Lecture Notes in Mathematics

Edited by A. Dold, B. Eckmann and F. Takens

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The Numerical Solution of Differential-Algebraic Systems by Runge-Kutta Methods

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Preface

The term differential-algebraic equation has been coined to comprise differential equations with constraints (differential equations on manifolds) and singular implicit differential equations. Such problems arise and have to be solved in a variety of applications, e.g., constrained mechanical systems, fluid dynamics, chemical reaction kinetics, simulation of electrical networks, and control engineering. From a more theoretical viewpoint, the study of differential-algebraic problems gives insight into the behaviour of numerical methods for stiff ordinary differential equations. As a consequence, this subject has attracted the interest of many engineers and mathematicians in the last years.

The purpose of these lecture notes is to give a self-contained and comprehensive exposition of the numerical solution of differential-algebraic systems arising in applications, when treated by Runge-Kutta methods, here included also extrapolation methods. While multistep methods (BDF) have been considered since the early seventies (Gear (1971)), the study of Runge-Kutta methods for differential-algebraic systems has begun only a few years ago. Runge-Kutta methods also have interesting computational and theoretical properties. They combine high order with good stability, allow a simple step size selection, are self-starting and have advantages in parallel computing.

The first two sections are introductory and review differential-algebraic problems and Runge-Kutta methods for their numerical solution. In Sections 3 to 6 we study existence and uniqueness of the numerical solution, influence of perturbations, local error and convergence, and asymptotic expansions. We investigate in Sections 7 and 8 the convergence of simplified Newton iterations for the arising nonlinear systems, and the problems of local error estimation and inconsistent starting values. In the final sections we describe a FORTRAN program and apply it to several concrete examples. The sections end with notes which relate the results to the existing literature. Most of the presented material has not been published previously.

We have tried to treat the subject in its various aspects ranging from theory via numerical analysis to implementation and applications. Many of the presented ideas and techniques are not restricted to Runge-Kutta methods, but can also be applied to other integration methods, such as linearly implicit methods and multistep methods.

These lecture notes have their origin in a one-semester graduate course given by one of the authors at the University of Rennes, and in a series of seminars at the University of Geneva, in the years 1987 and 1988.

Contents

1. Description of differential-algebraic problems

We consider problems whose general form is that of an implicit differential equation

$$F(Y', Y) = 0 \tag{1.1}$$

where F and Y are of the same dimension, and F is assumed to have sufficiently many bounded derivatives. A non-autonomous system $F(Y', Y, x) = 0$ is brought to the form (1.1) by adding the equation for the independent variable, $x' = 1$. The initial value $Y(0)$ is supposed to be specified, and the solution $Y(x)$ is sought on a bounded interval $[0, \bar{x}]$. If $\partial F/\partial Y'$ is invertible, then we can formally solve for Y' in (1.1) to obtain an ordinary differential equation. Here we are interested in the case when $\partial F/\partial Y'$ is singular. A convenient classification of such problems is provided by the concept of index.

Index of a differential-algebraic system

We introduce the index as a measure of the sensitivity of the solutions to perturbations in the equation. The relation to other definitions of the index will be discussed at the end of this section.

Definition 1.1. Equation (1.1) has *perturbation index m* along a solution Y on $[0, \bar{x}]$, if m is the smallest integer such that, for all functions $\widehat{Y}$ having a defect

$$F(\widehat{Y}', \widehat{Y}) = \delta(x), \tag{1.2}$$

there exists on $[0, \bar{x}]$ an estimate

$$\|\widehat{Y}(x) - Y(x)\| \le C\big(\|\widehat{Y}(0) - Y(0)\| + \max_{0\le\xi\le x} \|\delta(\xi)\| + \ldots + \max_{0\le\xi\le x} \|\delta^{(m-1)}(\xi)\|\big) \tag{1.3}$$

whenever the expression on the right-hand side is sufficiently small. Here C denotes a constant which depends only on F and the length of the interval.

In the numerical solution of equation (1.1), the influence of perturbations in the discretized equation is of fundamental importance in the analysis of convergence and of roundoff errors. The occurence of the $(m-1)$-th derivative in (1.3) will translate in the numerical solution into a division of the discrete perturbation by h^{m-1}, where h is the (small) discretization parameter.

It is worthwhile to remark that stronger estimates than (1.3) may be available for some components of the difference to the solution.

In obvious terminology we call an equation of index m if it has index m along any solution. As defined above, the perturbation index can not be less than one.

The index 0 case can be included if one interprets $\delta^{(-1)}(\xi)$ as the integral over δ. More precisely, we say that (1.1) has perturbation index 0, if

$$\|\widehat{Y}(x) - Y(x)\| \leq C\big(\|\widehat{Y}(0) - Y(0)\| + \max_{0\leq\xi\leq x} \|\int_0^\xi \delta(t)dt\|\big).$$

It follows from Gronwall's Lemma that this is satisfied for ordinary differential equations $Y' = f(Y)$. Let us now turn to classes of systems of index 1, 2 and 3 which frequently arise in applications. Concrete examples are presented in Section 9.

Systems of index 1

The simplest situation is that of a system of the form

$$y' = f(y, z) \qquad (1.4.a)$$
$$0 = g(y, z) \qquad (1.4.b)$$

(as always in this article, with sufficiently differentiable functions f and g) where

$$g_z \text{ has a bounded inverse} \qquad (1.5)$$

in a neighbourhood of the solution. Here and in the following we adopt the convention to denote partial derivatives by subscripts, so that $g_z = \partial g/\partial z$. The initial value (y_0, z_0) is to be consistent, i.e. $g(y_0, z_0) = 0$.

By the Implicit Function Theorem, z can be extracted from (1.4.b) as a function of y. Inserting it into (1.4.a) then gives an ordinary differential equation. This implies in particular local existence, uniqueness and regularity of the solution. Let us now consider the perturbed system

$$\widehat{y}\,' = f(\widehat{y}, \widehat{z}) + \delta_1(x)$$
$$0 = g(\widehat{y}, \widehat{z}) + \delta_2(x).$$

By the Implicit Function Theorem we get

$$\|\widehat{z}(x) - z(x)\| \leq C_1\big(\|\widehat{y}(x) - y(x)\| + \|\delta_2(x)\|\big),$$

as long as $\|\delta_2(x)\|$ is small and $\widehat{y}(x)$ is sufficiently close to $y(x)$. We substract (1.4.a) from the corresponding perturbed equation, integrate from 0 to x, use a Lipschitz condition for f and the above estimate for $\widehat{z}(x) - z(x)$. This gives for $e(x) = \|\widehat{y}(x) - y(x)\|$

$$e(x) \leq e(0) + C_2\int_0^x e(t)dt + C_3\int_0^x \|\delta_2(t)\|dt + \|\int_0^x \delta_1(t)dt\|,$$

and Gronwall's inequality implies

$$\|\widehat{y}(x) - y(x)\| \leq C_4 \big(\|\widehat{y}(0) - y(0)\| + \int_0^x \|\delta_2(t)\|dt + \max_{0\leq\xi\leq x} \|\int_0^\xi \delta_1(t)dt\|\big).$$

Inserting this into the estimate for $\widehat{z}(x) - z(x)$ we obtain finally an estimate (1.3) which does not depend on derivatives of the perturbation. The system is thus of index 1.

Problems of the form

$$BY' = a(Y) \tag{1.6}$$

with a constant singular matrix B can be transformed into the form (1.4) by decomposing B (e.g. by Gaussian elimination) as

$$B = S \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} T \tag{1.7}$$

with invertible S and T. Premultiplication of (1.6) by S^{-1} and use of the transformed variables

$$TY = \begin{pmatrix} y \\ z \end{pmatrix}$$

gives a system (1.4). Condition (1.5) then reads

$$\Big[\Big(\frac{\partial}{\partial Y}(S^{-1}a)\Big)T^{-1}\Big]_{22} \quad \text{has a bounded inverse,} \tag{1.8}$$

where $[\ldots]_{22}$ denotes the lower right block of the matrix (of the dimension of the null-space of B), according to the decomposition (1.7). The initial value Y_0 is consistent when $a(Y_0)$ is in the range of B.

Systems of index 2

We consider the problem

$$y' = f(y, z) \tag{1.10.a}$$
$$0 = g(y) \tag{1.10.b}$$

under the assumption that

$$g_y f_z \quad \text{has a bounded inverse} \tag{1.11}$$

in a neighbourhood of the solution. Differentiating (1.10.b) and substituting y' from (1.10.a) shows that the solution also has to satisfy the equation

$$0 = g_y(y) f(y, z) \tag{1.10.c}$$

so that it lies on the intersection of the manifolds defined by (1.10.b) and (1.10.c). A consistent initial value (y_0, z_0) now has to satisfy the constraint (1.10.b) for the y-component, and condition (1.10.c) then determines the z-component locally uniquely because of (1.11).

Equations (1.10.a) and (1.10.c) together are under the condition (1.11) of the index 1 form (1.4) with (1.5). Since we have differentiated once to arrive at this form, the estimate (1.3) contains the derivative of a perturbation in (1.10.b), and the system is thus of index 2. More formally, we consider the perturbed system

$$\begin{aligned} \widehat{y}\,' &= f(\widehat{y}, \widehat{z}) + \delta(x) \\ 0 &= g(\widehat{y}) + \theta(x). \end{aligned}$$

Differentiating the second equation gives

$$0 = g_y(\widehat{y}) f(\widehat{y}, \widehat{z}) + g_y(\widehat{y}) \delta(x) + \theta'(x).$$

We can now use the estimates of the index 1 case to obtain

$$\begin{aligned} \|\widehat{y}(x) - y(x)\| &\le C\big(\|\widehat{y}(0) - y(0)\| + \int_0^x (\|\delta(\xi)\| + \|\theta'(\xi)\|) d\xi\big) \\ \|\widehat{z}(x) - z(x)\| &\le C\big(\|\widehat{y}(0) - y(0)\| + \max_{0\le\xi\le x} \|\delta(\xi)\| + \max_{0\le\xi\le x} \|\theta'(\xi)\|\big). \end{aligned} \tag{1.12}$$

The system (1.10) can be considered as an extreme case of equations (1.4) with *singular* g_z. For such problems, under the assumption that g_z has constant rank in a neighbourhood of the solution, it is possible to perform a transformation into the form (1.10) which does not change the index and, even more importantly, under which the numerical methods to be studied are invariant. This transformation can be described as a nonlinear version of Gaussian elimination: Let us denote by z_1 the first component of z. From the assumption that g_z has constant rank it follows that either there exists a component of g such that $\partial g_i / \partial z_1 \neq 0$ locally, or $\partial g / \partial z_1$ vanishes identically so that g is already independent of z_1. In the first case we can express z_1 as a function of y and the remaining components of z by the Implicit Function Theorem, and thereby eliminate z_1 in the other equations. Repeating this procedure with z_2, z_3, etc., we arrive finally at a system of the form (1.10) where z now consists of those components of the original z in (1.4) which have not been eliminated.

Our next aim is to describe two important classes of equations which either are of the form (1.10), (1.11) or are closely related to it. These two classes are:

a) Systems with a solution-dependent singular matrix multiplying the solution derivative, which arise in electrical circuit analysis and in chemical reaction kinetics.

b) Equations of motion of constrained mechanical systems.

Ad a): An index 2 system (1.10) will be obtained formally from a transformation (to be described below) of a system

$$B(y)y' = a(y) \tag{1.13}$$

where $B(y)$ is a solution-dependent singular matrix satisfying (1.7) and (1.8). Since the numerical methods to be studied in this article are invariant under that transformation, convergence estimates for the y-component of (1.10) will apply immediately to the direct solution of (1.13).

We first rewrite (1.13) as an augmented system

$$\begin{aligned} y' &= z \\ 0 &= a(y) - B(y)z. \end{aligned}$$

Supposing that B is of constant rank, we can again decompose

$$B(y) = S(y) \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} T(y) \tag{1.14}$$

with invertible S and T. When B is sufficiently differentiable, also S and T can be chosen smooth in a neighbourhood of each y. We premultiply the second equation of the augmented system by $S^{-1}(y)$ and obtain with the block notation

$$(S^{-1}a)(y) = \begin{pmatrix} f(y) \\ g(y) \end{pmatrix}, \quad T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix},$$

the equivalent system

$$\begin{aligned} y_1' &= z_1 \\ y_2' &= z_2 \\ 0 &= f(y) - T_{11}(y)z_1 - T_{12}(y)z_2 \\ 0 &= g(y). \end{aligned}$$

Since T is invertible, we can (apart from a permutation of columns) assume also T_{11} invertible. We then eliminate the third line of the above system by calculating z_1 and substituting it into the first line. This gives a system of the form (1.10), with (y, z_2) in the role of (y, z) of (1.10). Condition (1.11) reads in the present situation

$$(-g_{y_1} T_{11}^{-1} T_{12} + g_{y_2}) \text{ is invertible,}$$

and a calculation shows that this is equivalent to (1.8).

With the help of the above transformation one derives that the difference between the solution of (1.13) and that of a perturbed system $B(\widehat{y})\widehat{y}' = a(\widehat{y})+\delta(x)$ is bounded by

$$\|\widehat{y}(x) - y(x)\| \leq C\big(\|\widehat{y}(0) - y(0)\| + \int_0^x \|\delta(\xi)\| d\xi + \int_0^x \|\delta'(\xi)\| d\xi\big)$$

whenever the expression on the right-hand side is sufficiently small. This estimate is stronger than (1.3) in that the uniform norm is replaced by the L^1 norm. In contrast to the case (1.6) of constant B, the dependence of the estimate on δ' cannot, in general, be removed for solution-dependent $B(y)$. This is seen from the following example:

$$\begin{aligned} y_1' - y_3 y_2' + y_2 y_3' &= 0, \quad y_1(0) = 0 \\ 0 &= y_2 \\ 0 &= y_3. \end{aligned}$$

If we add the perturbation $\delta(x) = (0, \epsilon \sin\omega x, \epsilon \cos\omega x)^T$, then we have $\widehat{y}_1' = \epsilon^2\omega$, and letting $\omega \to \infty$ we see that the $\|\delta'\|$ term cannot be omitted in (1.3).

We remark, however, that there is no dependence on δ' for systems of the special form

$$\begin{aligned} b_y(y)y' &= f(y) \\ 0 &= g(y) \end{aligned}$$

with invertible $(b_y^T, g_y^T)^T$, where $b_y = \partial b/\partial y$ for some function $b(y)$. This follows from the observation that the system obtained by adding the equation $0 = b(y) - v$ and replacing $b_y(y)y'$ by v' is of the index 1 form (1.4), (1.5) with (v, y) in the role of (y, z). Numerical methods are not invariant under this transformation, because v' and $b_y(y)y'$ are discretized differently for non-constant b_y.

Ad b): Problems of the very form (1.10) appear in mechanical modeling of constrained systems. A multi-body system described by (generalized) coordinates q and (generalized) velocity $u = q'$ may be subjected to geometric constraints $g(q) = 0$ and/or kinematic constraints $K(q)u + k(q) = 0$. In terms of the kinetic energy $T(q, u)$, the Lagrange equations of motion are

$$\frac{d}{dt}\left(\frac{\partial T}{\partial u}\right) - \frac{\partial T}{\partial q} = Q + H^T\lambda$$

where $Q(q, u)$ represents the (generalized) effective forces, λ is the Lagrangean multiplier, and $H^T = (G^T, K^T)$ with $G = g_q$. Differentiating out and collecting all equations gives a system of the form

$$\begin{aligned} q' &= u && (1.15.a)\\ M(q)u' &= f(q,u) + H^T(q)\lambda && (1.15.b)\\ 0 &= g(q) && (1.15.c)\\ 0 &= K(q)u + k(q) && (1.15.d) \end{aligned}$$

where $M = T_{uu}$ is a positive definite matrix.

Let us first consider the case when no constraints (1.15.c) are present. The system (1.15.a,b,d) is of the form (1.10) (apart from solving for u' in (1.15.b)) with (q, u) and λ in the roles of y and z. If the constraints in (1.15.d) are independent, so that $H = K$ has full row rank, then $KM^{-1}K^T$ is invertible, and condition (1.11) is satisfied.

In the presence of geometric constraints (1.15.c) the system (1.15) is no longer of index 2. A reduction to index 2 may be obtained by using the differentiated constraint $G(q)u = 0$, which is of the form (1.15.d), instead of (1.15.c) (or using a linear combination of both). A difficulty with this approach is that, in the course of the numerical integration, one may leave the original constraint (1.15.c). To avoid this, Gear, Gupta & Leimkuhler (1985) propose to use the differentiated constraint and to add (1.15.c) via a Lagrangean multiplier μ (which vanishes on the exact solution):

$$\begin{aligned} q' &= u + G^T(q)\mu && (1.16.a)\\ M(q)u' &= f(q,u) + H^T(q)\lambda && (1.16.b)\\ 0 &= g(q) && (1.16.c)\\ 0 &= G(q)u && (1.16.d)\\ 0 &= K(q)u + k(q). && (1.16.e) \end{aligned}$$

If the rows of H (and hence also those of G) are linearly independent, then (1.16) is of the form (1.10) with $y = (q, u)$ and $z = (\lambda, \mu)$, and condition (1.11) is satisfied.

Systems of index 3

Problems of the form

$$\begin{aligned} y' &= f(y,z) && (1.17.a)\\ z' &= k(y,z,u) && (1.17.b)\\ 0 &= g(y) && (1.17.c) \end{aligned}$$

are of index 3, if

$$g_y f_z k_u \text{ has a bounded inverse} \qquad (1.18)$$

in a neighbourhood of the solution. This is seen by differentiating (1.17.c) twice, which gives (omitting the function arguments)

$$0 = g_y f \tag{1.17.d}$$

$$0 = g_{yy}(f,f) + g_y f_y f + g_y f_z k. \tag{1.17.e}$$

Equations (1.17.a,b) together with (1.17.e) are under condition (1.18) of the index 1 form (1.4) with (1.5). The error estimate (1.3) now depends on the second derivative of a defect in (1.17.a-c), yielding index 3. Consistent initial values have to satisfy the three conditions (1.17.c-e).

An example of such an index 3 problem is given by a holonomic mechanical system, for which the equations (1.15) can be formulated without constraints (1.15.d). Here (q, u, λ) play the role of (y, z, u) in (1.17). Condition (1.18) is satisfied if $H = G$ has linearly independent rows. In the presence of constraints (1.15.d) the problem (1.15) is still of index 3 if H has full row rank (since differentiation of (1.15.c) then gives an index 2 system of the form (1.10)). It is then, however, of a slightly more general form than (1.17).

The pendulum

Let us illustrate the above discussion by the mathematical pendulum. The equations of motion of a point-mass m suspended at a massless rod of length l under the influence of gravity g, in cartesian coordinates (p, q), are

$$\begin{aligned} p' &= u \\ q' &= v \end{aligned} \tag{1.19.a}$$

$$\begin{aligned} mu' &= -p\lambda \\ mv' &= -q\lambda - g \end{aligned} \tag{1.19.b}$$

$$0 = p^2 + q^2 - l^2. \tag{1.19.c}$$

Here (u, v) is the velocity and λ is the rod tension. In this formulation the system is of the index 3 form (1.17.a-c). Differentiating (1.19.c) gives

$$0 = pu + qv \tag{1.19.d}$$

which geometrically corresponds to the fact that the velocity is tangential to the manifold given by (1.19.c), i.e., orthogonal to the gradient $2(p, q)$. The system (1.19.a,b,d) is of the index 2 form (1.10.a,b). Differentiating once more and using (1.19.c) yields

$$0 = m(u^2 + v^2) - gq - l^2\lambda. \tag{1.19.e}$$

The system (1.19.a,b,e) is of the index 1 form (1.4.a,b). The index 2 reformulation of Gear, Gupta & Leimkuhler (1985) reads in the present case

$$\begin{aligned} p' &= u - p\mu \\ q' &= v - q\mu \\ mu' &= -p\lambda \\ mv' &= -q\lambda - g \\ 0 &= p^2 + q^2 - l^2 \\ 0 &= pu + qv\,. \end{aligned} \tag{1.20}$$

Singularly perturbed problems

A sequence of differential-algebraic systems of arbitrarily high index arises in the study of singular perturbation problems:

$$y' = f(y,z) \tag{1.21.a}$$

$$\epsilon z' = g(y,z), \qquad 0 < \epsilon \ll 1 \tag{1.21.b}$$

where it is supposed that

$$\langle g_z v, v\rangle \le -\|v\|^2 \quad \text{for all vectors } v \tag{1.22}$$

holds for some scalar product in a neighbourhood of the solution. On any fixed interval bounded away from 0 (outside an initial transient phase), the solution is known to possess an ϵ-expansion (see e.g. O'Malley (1988))

$$\begin{aligned} y(x) &= y_0(x) + \epsilon y_1(x) + \epsilon^2 y_2(x) + \ldots + \epsilon^N y_N(x) + \mathbf{O}(\epsilon^{N+1}) \\ z(x) &= z_0(x) + \epsilon z_1(x) + \epsilon^2 z_2(x) + \ldots + \epsilon^N z_N(x) + \mathbf{O}(\epsilon^{N+1}) \end{aligned} \tag{1.23}$$

with smooth ϵ-independent coefficients y_k, z_k. Inserting (1.23) into (1.21) and comparing powers of ϵ shows that the expansion coefficients are solution of a sequence of differential-algebraic systems

$$\begin{aligned} y_0' &= f(y_0, z_0) \\ 0 &= g(y_0, z_0) \end{aligned} \tag{1.24.0}$$

$$\begin{aligned} y_1' &= f_y(y_0, z_0)y_1 + f_z(y_0, z_0)z_1 \\ z_0' &= g_y(y_0, z_0)y_1 + g_z(y_0, z_0)z_1 \end{aligned} \tag{1.24.1}$$

and in general

$$\begin{aligned} y_k' &= f_y(y_0,z_0)y_k + f_z(y_0,z_0)z_k + \varphi_k(y_0,z_0,\ldots,y_{k-1},z_{k-1}) \\ z_{k-1}' &= g_y(y_0,z_0)y_k + g_z(y_0,z_0)z_k + \psi_k(y_0,z_0,\ldots,y_{k-1},z_{k-1}). \end{aligned} \tag{1.24.k}$$

The functions y_0, z_0 are completely determined by (1.24.0), which is an index 1 system of the form (1.4), with condition (1.5) being implied by (1.22). If y_0, z_0 are considered known, then (1.24.1) is again an index 1 system for y_1, z_1. Equations (1.24.0) and (1.24.1) together are, however, of index 2, because a perturbation in z_0 enters differentiated into (1.24.1). * Similarly the system (1.24.0)-(1.24.k) is of index $k+1$.

Our interest in the system (1.24) comes from the fact that the numerical solution of the stiff problem (1.21) possesses an ϵ-expansion whose coefficients are the numerical solution of the differential-algebraic system (1.24). This permits to give sharp error bounds for the numerical solution of (1.21) as will be explained at the end of Section 2.

Singular singularly perturbed problems

As an example of a stiff mechanical system we consider the pendulum suspended at a massless stiff spring with Hooke's constant $1/\epsilon^2$, $0 < \epsilon \ll 1$. With the normalisation $m = 1$, $l = 1$, $g = 1$ the equations of motion are

$$\begin{aligned} p' &= u \\ q' &= v \end{aligned} \tag{1.25.a}$$

$$\begin{aligned} u' &= -\frac{1}{\epsilon^2}\frac{p}{\sqrt{p^2+q^2}}(\sqrt{p^2+q^2}-1) \\ v' &= -\frac{1}{\epsilon^2}\frac{q}{\sqrt{p^2+q^2}}(\sqrt{p^2+q^2}-1) - 1. \end{aligned} \tag{1.25.b}$$

It can be shown that the solution either has an asymptotic ϵ^2-expansion with smooth ϵ-independent coefficients

$$p(x) = p_0(x) + \epsilon^2 p_1(x) + \epsilon^4 p_2(x) + \ldots + \epsilon^{2N} p_N(x) + \mathbf{O}(\epsilon^{2N+2}) \tag{1.26}$$

and similarly for q, u, v with coefficients q_i, u_i, v_i, or it oscillates rapidly with frequency of magnitude $1/\epsilon$ around such a solution. Let us now suppose that we

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* The combined system (1.24.0), (1.24.1) is, in fact, of the form (1.10), (1.11), with (y_0, z_0, y_1) and z_1 in the roles of y and z.