentiation index is widely used, it has a major drawback, since it is not suited for over- and underdetermined systems. The reason for this is that it is based on a solvability concept that requires unique solvability. In our presentation, we will therefore focus on the concept of the *strangeness index* [123], [128], [129], [132], which generalizes the differentiation index to over- and underdetermined systems. We will not discuss other index concepts such as the *geometric index* [190], the *tractability index* [100], [148], [149] or the *structural index* [161]. A different index concept that is of great importance in the numerical treatment of differential-algebraic equations is the *perturbation index* that was introduced in [105] to measure the sensitivity of solutions with respect to perturbations of the problem. For a detailed analysis and a comparison of various index concepts with the differentiation index, see [53], [92], [147], [150], [156], [189].

At this point, it seems appropriate to introduce some philosophical discussion concerning the counting in the different index definitions. First of all, the motivation to introduce an index is to classify different types of differential-algebraic equations with respect to the difficulty to solve them analytically as well as numerically. In view of this classification aspect, the differentiation index was introduced to determine how far the differential-algebraic equation is away from an ordinary differential equation, for which the analysis and numerical techniques are well established. But purely algebraic equations, which constitute another important special case of (1.1), are equally well analyzed. Furthermore, it would certainly not make sense to turn a uniquely solvable classical linear system $Ax = b$ into a differential equation, since then the solution would not be unique anymore without specifying initial conditions. In view of this discussion, it seems desirable to classify differential-algebraic equations by their distance to a decoupled system of ordinary differential equations and purely algebraic equations. Hence, from our point of view, the index of an ordinary differential equation and that of a system of algebraic equations should be the same.

This differs from the differentiation index, for which an ordinary differential equation has index zero, while an algebraic equation has index one. Although the research community and also people working in applications have widely accepted this way of counting, in the concept of the strangeness index ordinary differential equations and purely algebraic equations both have index zero. We will present further arguments for this way of counting on several occasions throughout this textbook.

1.3 Applications

We will now discuss some elementary examples of differential-algebraic equations arising in applications such as electrical networks, multibody systems, chemical engineering, semidiscretized Stokes equations and others.

Let us first consider an example arising in electrical circuit simulation. For this topic, there is an extensive literature that includes the classification of properties of the arising differential-algebraic equations depending on the components of the network, see, e.g., [18], [83], [84], [103], [104], [214].

Example 1.2. To obtain a mathematical model for the charging of a capacitor via a resistor, we associate a potential x_i, $i = 1, 2, 3$, with each node of the circuit, see Figure 1.1. The voltage source increases the potential x_3 to x_1 by U, i.e.,

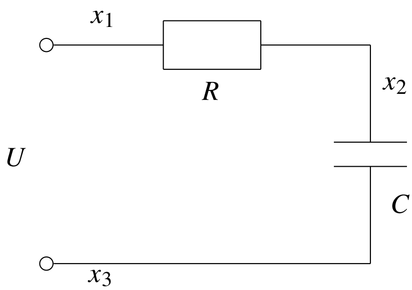

Figure 1.1. A simple electrical network

$x_1 - x_3 - U = 0$. By Kirchhoff's first law, the sum of the currents vanishes in each node. Hence, assuming ideal electronic units, for the second node we obtain that $C(\dot{x}_3 - \dot{x}_2) + (x_1 - x_2)/R = 0$, where R is the size of the resistance of the resistor and C is the capacity of the capacitor. By choosing the zero potential as $x_3 = 0$, we obtain as a mathematical model the differential-algebraic system

$$\begin{aligned} x_1 - x_3 - U &= 0, \\ C(\dot{x}_3 - \dot{x}_2) + (x_1 - x_2)/R &= 0, \\ x_3 &= 0. \end{aligned} \tag{1.6}$$

It is clear that this simple system can be solved for x_3 and x_1 to obtain an ordinary differential equation for x_2 only, combined with algebraic equations for x_1, x_3. This system has differentiation index one.

A second major application area is the simulation of the dynamics of multibody systems, see, e.g., [79], [196], [201], [205].

Example 1.3. A physical pendulum is modeled by the movement of a mass point with mass m in Cartesian coordinates (x, y) under the influence of gravity in a distance l around the origin, see Figure 1.2. With the kinetic energy $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2)$ and the potential energy $U = mgy$, where g is the gravity

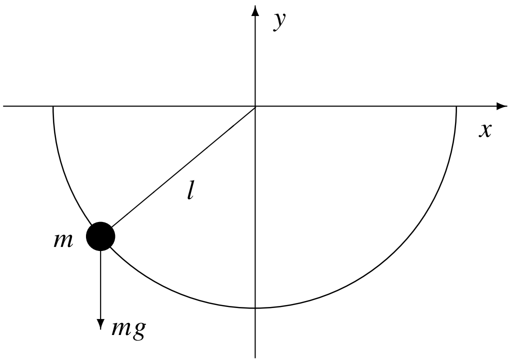

Figure 1.2. A mechanical multibody system

constant, using the constraint equation $x^2 + y^2 - l^2 = 0$, we obtain the Lagrange function

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - mgy - \lambda(x^2 + y^2 - l^2)$$

with Lagrange parameter λ. The equations of motion then have the form

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$$

for the variables $q = x, y, \lambda$, i.e.,

$$\begin{aligned} m\ddot{x} + 2x\lambda &= 0, \\ m\ddot{y} + 2y\lambda + mg &= 0, \\ x^2 + y^2 - l^2 &= 0. \end{aligned} \tag{1.7}$$

It is obvious that this system cannot have differentiation index one, it actually has differentiation index three.

Differential-algebraic equations are also frequently used in the mathematical modeling of chemical reactions, see, e.g., [161].

Example 1.4. Consider the model of a chemical reactor in which a first order isomerization reaction takes place and which is externally cooled.

Denoting by c_0 the given feed reactant concentration, by T_0 the initial temperature, by $c(t)$ and $T(t)$ the concentration and temperature at time t, and by R the reaction rate per unit volume, the model takes the form

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{c} \\ \dot{T} \\ \dot{R} \end{bmatrix} = \begin{bmatrix} k_1(c_0 - c) - R \\ k_1(T_0 - T) + k_2 R - k_3(T - T_C) \\ R - k_3 \exp\left(-\frac{k_4}{T}\right)c \end{bmatrix}, \tag{1.8}$$

where T_C is the cooling temperature (which can be used as control input) and k_1, k_2, k_3, k_4 are constants. If T_C is given, this system has differentiation index one. If T_C is treated as a control variable, the system is underdetermined and the differentiation index is not defined.

Another common source of differential-algebraic equations is the semidiscretization of systems of partial differential equations or coupled systems of partial differential equations and other types of equations, see, e.g., [5], [11], [102], [202].

Example 1.5. The nonstationary Stokes equation is a classical linear model for the laminar flow of a Newtonian fluid [225]. It is described by the partial differential equation

$$u_t = \Delta u + \nabla p, \quad \nabla \cdot u = 0, \tag{1.9}$$

together with initial and boundary conditions. Here u describes the velocity and p the pressure of the fluid. Using the method of lines [209], [211] and discretizing first the space variables with finite element or finite difference methods typically leads to a linear differential-algebraic system of the form

$$\dot{u}_h = Au_h + Bp_h, \quad B^T u_h = 0, \tag{1.10}$$

where u_h and p_h are semi-discrete approximations for u and p. If the nonuniqueness of a free constant in the pressure is fixed by the discretization method, then the differentiation index is well defined for this system. For most discretization methods, it is two, see, e.g., [222].

The study of classical control problems in the modern behavior framework [132], [167] immediately leads to underdetermined DAEs.

Example 1.6. The classical linear control problem to find an input function u that stabilizes the linear control system

$$\dot{x} = Ax + Bu, \quad x(t_0) = x_0 \tag{1.11}$$

can be viewed in the so-called behavior context ([116], [117], [167]) as determining a solution of the underdetermined linear differential-algebraic equation

$$[\, I \;\; 0 \,]\dot{z} = [\, A \;\; B \,]z, \quad [\, I \;\; 0 \,]z(t_0) = x_0 \tag{1.12}$$

such that for $z = \left[\begin{smallmatrix} x \\ u \end{smallmatrix}\right]$ the part $[\, I \;\; 0 \,]z$ is asymptotically stable.

Differential-algebraic equations also play an important role in the analysis and numerical solution of singular perturbation problems, where they represent the limiting case, see, e.g., [108], [159], [221].

Example 1.7. The van der Pol equation

$$\begin{aligned} \dot{y} &= z, \\ \epsilon \dot{z} &= (1 - y^2)z - y, \end{aligned} \tag{1.13}$$

possesses the differential-algebraic equation

$$\begin{aligned} \dot{y} &= z, \\ 0 &= (1 - y^2)z - y \end{aligned} \tag{1.14}$$

as limiting case for $\epsilon \to 0$. The analysis and understanding of (1.14) is essential in the construction of numerical methods that can solve the equation (1.13) for small parameters ϵ.

Many more application areas could be mentioned here, but these few examples already demonstrate the wide applicability of differential-algebraic equations in the mathematical modeling and the numerical solution of application problems.

1.4 How to use this book in teaching

This book is laid out to be and has been used in teaching graduate courses in several different ways.

Chapters 2, 3, and 4 together form a one semester course (approximately 60 teaching hours) on the analysis of differential-algebraic equations. As a prerequisite for such a course, one would need the level that is reached after a first course on the theory of ordinary differential equations.

A course with smaller volume is formed by omitting Sections 2.5, 3.6, and 4.4 on control that depend on each other in this order but are not needed for other sections. An even shorter course is obtained by omitting Sections 2.4 and 3.5 on generalized solutions which depend on each other in this order but again are not needed for other sections. Section 3.4 on generalized inverses is useful for the sections on control but not needed for other sections and can therefore also be omitted to shorten the course. Section 4.2 on structured problems and Section 4.5 on differential equations on manifolds again are not needed for other sections and could be omitted.

A combined one semester course (approximately 60 teaching hours) on the analysis and numerical solution of differential-algebraic equations would need as a prerequisite the level that is reached after a first course on the theory of ordinary differential equations as well as a first course on numerical analysis including the basics of the numerical solution of ordinary differential equations. Such a course would consist of Chapter 2, Section 2.1, Chapter 3, Sections 3.1, 3.2, 3.3, and Chapter 4, Sections 4.1, 4.2, 4.3, concerning the analysis and Chapter 5, Chapter 6, Sections 6.1, 6.2, and Chapter 7 concerning the numerical solution of differential-algebraic equations.

The numerical part of the book, which strongly relies on the analysis part, would represent a separate course (approximately 30 teaching hours) on the numerical solution of initial and boundary value problems for differential-algebraic equations that includes Chapter 5, Chapter 6 Sections 6.1, 6.2 and Chapter 7. A slightly extended course would combine these with Sections 6.3 and 6.4.

The scheme below displays the dependencies between the different sections and may help to organize courses on the basis of this textbook.