

Implicit Riquier Bases for PDAE and their Semi-Discretizations [★]

Wenyuan Wu ^a Greg Reid ^a Silvana Ilie ^b

^a*Applied Mathematics Department, University of Western Ontario, London, N6A 5B7, Canada.*

^b*Department of Computer Science, University of Toronto, Toronto, Ontario, M5S 2E4, Canada*

Abstract

Complicated nonlinear systems of PDE with constraints (called PDAE) arise frequently in applications. Missing constraints arising by prolongation (differentiation) of the PDAE need to be determined to consistently initialize and stabilize their numerical solution. In this article we review a fast prolongation method, a development of (explicit) symbolic Riquier Bases, suitable for such numerical applications. Our symbolic-numeric method to determine Riquier Bases in implicit form, without the unstable eliminations of the exact approaches, applies to square systems which are dominated by pure derivatives in one of the independent variables.

The method is successful provided the prolongations with respect to a single dominant independent variable have a block structure which is uncovered by Linear Programming and certain Jacobians are nonsingular when evaluated at points on the zero sets defined by the functions of the PDAE. For polynomially nonlinear PDAE, homotopy continuation methods from Numerical Algebraic Geometry can be used to compute approximations of the points.

Our method generalizes Pryce's method for DAE to PDAE. Given a dominant independent time variable, for an initial value problem for a system of PDAE we show that its semi-discretization is also naturally amenable to our symbolic-numeric approach. In particular, if our method can be successfully applied to such a system of PDAE, yielding an implicit Riquier Basis, then under modest conditions, the semi-discretized system of DAE is also an implicit Riquier Basis.

Categories and Subject Descriptors: G.1.8 **General Terms:** Algorithms, Design

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Email addresses: wwu25@uwo.ca (Wenyuan Wu), reid@uwo.ca (Greg Reid), silvana@cs.toronto.edu (Silvana Ilie).

1. Introduction

The analysis of polynomial systems of equations is very challenging, and despite much progress, the analysis of polynomially nonlinear PDAE (Partial Differential Algebraic Equations) poses even greater challenges. The available symbolic differential and elimination methods which determine the missing constraints for such PDAE, while powerful, are *local*. These methods do not naturally treat initial boundary value problems (IBVP), which are so central in applications.

In this paper we discuss a symbolic-numeric approach to the computation of Riquier Bases for PDAE introduced in [30], and show that they can be useful in the numerical solution of IBVP. In particular we present new theoretical results, showing that our method can be naturally applied to the approximate solution of PDAE by semi-discretization (i.e. by the method of lines). Very little work has been done on combining prolongation methods with numerical methods for PDAE (see Mohammadi and Tuomela [13] for recent progress).

Differential elimination algorithms apply a finite number of differentiations and eliminations to uncover obstructions to formal integrability (i.e. finitely characterize the relations between all the Taylor coefficients of solutions at a point). Since many numerical solution methods, depend on or are equivalent to Taylor expansions, the determination of such obstructions or missing constraints can be an important prerequisite for such methods. Exact differential elimination algorithms that apply to exact polynomially nonlinear systems of PDAE are given in [3, 6, 14, 22, 18]. Such methods enable the identification of all hidden constraints of PDAE systems and the computation of initial data and associated formal power series solutions in the neighborhood of a given point. Algorithmic membership tests (specifically in the radical of a differential ideal) can be given [3, 6]. They can ease the difficulty of numerical solution of DAE systems [1]. See Lemaire [11] for a modern treatment of the existence and convergence of analytic solutions for differential systems which can be applied to Riquier Bases.

A major problem in these approaches is the exploding size of prolongations for more than one independent variable. In symbolic approaches much effort has been devoted to control the growth of this size by developing redundancy criteria (for integrability conditions), and making strong use of elimination with respect to rankings to decrease the size of the prolongations [2, 27]. However symbolic elimination can cause expression swell even in the case of one independent variable, for DAE problems arising in multi-body mechanics.

Very little work has been done on the corresponding problems for symbolic-numeric methods. Techniques which are helpful for the symbolic case are often unstable for the approximate case, since rankings (the differential analogue of term orders) which underly symbolic methods can cause pivoting on small quantities and result in instability.

In this paper we make progress on this problem for a certain class of PDAE. For this class, only prolongations with respect to *one independent variable* are needed. Paradoxically rankings are important in our approach but don't cause instability since no eliminations are made. Hence we also avoid the expression swell due to the eliminations mentioned above. A suitable ranking is determined by solving an integer linear programming problem to uncover a block structure in the PDAE system.

Another main idea in our paper is that such prolongations are essentially DAE like enabling us to generalize DAE techniques to the PDAE case. In our case we generalize a

method of Pryce for DAE in the framework of Riquier Theory. However we might imagine this being also used as a bridge for other DAE techniques (e.g. that of Sedoglavic [21]).

In particular, we give methods for computing approximate implicit Riquier Bases for square systems of analytic PDAE. There already exist exact methods for computing Riquier Bases for non-square polynomially nonlinear PDAE together with an input ranking of derivatives [19]. However these exact methods may not succeed if the intermediate systems can not be solved explicitly for their highest derivatives.

For polynomially nonlinear PDAE, our approximate Riquier Basis method uses an approximate method, homotopy continuation [24], to by-pass this difficulty. From a given set of solutions of a system of similar structure, homotopy paths converge to points on the zero set of the functions in the prolongations of the PDAE system. It is these points that are used to verify the conditions of the Implicit Function Theorem, allowing the implicit solution of the given functions for their highest derivatives.

In addition our method yields the method of Pryce [17] for systems of DAE as a special case. Prolongation will usually introduce more equations as well as more (jet) variables, *but not always*. If some equations after differentiation do not introduce new variables for whole system, then there is the possibility that the dimension of the system is lowered. Pryce [17] proposed a method to detect such “chances” that minimize the dimension by taking advantage of the special structure of some systems. Pryce’s method was the generalization of a method developed by Pantelides with historical roots in the work of Jacobi (see [15]). Ilie et al [8] show that Pryce’s method can be extended to give a polynomial cost method for numerical solution of DAE.

As we indicated the challenges for differential elimination methods are so great, that it is of considerable interest to develop techniques that are efficient for subclasses of problems. For example, consider IBVP for square systems of evolutionary PDAE. It is natural to apply our fast prolongation method with the time t as a dominant variable. If the method is successful, and produces an implicit Riquier Basis, it is also very natural to discretize the other (e.g. spatial) variables, to yield a system of DAE from the output of our prolongation method. Indeed we prove, that the semi-discretized system, under modest assumptions, is also an implicit Riquier Basis which facilitates its numerical integration. Some simulations, using a curtain of Pendula, are made to illustrate the approach. Riquier Bases are closely related to formally integrable and involutive systems. In [23] relations between involutive linear systems with constant coefficients and their semi-discretizations are investigated.

2. Zero Set of PDE in Jet Space

General systems of PDAE are naturally described in the setting of Jet spaces - a construction that underlies geometric and differential-algebraic approaches. At first sight this construction can seem perverse in its careful distinction between derivatives of actual solutions and the equations in indeterminates obtained by replacing these derivatives by formal jet variables. However this distinction, enables the rigorous manipulation of a formal structure corresponding the PDAE without first assuming that solutions exist, an essential prerequisite for any general theory of differential systems. The reader should be able to quickly become familiar with this approach by considering examples and probably has already implicitly used this construction in their own work (see [18] for an introduction).

Let \mathbb{F} be a field (\mathbb{R} or \mathbb{C} in this paper), $x = (x_1, \dots, x_n)$ be the independent variables and $u = (u^1, \dots, u^m)$ be the dependent variables for a system of PDAE and let $\mathbb{N} = \{0, 1, 2, \dots\}$. The usual commutative approaches to differential algebra and differential elimination theory [19, 3] consider a set of indeterminates $\Omega = \{v_\alpha^i \mid \alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n, i = 1, \dots, m\}$ where each member of Ω corresponds to a partial derivative by:

$$v_\alpha^i \leftrightarrow (\mathbf{D}_{x_n})^{\alpha_n} \cdots (\mathbf{D}_{x_1})^{\alpha_1} u^i(x_1, \dots, x_n) := \mathbf{D}^\alpha u^i(x_1, \dots, x_n).$$

Formal commutative total derivative operators are introduced to act on members of Ω by a unit increment of the j -th index of their vector subscript: $\mathbf{D}_{x_j} v_\alpha^k := v_{\alpha+1_j}^k$ where $\alpha+1_j = (\alpha_1, \dots, \alpha_j+1, \dots, \alpha_n)$. The usual total derivatives \mathbf{D}_{x_j} act on functions of $\{x\} \cup \Omega$ by:

$$\mathbf{D}_{x_j} = \frac{\partial}{\partial x_j} + \sum_{v \in \Omega} (\mathbf{D}_{x_j} v) \frac{\partial}{\partial v} \quad (1)$$

where $\frac{\partial}{\partial v}$ are the usual partial derivatives.

A q -th order differential system with ℓ equations is associated with a locus (or zero set) of points

$$Z(f) := \{(x, v_\alpha^i) \in J^q(\mathbb{F}^n, \mathbb{F}^m) : f^k(x, v_\alpha^i) = 0, k = 1, \dots, \ell\} \quad (2)$$

where $J^q(\mathbb{F}^n, \mathbb{F}^m) \simeq \mathbb{F}^n \times \mathbb{F}^m \times \mathbb{F}^{m_1} \times \dots \times \mathbb{F}^{m_q}$ is the jet space of order q and $f^k : J^q(\mathbb{F}^n, \mathbb{F}^m) \rightarrow \mathbb{F}$, $k = 1, \dots, \ell$ are the maps defining the differential equations. Here $m_r := m \cdot \binom{r+n-1}{r}$ is the number of jet variables corresponding to r -th order derivatives.

One class of systems considered in this paper will be differential polynomials in $\mathbb{F}[x_1, \dots, x_n; v_\alpha^i]$, the ring of all polynomials over \mathbb{F} in finite subsets of indeterminates $\{x\} \cup \Omega$. The other case, which is required by our use of the Implicit Function Theorem, is where the f^k are \mathbb{F} -analytic functions in a neighborhood of a point $(x^0, (v_\alpha^i)^0)$. We always work locally over some \mathbb{F} -Euclidian space. So we don't use the more global geometric features of Jet Geometry, such as bundles, contact structures, etc (see [22]).

The pendulum the classic illustrative example of higher indexDAE. Such systems are ubiquitous in multi-body dynamics. From CAD like graphical descriptions of links, joints, motors, etc, there are several software packages (e.g. Adams, Dads and WorkingModel), that automatically produce the equations of motion.

EXAMPLE 2.1 (The Pendulum). For the pendulum of unit mass, under constant gravity g , we have

$$\begin{cases} X_{tt} + \lambda X = 0 \\ Y_{tt} + \lambda Y = -g \\ X^2 + Y^2 = 1 \end{cases} \quad (3)$$

with independent variable $t \in \mathbb{F}$ and dependent variables $(X, Y, \lambda) \in \mathbb{F}^3$. Here $Z(f) = \{(t, X, Y, \lambda, X_t, Y_t, \lambda_t, X_{tt}, Y_{tt}, \lambda_{tt}) \in J^2(\mathbb{F}, \mathbb{F}^3) : X_{tt} + \lambda X = 0, Y_{tt} + \lambda Y + g = 0, X^2 + Y^2 - 1 = 0\}$ is a 7 dimensional submanifold of $\mathbb{F}^{10} \simeq J^2(\mathbb{F}, \mathbb{F}^3)$. Here derivatives of solutions such as $\frac{d^2 X(t)}{dt^2}$ have been replaced by formal jet variables X_{tt} , etc. Following notational convention the same letters are used to denote these variables, although strictly they are indeterminate quantities and not derivatives of solutions. Here $\Omega = \{X, Y, \lambda, X_t, Y_t, \lambda_t, \dots\}$ and (26) is the formal total derivative operator

$$\mathbf{D}_t = \frac{\partial}{\partial t} + X_t \frac{\partial}{\partial X} + Y_t \frac{\partial}{\partial Y} + \lambda_t \frac{\partial}{\partial \lambda} + X_{tt} \frac{\partial}{\partial X_t} + \dots \quad (4)$$

3. Rankings of Derivatives

Rankings of derivatives which are total orderings on the set of all derivatives are fundamental in our approach. Every equation has a highest derivative in a given ranking. A detailed formal treatment of this subject, and the classification of all such rankings are given in Rust [19]. Rankings are fundamental in *Differential Algebra* [9].

Definition 3.1 (Ranking [19]). A *positive ranking* \prec of Ω is a total ordering on Ω which satisfies:

$$v_\alpha^i \prec v_\beta^j \Rightarrow v_{\alpha+\gamma}^i \prec v_{\beta+\gamma}^j, \quad (5)$$

$$v_\alpha^i \prec v_{\alpha+\gamma}^i, \quad (6)$$

for all $\alpha, \beta, \gamma \in \mathbb{N}^n$.

Let $\text{HD}f$ denote the greatest member in Ω in f with respect the ranking \prec .

EXAMPLE 3.1. An example of a ranking for the system given in Example 2.1 is:

$$X \prec Y \prec \lambda \prec X_t \prec Y_t \prec \lambda_t \prec X_{tt} \prec Y_{tt} \prec \lambda_{tt} \prec \dots \quad (7)$$

It is easily seen that (7) is invariant under differentiation, so (5) is satisfied. In addition any derivative of a member is greater than itself, so (6) is satisfied. In this ranking $\text{HD}(X_{tt} + \lambda X) = X_{tt}$, $\text{HD}(Y_{tt} + \lambda Y - g) = Y_{tt}$, and $\text{HD}(X^2 + Y^2 - 1) = Y$.

There are many ways to specify a ranking. In this paper we use a matrix representation following Riquier and Rust [19, 20]. First we introduce a map ψ from Ω to \mathbb{Z}^{m+n} :

$$\psi : \frac{\partial^{\alpha_1 + \dots + \alpha_n} u^j}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}} \mapsto (0, \dots, 0, 1, 0, \dots, 0, \alpha_1, \dots, \alpha_n)^t \quad (8)$$

where the “1” and “ α_1 ” appear in j -th and $(m+1)$ -th coordinate respectively.

An ordering of the elements in \mathbb{Z}^{m+n} denoted by $<$ is defined by lexical order (comparing the values at the first coordinate, then the second coordinate, and so on).

Definition 3.2 (Ranking by Matrix). Suppose M is an $l \times (m+n)$ matrix with nonnegative integer entries and satisfies: $\theta \neq \tau \Rightarrow M \cdot \psi(\theta) \neq M \cdot \psi(\tau)$. We define \prec_M to be a ranking with respect to M , if $\theta, \tau \in \Omega$, we have $\theta \prec_M \tau \Leftrightarrow M \cdot \psi(\theta) < M \cdot \psi(\tau)$.

The non-uniqueness of rankings will be a key aspect of our approach. For example any permutation of X, Y, λ leads to an alternative ranking in to that given in (7).

4. Signature Matrix of t-Dominated Systems using Rankings

The methods developed in this paper are applicable to a class of PDAE that are *dominated by pure derivatives* in one of their independent variables with respect to some (partial) ranking described in Section 3.

By a *pure derivative* with respect to an independent variable x_i , we mean a derivative of form $\left(\frac{\partial}{\partial x_i}\right)^k u^j$ where $k \in \mathbb{N}$. By Definition 4.1 given later, a PDAE system which is *dominated by pure derivatives* with respect to an independent variable x_i , must at least contain such a derivative in each of its equations. For example $u_{tt} - c^2 u_{xx} = 0$ and

$v - u_x = 0$ both contain pure t -derivatives in their equations (u_{tt} and v respectively). But $u_{xt} - u_{xxt} = 0$ contains neither a pure t or x -derivative.

To prepare us for our definition of t -dominated systems we need to consider rankings which are consistent with highest t -derivatives. For example, for two independent variables t, x and for each u^j , such a ranking should satisfy:

$$u^j \prec u_x^j \prec u_{xx}^j \prec \cdots \prec u_t^j \prec u_{tx}^j \prec \cdots \quad (9)$$

It is easy to extend this (partial) ranking to the case when x is a vector (e.g. using lexical order on x). In the general case $t = x_k$ for an x_k -dominated system. We caution however that t may not represent time for some physical t -dominated systems.

We hide the details about the differential order of the other independent variables by defining a weight map $\varphi : \Omega \rightarrow \mathbb{R}$ with respect to t as follows:

$$\varphi(v_\alpha^i) := \begin{cases} \alpha_k, & \text{if } \alpha_p = 0, \text{ for every } p \neq k ; \\ \alpha_k + \epsilon, & \text{otherwise.} \end{cases} \quad (10)$$

where “ ϵ ” is a symbolic parameter.

For example $\varphi(u_{tt}) = 2$, $\varphi(u_{xxt}) = 1 + \epsilon$ and $\varphi(u) = 0$.

The leading derivative of each equation R_i with respect to each u^j using the (partial) ranking (9), is denoted by $\text{LD}(R_i, u^j)$. Applying (10) to the leading derivatives of R , we obtain an $\ell \times m$ matrix $(\sigma_{i,j})$ which is called the *signature matrix* (with respect to t) of R (see Pryce [17] for the DAE case):

$$(\sigma_{i,j})(R) := \begin{cases} \varphi(\text{LD}(R_i, u^j)), & \text{if } R_i \text{ depends on } u^j \text{ or any of its derivatives;} \\ -\infty, & \text{otherwise.} \end{cases} \quad (11)$$

For example consider the single PDE: $u_{tt} - c^2 u_{xx} = 0$; $(v_{ttt})^2 - v_{xt} + v_{xx} = 0$; $w_{xt} - w_t = 0$. The 1×1 signature matrices (with respect to t) for these PDE are respectively: $\sigma = (2)$; $\sigma = (3)$; $\sigma = (1 + \epsilon)$. The 2×2 signature matrix (with respect to t) of the system $\{u_{xt} - (v_{tt})^2 = 0, (v_{ttt})^2 + (v_x)^2 = 0\}$ is $(\sigma_{i,j}) = \begin{pmatrix} (1+\epsilon) & 2 \\ -\infty & 3 \end{pmatrix}$.

We define the *leading class* derivatives of a system R by

$$\text{LCD}(R) := \{\text{LD}(R, u^j) : 1 \leq j \leq m\}.$$

For example, $R = \{u_{xt} - (v_{tt})^2 = 0, (v_{ttt})^2 + (v_x)^2 = 0\}$, then $\text{LCD}(R) = \{u_{xt}, v_{ttt}\}$.

If for each equation R_i , $\text{LCD}(R_i)$ are pure t -derivatives, then regarding the other independent variables as parameters the PDAE has an DAE-like structure:

Definition 4.1. We say R is dominated by pure derivatives in the independent variable t if there is no ϵ appearing in $(\sigma_{i,j})(R)$.

Thus $u_{tt} - c^2 u_{xx} = 0$ and $(v_{ttt})^2 - v_{xt} + v_{xx} = 0$ are t -dominated. In contrast $w_{xt} - w_t = 0$ and the system $\{u_{xt} - (v_{tt})^2 = 0, (v_{ttt})^2 + (v_x)^2 = 0\}$ are not t -dominated.

Such t -dominated systems are not as special as they appear.

Proposition 1. [Genericity of t -dominated Systems] Let t be any independent variable. A generic \mathbb{F} -analytic or polynomially nonlinear PDAE system R with order q is t -dominated. Any \mathbb{F} -analytic or polynomially nonlinear PDAE system R with order q is

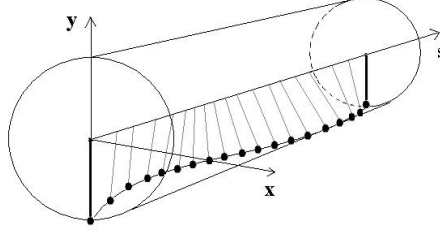


Fig. 1. Pendulum Curtain

t -dominated after a random linear coordinate transformation in the independent variables with coefficients in \mathbb{F} .

PROOF. Let R be a generic PDAE. So each R_i contains all pure t derivatives with order q , which are the leading class derivatives with respect to Ranking (9). For any nonlinear PDAE R , after a random linear coordinate change, any derivative with order q becomes a linear combination of all the q -th order derivatives. So R contains all pure q -th order t derivatives which are the leading class derivatives. \square

EXAMPLE 4.1 (Changing the Coordinates). The equation $R = \delta_1 u_{xx} + u_{xy} + \delta_2 u_{yy} = 0$ is both x and y dominated. However for small δ_1, δ_2 , the resulting Jacobians $\frac{\partial R}{\partial u_{xx}} = \delta_1$ and $\frac{\partial R}{\partial u_{yy}} = \delta_2$ in our method are poorly conditioned. The problem is well conditioned with respect to its leading derivatives after a coordinate change.

Remark 4.2. A symbolic random linear coordinate transformation often destroys the sparsity of the original system, which can cause dramatic increase in size of the system if subsequent eliminations are applied. However our use of numeric transformations in fixed precision lessens expression growth. Also, no eliminations will be used in our method.

Our main illustrative example in the paper is:

EXAMPLE 4.2 (Pendulum Curtain). Consider a curtain made of many pendula hanging under gravity g as shown in Figure 1. The Pendula are restricted to move on the surface of the cylinder and in planes perpendicular to the s -axis displayed in Figure 1. The pendula form a continuous curtain in the limit. For small deviations from the vertical equilibrium position the equations for $X(t, s)$, $Y(t, s)$ and Lagrange multiplier $\lambda(t, s)$ for the continuous curtain satisfy

$$\begin{cases} X_{tt} + \lambda X = \kappa X_{ss} \\ Y_{tt} + \lambda Y + g = \kappa Y_{ss} \\ X^2 + Y^2 = 1 \end{cases} \quad (12)$$

The signature matrix for (12) with columns corresponding to X , Y and λ is:

$$(\sigma_{i,j}) = \begin{pmatrix} 2 & -\infty & 0 \\ -\infty & 2 & 0 \\ 0 & 0 & -\infty \end{pmatrix} \quad (13)$$

Since (13) does not contain ϵ the system (12) is t -dominated.

5. Generalizing Pryce's Prolongation Method to PDE

5.1. Square Systems

Let R be a square (i.e. #equations = #unknowns) and t -dominated system. From Section 4, the signature matrix $(\sigma_{i,j})(R)$ contains information on differential order and ignores details on the degrees and coefficients of a system R . We introduce a fast method based on $(\sigma_{i,j})(R)$ to differentiate R with respect to t in a manner which includes its missing constraints. Pryce's method for square DAE is a special case with roots in the work of Jacobi (see [15]) and yields a local existence and uniqueness result. We state a local existence and uniqueness result for square PDAE.

Pryce's method [17] finds all the local constraints for a large class of square DAE using only prolongation. We will generalize this construction to PDAE. Suppose R_i is differentiated c_i times ($c_i \geq 0$). The new system after differentiation is denoted by $\mathbf{D}_t^c R$. Suppose the highest order of u^j appearing in $\mathbf{D}_t^c R$ is d_j . From the definition of $(\sigma_{i,j})$, clearly d_j is the largest of $c_i + \sigma_{ij}$, which implies that

$$d_j - c_i \geq \sigma_{ij}, \quad \text{for all } i, j. \quad (14)$$

Obviously there are at most $m + \sum d_j$ pure t -derivative jet variables and $m + \sum c_i$ equations in $\mathbf{D}_t^c R$ (considering independent variables and all non- t -derivatives as parameters). The dimension of $\mathbf{D}_t^c R$ is $\sum d_j - \sum c_i$. Roughly speaking, to find all the constraints is equivalent to minimizing the dimension of $\mathbf{D}_t^c R$. This can be formulated as an integer linear programming (LP) problem in the variables $c = (c_1, \dots, c_m)$ and $d = (d_1, \dots, d_m)$:

$$\left\{ \begin{array}{l} \text{Minimize } z = \sum d_j - \sum c_i, \\ \text{where } d_j - c_i \geq \sigma_{ij}, \\ c_i \geq 0 \end{array} \right. \quad (15)$$

Remark 5.1. This integer LP problem is dual to an assignment problem [17]. The task is to choose just one element in each row and column of the signature matrix, then maximize the sum of these m elements. The maximum is called the Maximal Transversal Value (MTV). If this value exists, then (15) has finite solution. Such problems can be solved (and existence of MTV can be checked) efficiently and in polynomial time by the Hungarian Method.

EXAMPLE 5.1. Recall that the Pendulum Curtain Example 4.2 has signature matrix (13) with no ϵ and so is t -dominated. Thus we can apply the method above using the signature matrix.

Recall that c_i means the i -th equation needs to be differentiated c_i times ($c_i \geq 0$) and d_j is the highest order of u^j after the prolongation. Solving (15) by LPSolve in the Optimization package of Maple10, we obtain $c = (0, 0, 2)$ and $d = (2, 2, 0)$.

B_0	B_1	\cdots	B_{k_c-1}	B_{k_c}
$R_1^{(0)}$	$R_1^{(1)}$	\cdots	$R_1^{(c_1-1)}$	$R_1^{(c_1)}$
	$R_2^{(0)}$	\cdots	$R_2^{(c_2-1)}$	$R_2^{(c_2)}$
		\vdots	\vdots	\vdots
		$R_m^{(0)}$	\cdots	$R_m^{(c_m)}$

Table 1. The triangular block structure of $\mathbf{D}_t^c R$ for the case of $c_i = c_{i+1} + 1$. For $0 \leq i < k_c$, B_i has fewer jet variables than B_{i+1} .

5.2. Block Triangular Structures

After we obtain the number of prolongation steps c_i for each equation, we can construct the partial prolonged system $\mathbf{D}_t^c R$ using c . We note that $\mathbf{D}_t^c R$ has a favorable block triangular structure which enables us to compute points on $Z(\mathbf{D}_t^c R)$ more efficiently. Without loss of generality, we assume $c_1 \geq c_2 \geq \cdots \geq c_m$, and let $k_c = c_1$, which is closely related to the *index* of system R (see [17]). The r -th partial differentiation of a PDE R_j with respect to t is denoted by $R_j^{(r)}$. Then we can partition $\mathbf{D}_t^c R$ into $k_c + 1$ parts (see Table 1) for $0 \leq i \leq k_c$ given by

$$B_i := \{R_j^{(i+c_j-k_c)} : 1 \leq j \leq m, i + c_j - k_c \geq 0\}. \quad (16)$$

For each $B_i, 0 \leq i \leq k_c$, we denote the leading class variables by $U_i := \text{LCD}(B_i)$, which are pure t -derivatives, and define the Jacobian Matrix

$$\mathcal{J}_i := \left(\frac{\partial B_i}{\partial U_i} \right). \quad (17)$$

Proposition 2. Let $\mathcal{J}(\mathbf{D}_t^c R) := \{\mathcal{J}_i\}$ be the set of Jacobian matrices of $\{B_i\}$. For any $0 \leq i < j \leq k_c$, \mathcal{J}_i is a sub-matrix of \mathcal{J}_j . Moreover, if \mathcal{J}_{k_c} has full rank, then any \mathcal{J}_i also has full rank.

PROOF. The first result is by the chain rule and the fact that if θ is the leading variable of a PDAE F then θ_t is the leading variable of $\mathbf{D}_t F$.

Because \mathcal{J}_{k_c} is an $m \times m$ full rank matrix, its rows are linearly independent. Since \mathcal{J}_i is a sub-matrix of \mathcal{J}_{k_c} , we can assume it consists of the first p rows and first q columns of \mathcal{J}_{k_c} , where q is the number of elements in U_i . If $q = m$, then $\text{rank}(\mathcal{J}_i) = p$. If $q < m$, then the entries in its first p rows and last $m - q$ columns must be 0. So $\text{rank}(\mathcal{J}_i) = p$. \square

In the following section we will show that the output of the t -prolongation implicitly yields a Riquier Basis for which an associated existence theorem is available.

6. Implicit Riquier Bases

In Section 6.1, we state Theorem 6.5 for the existence and uniqueness of formal power series solutions of a Riquier Basis. This theorem is the result of a Gröbner style development and extension of Riquier's classical existence results for PDAE. The details can be found in the works of Rust et al. [20, 19]. The corresponding exact symbolic differential elimination algorithms were implemented [27] in distributed Maple; which also refers to applications of the algorithms.

Given a ranking of partial derivatives, such bases are in solved form with respect to their highest derivatives. They are symbolically determined by successively including integrability conditions and performing eliminations on the resulting systems. The solved form requirement means that in the exact case they are essentially restricted to PDAE which are linear in their highest derivatives.

In this paper for numerical purposes we need an implicit form of Riquier and Rust's results. This is given in Section 6.2 and enables us to use the Implicit Function Theorem coupled with Numerical Algebraic Geometry to avoid explicitly solving PDAE for their highest derivatives or specifying a ranking.

6.1. The Formal Riquier Existence Theorem

We say that f is \prec -monic with respect to a ranking \prec if f has the form $f = \text{HD}f + g$, with $\text{HD}g \prec \text{HD}f$. For example the equation $X^2 + Y^2 - 1 = 0$ of the Pendulum system of (3) is not \prec -monic with respect to the ranking given in (7) since it is nonlinear in Y , its highest derivative.

Definition 6.1. $[\mathcal{M}, \mathcal{V}]$ In the remainder of the paper, fix a finite set \mathcal{M} of \prec -monic functions of which are \mathbb{F} -analytic functions on some subset \mathcal{V} of $J^r(\mathbb{F}^n, \mathbb{F}^m)$ for some finite r . The subset \mathcal{V} is connected and open in the usual \mathbb{F} -Euclidean topology.

Definition 6.2. [Principal and Parametric Derivatives] The *principal derivatives* of \mathcal{M} are defined as

$$\text{Prin}\mathcal{M} := \{v \in \Omega \mid \exists f \in \mathcal{M} \text{ and } \alpha \in \mathbb{N}^n \text{ with } v = \text{HD}\mathbf{D}^\alpha f\}$$

The *parametric derivatives* of \mathcal{M} , which we denote $\text{Par}\mathcal{M}$, are those derivatives (including those of zero order) that are not principal.

The parametric and principal derivatives enable us to specify initial data.

Definition 6.3. A *specification of initial data* for \mathcal{M} is a map $\phi : \{x\} \cup \text{Par}\mathcal{M} \rightarrow \mathbb{F}$. For $x^0 \in \mathbb{F}^m$, we say that ϕ is a specification at x^0 if $\phi(x) := (\phi(x_1), \phi(x_2), \dots, \phi(x_m)) = x^0$.

For an analytic function g on jet space, let $\phi(g)$ be the function of the principal derivatives obtained from g by evaluating x and the parametric derivatives using ϕ :

$$\phi(g) := g(\phi(x), (\phi(v))_{v \in \text{Par}\mathcal{M}}).$$

Definition 6.4. \mathcal{M} is called a *Riquier Basis* if for all $\alpha, \alpha' \in \mathbb{N}^m$ and $f, f' \in \mathcal{M}$ with $\text{HD}\mathbf{D}^\alpha f = \text{HD}\mathbf{D}^{\alpha'} f'$, the integrability condition $\mathbf{D}^\alpha f - \mathbf{D}^{\alpha'} f'$ is reduced to zero by a sequence of one-step reductions by members of \mathcal{M} .

See [20] for the definition of *one-step reduction* used above. Recall that \mathcal{M} and \mathcal{V} are as given in Definition 6.1.

Theorem 6.5 (Formal Riquier Existence Theorem). Let \mathcal{M} be a Riquier Basis such that each $f \in \mathcal{M}$ is polynomial in the principal derivatives. For $x^0 \in \mathbb{F}^n$, let ϕ be a specification of initial data for \mathcal{M} at x^0 such that $\phi(f)$ is well-defined for all $f \in \mathcal{M}$. Then there is formal power series solution $u(x) \in \mathbb{F}[[x - x^0]]^n$ to \mathcal{M} at x^0 such that $\mathbf{D}^\alpha u^i(x^0) = \phi(v_\alpha^i)$ for all $v_\alpha^i \in \text{Par}\mathcal{M}$. Furthermore, every formal power series solution to \mathcal{M} at x^0 may be obtained in this way for some ϕ .

Note that the set of integrability conditions given by Definition 6.4 is generally infinite. This infinite number of conditions is shown in [19] to be a consequence of a finite set of integrability conditions given below; thus enabling finite implementation [27]. Further more refined redundancy criteria for integrability conditions are given in [27].

Definition 6.6. Let $f, f' \in \mathcal{M}$ with $\text{HD}f = \mathbf{D}^\alpha u^i$ and $\text{HD}f' = \mathbf{D}^{\alpha'} u^{i'}$, and β be the least common multiple of α and α' . Then if $i = i'$, define the *minimal integrability condition* of f and f' to be $\text{IC}(f, f') = \mathbf{D}^{\beta-\alpha} f - \mathbf{D}^{\beta-\alpha'} f'$. If $i \neq i'$, then $\text{IC}(f, f')$ is said to be undefined.

Theorem 6.7. Suppose that for each pair $f, f' \in \mathcal{M}$ with $\text{IC}(f, f')$ well-defined we have $\text{IC}(f, f')$ is reduced to 0 by a sequence of one-step reductions. Then \mathcal{M} is a Riquier Basis.

6.2. Implicit Riquier Existence Theorem

A Riquier Basis is in solved form with respect to its highest derivatives, and can be taken to be monic and auto-reduced. In contrast, an Implicit Riquier Basis is locally equivalent to a Riquier Basis by Implicit Function Theorem, but is in implicit form:

Definition 6.8. [Implicit Riquier Basis] An analytic q -th order differential system R is an implicit Riquier Basis at a point P of its zero set $Z(R) \subseteq J^q(F^n, F^m)$ if there is a neighborhood N_P of P in J^q , such that $Z(R) \cap N_P$ is equal to the zero set of a Riquier Basis of R with respect to some ranking in N_P .

The connection is given in Remark 6.11. Numerical Algebra Geometry allows us to approximate points on the zero set of a PDAE and check the criteria for an implicit basis.

If the Jacobian matrix for a DAE is nonsingular, then Pryce's method can successfully construct the unique local solution at a given consistent initial point. For the PDAE case, we show that if \mathcal{J}_{k_c} is nonsingular at some point P , which satisfies system $\mathbf{D}_t^c R$, then any order derivative of each u^j is determined by P . So the Taylor series coefficients of the solution passing through P can be computed to arbitrary order under a specification of initial data.

For each dependent variable we have a ranking of type (9). To apply the Riquier Existence Theorem, we need to merge these partial rankings (9) to a total ranking which is consistent with all the partial rankings.

Proposition 3. Let the leading class derivatives of R be $\{\theta_1, \dots, \theta_m\}$ with respect to the partial ranking (9) and let B be the set of all the other derivatives of R . Then there exists a positive ranking \prec which: satisfies the partial ranking (9); has $\theta_1 \succ \theta_2 \succ \dots \succ \theta_m$; satisfies $\theta_i \succ b$ for any $b \in B$.

PROOF. Case 1: $m \geq n$. Suppose the dependent variable index of θ_i is i and $t = x_1$. If the dependent and independent variable indices do not satisfy this condition, then it can be satisfied after a permutation of the variables. Let $\begin{pmatrix} I^{m \times m} \\ X^{n \times m} \end{pmatrix} = (\psi(\theta_1), \dots, \psi(\theta_m))$. And suppose c is the maximum entry of X . Then let $M' = c \cdot 1^{m \times m} - \begin{pmatrix} X \\ 0 \end{pmatrix}^{m \times m}$.

Finally we construct an $(m+1) \times (m+n)$ matrix

$$M = \begin{pmatrix} M' & I^{n \times n} \\ \mathbf{v} & 0^{(m-n+1) \times n} \end{pmatrix}, \quad (18)$$

where $\mathbf{v} = (m, m-1, \dots, 1)$. All the entries of M are non-negative. Suppose $\theta, \tau \in \Omega$ and $\theta \neq \tau$. Consider first the case where θ, τ are derivatives of different dependent variables. Then the last coordinates of $M \cdot \psi(\theta)$ and $M \cdot \psi(\tau)$ are different. The other case is that θ, τ are derivatives of the same dependent variable. Then their ranks are determined by the last n columns of M , which is the lexical order over independent variables. In this case, $M \cdot \psi(\theta) \neq M \cdot \psi(\tau)$. So M is a matrix representation of a ranking which satisfies Ranking (9).

Suppose $i < j$, then we can check $\theta_i \succ \theta_j$. This is true because $\binom{\gamma_i}{m-i+1} = M \cdot \psi(\theta_i) > M \cdot \psi(\theta_j) = \binom{\gamma_j}{m-j+1}$, where $\gamma_j = M'_j + \binom{X_j}{0} = c \cdot 1^{m \times 1} = \gamma_i$.

Suppose $\tau \in B$ with dependent variable u^i , then we can show $\theta_j \succ \tau$, for any j . Since \prec_M satisfies Ranking (9), we have $\binom{\gamma_\tau}{m-i+1} = M \cdot \psi(\tau) < M \cdot \psi(\theta_i) = \binom{\gamma_i}{m-i+1}$, which implies $\gamma_\tau < \gamma_i$. So $\gamma_\tau < \gamma_j = \gamma_i$, for any $1 \leq j \leq m$.

Therefore, $M \cdot \psi(\tau) < M \cdot \psi(\theta_j)$, which implies for any θ_j and any $\tau \in B$ we have $\tau \prec_M \theta_j$ completing the proof in Case 1 ($m \geq n$).

Case 2: $m < n$. In the proof, we only need to change the construction slightly by setting $M' = c \cdot 1^{n \times m} - X$. Similarly we construct an $(n+1) \times (m+n)$ matrix $M = \begin{pmatrix} M' & I^{n \times n} \\ \mathbf{v} & 0^{1 \times n} \end{pmatrix}$. \square

Lemma 6.9. Let $C = \begin{pmatrix} A^{n \times m} \\ B^{\ell \times m} \end{pmatrix}$ and $n + \ell \leq m$. If C is a full rank matrix, then any rank n square sub-matrix of A can be extended to a rank $n + \ell$ square sub-matrix of C .

PROOF. Because C is a full rank matrix and $n + \ell \leq m$, $\text{rank}(C) = n + \ell$. Suppose the first n columns of A form a full rank matrix, so the first n columns of C are linearly independent. A set of linearly independent columns can be extended to a basis of the column space of C . Hence we can find ℓ columns which generate a basis for the column space of C together with the first n columns. \square

Lemma 6.10. Let R be a square t -dominated \mathbb{F} -analytic system of PDAE. Suppose the maximal transversal value of $(\sigma_{ij})(R)$ exists. Let $\mathbf{D}_t^c R$ be the system obtained by the t -prolongation method of Section 5. If \mathcal{J}_{k_c} is nonsingular at some point P in $Z(\mathbf{D}_t^c R)$, then there exists a positive ranking \prec that determines a set of local solved forms $w^{(i)} = f^{(i)}(z)$ for each block B_i , such that $\mathbf{D}_t w^{(i-1)} \subseteq w^{(i)}$ where each $w^{(i)}$ is a set of pure t -derivatives.

PROOF. Because \mathcal{J}_{k_c} is nonsingular at P , each \mathcal{J}_i is full rank by Proposition 2. So B_0 is full rank and we can find an invertible sub-matrix M_0 of \mathcal{J}_0 , and solve for the corresponding set of variables $w^{(0)}$, which is a subset of $\text{LCD}(B_0)$, locally using the Implicit Function Theorem. The $w^{(0)}$ are t -derivatives of the dependent variables. Let the solved forms of B_0 be $w^{(0)} = f^{(0)}(z)$, where z is the set of unsolved variables of B_0 . Let S_0 be the set of the corresponding dependent variables of $w^{(0)}$. For the next block B_1 we can choose an invertible sub-matrix M_1 of \mathcal{J}_1 which contains M_0 by Lemma 6.9. So $\mathbf{D}_t w^{(0)} \subseteq w^{(1)}$. Let S_i be the set of dependent variables of $w^{(i)} \setminus (S_0 \cup \dots \cup S_{i-1})$. Continue the process until the last block B_{k_c} . Then we can check that $\mathbf{D}_t w^{(i-1)} \subseteq w^{(i)}$ and the union of all the S_i is the set of all dependent variables.

Suppose that $w^{(k_c)} = \{\theta_1, \dots, \theta_m\}$. Then after appropriate re-indexing $w^{(k_c)}$ satisfies the condition: for any $1 \leq i < j \leq m$, if the dependent variables of θ_i and θ_j belong to S_p

and S_q respectively then $p \leq q$. Therefore we can define a positive ranking \prec by Proposition 3 such that this ranking is consistent with all the solved forms $\{w^{(i)} = f^{(i)}(z)\}$. In other words, for each solved form $\hat{w} = \hat{f}(z)$ we have $\hat{w} \succ v$ for any $v \in z$. \square

Let $w_0 \in \mathbb{F}^k$, $z_0 \in \mathbb{F}^\ell$ and $\mathcal{U} \subset \mathbb{F}^k \times \mathbb{F}^\ell$ be a neighborhood of (w_0, z_0) . Let $F : \mathcal{U} \rightarrow \mathbb{F}^k$ be an analytic function with $F(w_0, z_0) = 0$ and $\text{rank} \frac{\partial F}{\partial w} = k$ at $(w_0, z_0) \in \mathcal{U}$. That is, the Jacobian of F has maximal rank with respect to w at (w_0, z_0) . Then by the Implicit Function Theorem there exists an analytic function $f : \mathbb{F}^\ell \rightarrow \mathbb{F}^k$, such that the zero set of $\{(w, z) : F(w, z) = 0\}$ is equal to $\{(w, z) : w = f(z)\}$ in a neighborhood of \mathcal{N} of (w_0, z_0) [5]. Expansion of $F(w, z)$ in $\zeta = w - f(z)$ about $\zeta_0 = w_0 - f(z_0) = 0$ shows that there exists an analytic function H such that $F(w, z) = H(w, z)(w - f(z))$. Differentiation of this function with respect the vector of variables w and exploiting $\text{rank} \frac{\partial F}{\partial w} = k$ at $(w_0, z_0) \in \mathcal{U}$ yields:

Remark 6.11. There exists a neighborhood of \mathcal{N} of (w_0, z_0) and an analytic function $H : \mathcal{N} \rightarrow \mathbb{F}^{k \times k}$ such that

$$F(w, z) = H(w, z)(w - f(z)) \quad (19)$$

and $H(w, z)$ is invertible in \mathcal{N} .

Theorem 6.12. Let R be a square t -dominated \mathbb{F} -analytic system of PDAE. Suppose the maximal transversal value of $(\sigma_{ij})(R)$ exists. Let $\mathbf{D}_t^c R$ be the system computed by our t -prolongation method. If \mathcal{J}_{k_c} is nonsingular at some point P in $Z(\mathbf{D}_t^c R)$, then $\mathbf{D}_t^c R$ is an Implicit Riquier Basis in a neighborhood of P .

PROOF. By Proposition 3, there is a ranking in which all leading class derivatives are pure t -derivatives. And by Lemma 6.10, there exists a solved form $w = f(z)$ of $\mathbf{D}_t^c R$ in a sufficiently small neighborhood \mathcal{N}_P , where w is the union of all $w^{(i)}$ defined in Lemma 6.10. We will show that $w = f(z)$ is a Riquier Basis in \mathcal{N}_P . First note that the principal derivatives of $w = f(z)$ are given by w . Thus $w = f(z)$ is certainly polynomial in w as required by Theorem 6.5. Secondly, it remains to be proved that the integrability conditions of $w = f(z)$ are satisfied. So without loss of generality, we consider two particular equations $\hat{w} - \hat{f}(z) = 0$ and $\tilde{w} - \tilde{f}(z) = 0$ with $(\mathbf{D}_t)^\gamma \hat{w} = \tilde{w}$. By Theorem 6.7, the corresponding integrability condition is $(\mathbf{D}_t)^\gamma (\hat{w} - \hat{f}(z)) - (\tilde{w} - \tilde{f}(z))$. By the more refined redundancy criterion given in Corollary 5.3.2 of [19], this can be reduced to case $\gamma = 1$:

$$\mathbf{D}_t(\hat{w} - \hat{f}(z)) - (\tilde{w} - \tilde{f}(z)) \quad (20)$$

where $\hat{w} - \hat{f}(z) = 0$ and $\tilde{w} - \tilde{f}(z) = 0$ are two particular equations out of the solved forms $w^{(i-1)} = f^{(i-1)}(z)$ and $w^{(i)} = f^{(i)}(z)$ respectively, with $\mathbf{D}_t \hat{w} = \tilde{w}$.

Remark 6.11 implies that $w^{(i)} - f^{(i)}(z) = H_i^{-1} \cdot B_i$ in \mathcal{N}_P . Thus $\tilde{w} - \tilde{f}(z) = \tilde{h} \cdot B_i$ in \mathcal{N}_P , for some analytic function vector \tilde{h} . Similarly $\hat{w} - \hat{f}(z) = \hat{h} \cdot B_{i-1}$ in \mathcal{N}_P , for some analytic function vector \hat{h} . Then (20) is

$$\mathbf{D}_t(\hat{h} \cdot B_{i-1}) - \tilde{h} \cdot B_i \quad (21)$$

which has the general form

$$\mathbf{D}_t \hat{h} \cdot B_{i-1} + \hat{h} \cdot \mathbf{D}_t B_{i-1} - \tilde{h} \cdot B_i \quad (22)$$

Because $\mathbf{D}_t B_{i-1} \subseteq B_i$, condition (20) is zero on $\mathcal{N}_P \cap Z(\mathbf{D}_t^c R)$, which is equivalent to $\{(w, z) : w = f(z)\} \cap \mathcal{N}_P$. So (20) is zero when $w = f(z)$ in \mathcal{N}_P , which means (20) is identically equal to zero on the connected component containing \mathcal{N}_P by the properties of analytic functions (the Identity Theorem). Hence (20) can be reduced to zero by $w = f(z)$. Therefore $\mathbf{D}_t^c R$ is an implicit Riquier Basis in \mathcal{N}_P . \square

Remark 6.13. If the maximal transversal value of a signature matrix exists, then the vector c is determined only by the signature matrix. So a signature matrix corresponds to a class of t -dominated PDAE. For a square polynomially nonlinear PDAE system R in such a class, if the coefficient of each term is generic, then at a generic point in the variety defined by $\mathbf{D}_t^c R$ in Jet space, the Jacobian matrix \mathcal{J}_{k_c} is nonsingular. This fact together with Proposition 1 means the t -prolongation method can be successfully applied to a large class of PDAE.

7. Discretization of Prolonged PDAE to DAE

The solution of most systems of PDAE arising in applications can only be obtained numerically, by an appropriate discretization method, whether it is finite differences, finite elements, or other numerical methods. We assume that the problem under investigation is well-posed as an initial value problem in the t -variable. In this section we obtain results concerning the output PDAE of our method and their numerical discretization to DAE via the numerical method of lines. One strong advantage of the method of lines is that it transforms PDAE into a DAE to which one of the many existing efficient numerical solvers can be applied. By contrast little numerical software has been developed for directly addressing PDAE. In Section 9 we apply these results to the numerical solution of the Pendulum Curtain Example.

The output of our fast prolongation method to the special case of DAE (i.e. the output of Pryce's method) has already proven useful in assisting the numerical solution of DAE. In particular there is a subsequent Taylor series numerical discretization solution method, that exploits the block structure of the output [17]. Indeed, in [8, 7] it is shown that such methods, under appropriate conditions are of polynomial cost in the number of digits of requested accuracy. Other authors have also shown that prolongation methods can be helpful in the numerical solution of DAE [1].

It is natural and very useful to try to generalize such methods to the PDAE case. Few results are known for this case. However we mention the work of Mohammadi and Tuomela [13] who show on a series of overdetermined initial and BVP that numerical solution of constrained PDE systems can be simplified through a prior completion by prolongation.

7.1. Riquier Basis of Discretized DAE

In order to see the basic idea of the standard method of lines we consider a single PDE in the dependent variable u and 2 independent variables t, x of differential order at most 2. The method can be generalized to any differential order and any number of independent variables, see e.g. [28].

We consider problems posed over $\mathbb{F} = \mathbb{R}$, on a rectangle $x_{\min} < x < x_{\max}$ for $t > 0$. We discretize the spatial variable x into N intervals of equal length $\Delta x = (x_{\max} - x_{\min})/N$ with grid points located at $x^{(j)} = x_{\min} + j\Delta x$ where $j = 0, \dots, N$.

Consider first the case where the PDE contains no derivatives, that is it has form $R(x, t, u) = 0$. Then the PDE is a function $R : \mathbb{R}^3 \rightarrow \mathbb{R}$. Then the image of this system under our discretization map δ is defined to be: $R^{(j)} : \mathbb{R}^{N+2} \rightarrow \mathbb{R}$ where $R^{(j)}(t, u^{(j)}) = R(t, x^{(j)}, u^{(j)})$ for $j = 1, \dots, N-1$. In computations the $u^{(j)} =: \delta^{(j)}(u)$ are approximations of the solutions at time t and interior spatial grid points $x^{(j)}$. We interpret δ as a formal map between Jet spaces, transforming one set of functions defining differential equations into another set.

Consider the case where the PDE contains first order jet variables, that is it has form $R(x, t, u, u_x, u_t) = 0$ where R is a function $R : \mathbb{R}^5 \rightarrow \mathbb{R}$. Then the image of this system under δ is defined to be: $R^{(j)} : \mathbb{R}^{N+2} \rightarrow \mathbb{R}$ for $j = 1, \dots, N-1$, where

$$R^{(j)}(t, u^{(0)}, u^{(1)}, \dots, u^{(N)}) = R(t, x^{(j)}, u^{(j)}, \frac{u^{(j+1)} - u^{(j-1)}}{2\Delta x}, u_t^{(j)}). \quad (23)$$

In computations the $\delta^{(j)}(u_x) := \frac{u^{(j+1)} - u^{(j-1)}}{2\Delta x}$ are finite difference approximations of derivatives at time t and interior spatial grid points $x^{(j)}$. We will work locally and regard the boundary grid values of u , that is $u^{(0)}$ and $u^{(N)}$, parametrically in the resulting discretized DAE system. For example, applying the discretization operator to a PDAE $R(t, x, u_t, u_x, u_{tt}, u_{tx}, u_{xx})$ at a point $x^{(i)}$ yields for $i = 1, \dots, (N-1)$:

$$\delta^{(i)}(R) := R(t, x^{(i)}, u_t^{(i)}, \frac{u^{(i+1)} - u^{(i-1)}}{2\Delta x}, u_{tt}^{(i)}, \frac{u_t^{(i+1)} - u_t^{(i-1)}}{2\Delta x}, \frac{u^{(i+1)} - 2u^{(i)} + u^{(i-1)}}{(\Delta x)^2})$$

From the example above we can see

$$\delta^{(i)}(u_{tx}) = \frac{u_t^{(i+1)} - u_t^{(i-1)}}{2\Delta x} = \mathbf{D}_t \left(\frac{u^{(i+1)} - u^{(i-1)}}{2\Delta x} \right) = \mathbf{D}_t \delta^{(i)}(u_x). \quad (24)$$

In this paper, we always choose a finite difference scheme such that $\delta^{(i)}(\mathbf{D}_t v) = \mathbf{D}_t(\delta^{(i)}v)$, for all jet variables $v \in \Omega$. Essentially, δ performs a substitution operation, so δ commutes with arithmetic operations. We can also prove the following commutativity property.

Lemma 7.1. Let F be an analytic function of jet variables. Then

$$\mathbf{D}_t \circ \delta(F) = \delta \circ \mathbf{D}_t(F). \quad (25)$$

PROOF. We only need to prove the commutativity for each i :

$$\begin{aligned} \delta^{(i)} \circ \mathbf{D}_t(F) &= \delta^{(i)} \circ \frac{\partial}{\partial t}(F) + \delta^{(i)} \circ \sum_{v \in \Omega} (\mathbf{D}_t v) \frac{\partial}{\partial v}(F) \\ &= \delta^{(i)}(F_t) + \sum_{v \in \Omega} \delta^{(i)}(\mathbf{D}_t v) \cdot \delta^{(i)}(F_v) \\ &= F_t(t, \delta^{(i)}v) + \sum_{v \in \Omega} F_v(t, \delta^{(i)}v) \cdot \mathbf{D}_t(\delta^{(i)}v) \\ &= \mathbf{D}_t F(t, \delta^{(i)}v) = \mathbf{D}_t \circ \delta^{(i)}(F). \quad \square \end{aligned}$$

When we apply the discretization operator δ to a PDAE system R , we will have a DAE system $\delta(R)$. Now we will study how to find a Riquier Basis of $\delta(R)$ from the output of our fast prolongation method to PDAE.

By Lemma 6.10, there exists a solved form $w = f(z)$ of $\mathbf{D}_t^c R$ in a sufficiently small neighborhood \mathcal{N}_P provided \mathcal{J}_{k_c} is nonsingular at P , where w consists of the pure t -derivatives. We show that $w - f(z)$ is a Riquier Basis in Theorem 6.12. Here we will show that the DAE $\delta(w - f(z))$ is also a Riquier Basis with respect to an appropriate ranking.

To prove the existence of such a ranking, we use $(m + 2)$ -dimensional vectors to represent the jet variables of the discretized system in $J^q(\mathbb{F}^1, \mathbb{F}^{m \cdot (N-1)})$ produced by the map ψ :

$$\psi : \frac{\partial^d u^{j,(i)}}{\partial t^d} \mapsto (0, \dots, 0, 1, 0, \dots, 0, d, i)^t \quad (26)$$

where the “1” appears in j th coordinate and the “ d ” appears in $(m + 1)$ -th coordinate. Again for illustration we have restricted ourselves to 2 independent variables.

Proposition 4. *Suppose \succ is the positive ranking in $J^q(\mathbb{F}^2, \mathbb{F}^m)$ given in the proof of Proposition 3 which satisfies $\theta_1 \succ \theta_2 \succ \dots \succ \theta_m$ and $\mathbf{D}_{x_i} \theta_\ell \succ \theta_k$ for any i, ℓ, k . Then there exists a positive ranking in $J^q(\mathbb{F}^1, \mathbb{F}^{m \cdot (N-1)})$ such that*

- $\theta_\ell^{(i)} \succ \theta_k^{(i)}$, for any $\ell < k$
- $\theta_\ell^{(i)} \succ \theta_\ell^{(j)}$, for any $i > j$
- $\mathbf{D}_t \theta_\ell^{(i)} \succ \theta_k^{(j)}$, for any i, j, ℓ, k .

PROOF. Let M' be the $m \times m$ matrix given in the proof of Proposition 3 and $\mathbf{v} = (m, m - 1, \dots, 1)$. Now we construct an $(m + 2) \times (m + 2)$ matrix

$$M = \begin{pmatrix} M' & 1 & 0 \\ \mathbf{v} & \mathbf{0}^{m \times 1} & \mathbf{0}^{m \times 1} \\ \mathbf{0}^{1 \times m} & 0 & 1 \end{pmatrix}. \quad (27)$$

By the map ψ given in (26), we easily check that this matrix represents such a ranking. \square

By Theorem 6.12, we know that all integrability conditions can be reduced to zero by substitution of the solved form. The δ operator is also a substitution operation. Next we will show that these substitutions commute.

Proposition 5. *Let $\theta = f(z)$ be a system with jet variables θ, z in a solved form, where θ is a vector of pure t -derivatives and z is a vector of jet variables. If F is a function of θ and z , then*

$$\delta^{(i)}(F|_{\theta=f(z)}) = (\delta^{(i)} F)|_{\theta^{(i)}=\delta^{(i)}(f(z))}. \quad (28)$$

PROOF. Because θ is a vector of pure t -derivatives, we have $\delta^{(i)}(\theta) = \theta^{(i)}$ by the definition of the map δ . By substitution, $F(\theta, z)|_{\theta=f(z)} = F(f(z), z)$. Applying the discretization operator yields $\delta^{(i)}(F(f(z), z)) = F(\delta^{(i)}(f(z)), \delta^{(i)}(z))$.

On the right hand side, $\delta^{(i)} F(\theta, z) = F(\theta^{(i)}, \delta^{(i)}(z))$. Then substituting $\theta^{(i)} = \delta^{(i)}(f(z))$ into $F(\theta^{(i)}, \delta^{(i)}(z))$, we have $F(\delta^{(i)}(f(z)), \delta^{(i)}(z))$ which is same as the left hand side. \square

Theorem 7.2. Let R be a square t -dominated PDAE system with m dependent variables and independent variables t and x . Suppose the solved form $\theta - f(z)$ is a Riquier Basis of $\mathbf{D}_t^c R$ shown in Theorem 6.12 with a ranking given in Proposition 3. Then $\delta(\theta - f(z))$ is a DAE system with $m \cdot (N - 1)$ dependent variables and there exists a ranking such that $\delta(\theta - f(z))$ is a Riquier Basis.

PROOF. Using the same argument in Theorem 6.12, we only need to consider the integrability condition of $\hat{\theta} - \hat{f}(z)$ and $\tilde{\theta} - \tilde{f}(z)$ chosen from the solved form, such that $\mathbf{D}_t \hat{\theta} = \hat{\theta}$. Then the integrability condition is $F = \mathbf{D}_t(\hat{\theta} - \hat{f}(z)) - (\tilde{\theta} - \tilde{f}(z)) = \tilde{f}(z) - \mathbf{D}_t(\hat{f}(z))$. From the proof of Theorem 6.12, we know F can be reduced to zero by substituting $\theta = f(z)$.

By Proposition 4, there exists a ranking such that $\theta^{(i)}$ is the leading derivative of $\delta^{(i)}(\theta - f(z))$ respectively. Now let us consider the integrability condition of the discretized system $\hat{\theta}^{(i)} - \delta^{(i)}(\hat{f}(z))$ and $\tilde{\theta}^{(i)} - \delta^{(i)}(\tilde{f}(z))$. The integrability condition is $\delta^{(i)}(\tilde{f}(z)) - \mathbf{D}_t(\delta^{(i)}(\hat{f}(z))) = \delta^{(i)}(\tilde{f}(z)) - \delta^{(i)}(\mathbf{D}_t(\hat{f}(z))) = \delta^{(i)}(F)$ by Lemma 7.1.

By Proposition 5, we have $(\delta^{(i)}F)|_{\theta^{(i)}=\delta^{(i)}(f(z))} = \delta^{(i)}(F)|_{\theta=f(z)} = \delta^{(i)}(0) = 0$. Hence The integrability conditions of DAE can be also reduced to zero by substituting $\delta^{(i)}(\theta = f(z))$ into $\delta^{(i)}(F)$. \square

Theorem 7.3. Let R be a PDAE system. Suppose that the top block of $\mathbf{D}_t^c R$ given in Theorem 6.12 has nonsingular Jacobian in a sufficiently small neighborhood \mathcal{N}_P of a point $P \in Z(\mathbf{D}_t^c R)$ and there are no mixed derivatives in this Jacobian matrix. Then $\delta(\mathbf{D}_t^c R)$ is an implicit Riquier Basis of $\delta(R)$ in \mathcal{N}_P with the ranking given in Proposition 4.

PROOF. Since there are no mixed derivatives in R , the Jacobian matrix J of the top block of $\mathbf{D}_t^c R$ only contains pure t -derivatives. We have $\delta(J) = \text{diag}(J^{(1)}, J^{(2)}, \dots, J^{(N-1)})$, where $J^{(i)}$ is the matrix by replacing each jet variable θ with $\theta^{(i)}$. Then $\delta(J)$ is nonsingular in \mathcal{N}_P since each sub-matrix on the diagonal is nonsingular. And $\delta(J)$ is the Jacobian matrix of the top block of $\delta(\mathbf{D}_t^c R)$ and all the lower blocks are nonsingular by Proposition 2. Hence $\delta(\mathbf{D}_t^c R)$ is equivalent to the corresponding solved form which is a Riquier Basis by Theorem 7.2.

By Lemma 7.1, $\delta(\mathbf{D}_t^c R) = \mathbf{D}_t^c(\delta(R))$, so $\delta(\mathbf{D}_t^c R)$ is an implicit Riquier Basis of $\delta(R)$.

Remark 7.4. Although the proof depends on our finite difference scheme (23), theoretically our formal result can be generalized to any finite difference scheme which commutes with the formal derivative \mathbf{D}_t . Practically, an analysis of the numerical properties of the above discretization scheme is necessary, but this is beyond the scope of this paper. We only consider numerical schemes which satisfy stability requirements. We shall assume that the discretization of the prolonged PDAE and of the boundary conditions is chosen such that the numerical method is convergent.

8. Approximating Points on Zero Sets of PDE

The method we have developed depends on finding a point P on the zero set $Z(R)$ of the PDAE system R to test that the relevant Jacobians are nonsingular. Their nonsingularity at a point (and thus in a neighborhood) ensures that the conditions for the local existence and uniqueness Theorem 6.12 are satisfied.

We consider polynomially nonlinear PDAE as polynomial systems in Jet space. Our tool to numerically solve polynomial systems is homotopy continuation. In [24], a new field ‘‘Numerical Algebraic Geometry’’ was described which led to the development of homotopies to describe all irreducible components (all meaning: for all dimensions) of the solution set of a polynomial system by witness sets. These methods have been implemented in PHCpack [26].

We can compute $P \in Z(R)$ by exploiting the triangular block structure of the PDAE system after the partial prolongation (see Table 1).

Remark 8.1. In the case of DAE, we can compute the witness points of B_0 , which is the projection of the variety to the subspace, then substitute the solutions into B_1 to extend the solutions to higher dimensional space. Continuing this process, we can find the witness points of nonsingular components. This way is more efficient than solving the whole polynomial system directly. Let R be a polynomially nonlinear DAE $\{R_1, \dots, R_m\}$ with total degree d . Then the Bezout bound of $\mathbf{D}_t^c(R)$ in Jet space is $d^C d^m$, where $C = \sum c_i$. However if we solve it by bottom up substitution it only has at most d^m homotopy continuation paths to track, since any nonlinear equation will be linear with respect to highest Jet variables after prolongation.

Usually applications involve finding real solutions. For real differential polynomial systems using our approach, we need to find points on a real variety. Real algebraic geometry is a rapidly developing area with many recent developments [4, 12]. There are several techniques for compact varieties while approaches are less well-developed in the non-compact case. In our experiments, we heuristically selected some proper real linear equations to slice the variety to obtain real points on the zero set of the PDAE.

9. Application to the Pendulum Curtain PDAE

Consider the system introduced in Example 4.2. This is an IVP for the square system above, and it is a t -dominated system. Assume $\kappa > 0$ and that all variables are real. The system has singular Jacobian with respect to X_{tt}, Y_{tt}, λ . Applying the fast prolongation method in Example 5.1 gives $c = (0, 0, 2)$ and $d = (2, 2, 0)$.

The analysis for this PDAE example yields (see [17] for the case $\kappa = 0$):

$$\begin{aligned}
X_{tt} + \lambda X &= \kappa X_{ss} \\
Y_{tt} + \lambda Y + g &= \kappa Y_{ss} \\
XX_{tt} + YY_{tt} + X_t^2 + Y_t^2 &= 0 \\
XX_t + YY_t &= 0 \\
X^2 + Y^2 - 1 &= 0.
\end{aligned} \tag{29}$$

The top block B_2 of the system is the first three equations of (29) and has Jacobian matrix with respect to X_{tt}, Y_{tt}, λ which has full rank. The blocks B_1 and B_0 are the 4-th and 5-th equations of (29) respectively. To determine whether the system is actually an Implicit Riquier Basis, it remains to show that there is an \mathbb{R} -valued point P at which the relevant Jacobians for B_0, B_1, B_2 have full rank.

Numerical solution of IVP for DAE, requires the determination of a consistent initial point P at $t = 0$ and the computation of an approximate solution through that point. For PDAE a consistent initial point P on the constraints, is first determined. Secondly, initial data should be posed on the constraints at $t = 0$, in a spatial domain containing P . Thirdly appropriate BC need to be adjoined.

For simulations we choose $\hat{s} = 0.5$ at $t = 0$ and we build consistent initial conditions on the constraints in a neighborhood of this point. We find a point $(\hat{t}, \hat{s}, \hat{X}, \hat{Y})$ in J^0 for the lowest block B_0 satisfying $\hat{X}^2 + \hat{Y}^2 - 1 = 0$. For example take $(\hat{s}, \hat{t}, \hat{X}, \hat{Y}) = (0.5, 0.0, 0.4, -\sqrt{1-0.16})$. Now, we determine $\hat{P} = (\hat{t}, \hat{s}, \hat{X}, \hat{Y}, \hat{X}_t, \hat{Y}_t)$ for B_1 in J^1 satisfying $\hat{X}\hat{X}_t + \hat{Y}\hat{Y}_t = 0$. The top block B_2 has full rank with respect to X_{tt}, Y_{tt}, λ at \hat{P} .

We assign an initial condition of form $X(0, s) = F(s)$ in a neighborhood of $\hat{s} = 0.5$. Choosing $F(s) = 0.4 \exp(-(\frac{s-0.5}{0.1})^2)$ then $Y(0, s) = G(s)$ is determined by solving $G(s)^2 + F(s)^2 = 1$.

Secondly we can choose $X_t(0, s) = 0$ (say). This yields $Y_t(0, s) = 0$ corresponding to the curtain being released from rest with a bump initial condition. In general these initial conditions will be valid only locally on some interval $s_{\min} < s < s_{\max}$ and the nonsingularity conditions of the Jacobians need to be continually monitored. In our case these conditions are satisfied for $0 < s < 1$ at $t = 0$.

We apply the method of lines (see Section 7) on an equally spaced grid with $\Delta s = \frac{1}{N}$ (where $s_0 = 0$ and $s_N = 1$). Under the discretization map $\delta(X) = X^{(j)}$, $\delta(Y) = Y^{(j)}$ and $\delta(\lambda) = \lambda^{(j)}$ for $j = 1, \dots, N$, $\delta(X_s) = \frac{X^{(j+1)} - X^{(j-1)}}{2 \Delta s}$, etc. In particular we use central differences at the interior points of the grid.

We apply δ to the system (29) to obtain for $j = 1, \dots, N - 1$:

$$\begin{aligned} X_{tt}^{(j)} + \lambda^{(j)} X^{(j)} &= \kappa \frac{X^{(j+1)} - 2X^{(j)} + X^{(j-1)}}{(\Delta s)^2} \\ Y_{tt} + \lambda^{(j)} Y^{(j)} + g &= \kappa \frac{Y^{(j+1)} - 2Y^{(j)} + Y^{(j-1)}}{(\Delta s)^2} \\ X^{(j)} X_{tt}^{(j)} + Y^{(j)} Y_{tt}^{(j)} + (X_t^{(j)})^2 + (Y_t^{(j)})^2 &= 0 \\ X^{(j)} X_t^{(j)} + Y^{(j)} Y_t^{(j)} &= 0 \\ (X^{(j)})^2 + (Y^{(j)})^2 - 1 &= 0. \end{aligned} \tag{30}$$

By Theorem 7.3 this is an Implicit Riquier Basis at the point corresponding to the point \hat{P} at which the nonsingularity conditions were satisfied for the original PDAE system.

We note that the values of $X^{(j)}$, $Y^{(j)}$, $\lambda^{(j)}$ on the boundaries of the spatial grid where $j = 0, N$ are not specified. The next step is to specify appropriate BC. In particular for $t > 0$ on the boundaries $s = 0, 1$, for continuous solutions we require that the X , Y also satisfy the constraints which contain no spatial derivatives: $X^2 + Y^2 - 1 = 0$ and $XX_t + YY_t = 0$. We can also impose additional conditions at the boundaries which must be analyzed for compatibility with the two conditions above. For our example imposing general Dirichlet conditions at $s = 0$. This yields $X(0, t) = P(t)$, $Y(0, t) = Q(t)$, where P, Q are specified functions, and P, Q satisfy the square system: $P^2 + Q^2 - 1 = 0$ and $PP_t + QQ_t = 0$. This is easily checked to be an implicit Riquier Basis by the fast prolongation method. We chose $P(t) = 0$, $Q(t) = -1$. That is the left end of the curtain is held fixed at $(X, Y) = (0, -1)$. Similarly we chose the same condition at the right end of the curtain.

When these BC are discretized we obtain

$$X^{(0)}(t) = 0, Y^{(0)}(t) = -1, X^{(N)}(t) = 0, Y^{(N)}(t) = -1. \tag{31}$$

In summary the discretized system for our simulations is: the interior DAE given by (30) and the boundary DAE given by (31).

For the simulations we processed the square system at the top block of DAE with an implicit numerical solver in Maple's `dsolve` library. Time snapshots are shown in Figure 2. These were consistent with the results that we obtained in [30] by simultaneously discretizing both space and time for the PDAE. We performed experiments with various

initial and boundary conditions and values of κ . One of these was for an exponential bump located in the middle of the s -range (discussed above), where the curtain is released from rest. As expected this forms two waves, moving in opposite directions (see Figure 2).

10. Discussion

A significant problem in the development of symbolic-numeric differential elimination methods is to create methods to control the growth of prolongations. Although much progress has been made on the symbolic case [2], there are few results in the symbolic-numeric case.

In the current work we define a class of systems, for which only prolongations with respect to a single independent variable t are needed. In particular we discussed the generalization of Pryce's structure analysis technique in the framework of Riquier Bases. That structure analysis has its roots in the historical work of Jacobi (see the historical references in [15]). The recent work of [16] extends Jacobi's work for systems of ordinary differential equations using modern theoretical tools. Also see [25] for results for PDE.

Riquier's classical approach has fallen out of favor in recent times, since for a purely symbolic implementation, it is limited to systems linear in their highest derivatives and modern symbolic alternatives now exist [3, 27]. However in our article, Riquier's approach makes a comeback, by using the Implicit Function Theorem, which requires points on the zero set of the system. These points give initial data that are compatible with its integrability conditions. For highly implicit nonlinear systems, finding initial data can be very difficult. Basically the witness points computed by the homotopy continuation methods lying on our fast prolongation, efficiently gives us a representation of such data. For systems of differential polynomials over \mathbb{C} , we can use homotopy methods from Numerical Algebraic Geometry to compute approximations to such points [24]. For systems of differential polynomials over \mathbb{R} , there are also rapidly evolving methods [12, 4]. For analytic systems, methods are less systematic but progress can be made using Gaussian-Newton iteration from initial guesses close enough to a solution.

It may seem strange that such implicit representations could be useful, especially since the representations given by such symbolic elimination methods as [3] provide output systems in much closer to explicit solved or triangular form. However such eliminations can often cause severe expression swell. The Pryce method, appears to find a balance between working implicitly, while at the same time uncovering and exploiting the block structure of a system. Finally we note that such implicit representations, are an important choice in the numerics community. Solving a constant matrix system, at the intermediate steps of a numerical integration, is often preferred over first symbolically inverting, then evaluating the explicit solution at those intermediate steps.

An interesting research problem is to extend our method to non-square t -dominated systems [29]. The case of over-determined systems ($\ell > m$) is more challenging. One idea is to seek square sub-systems and apply the fast prolongation method to them separately. Then the output needs to be intersected with the remaining equations (perhaps by some type of generalized diagonal differential homotopy).

Our method provides a bridge between DAE and PDAE techniques. In particular, Theorem 7.3 gives a remarkable connection between a PDAE system and its discretized DAE system.

We note that properly posing BC for nonlinear systems and obtaining results, concerning the well-posedness of such problems, existence, uniqueness, and the consistency of numerical schemes for their solutions, is extremely challenging. Our contribution here is limited. Local compatibility, in the sense of absence of local constraints, is certainly a necessary condition, for such an analysis. The fast prolongation method gives us a way to analyze for such compatibility. We remark that the discretization map can include the BC in a natural way, which is not possible with the local differential elimination completion methods. See Krupchyk et al. [10] for very interesting work on linking formal properties to elliptic BVP.

Since the discretized system of a given PDAE will be a DAE, naturally we can apply Pryce’s method to the resulting system. An interesting and very important question is whether the structure analysis of the resulting DAE agrees with the the structure analysis of the original PDAE. Note that the signature matrix of the DAE depends on the discretization scheme. If they are the same, then the discretization step and structure analysis can commute. Consequently we can simply first apply our fast prolongation method to a PDAE then discretize the prolonged PDAE to yield a DAE system without hidden constraints. The solution of the DAE can be obtained and yield approximation to the solution of the PDAE system. This way is equivalent to but much more efficient than applying Pryce’s method directly to the discretized system of the given PDAE. In [23] relations between involutive linear systems with constant coefficients and their semi-discretizations are investigated. For a certain class of “weakly overdetermined systems” it is shown that the resulting DAE have no hidden constraints if and only if the PDAE system is involutive. Interesting discussion on indices and estimates for drift off the constraints is also given.

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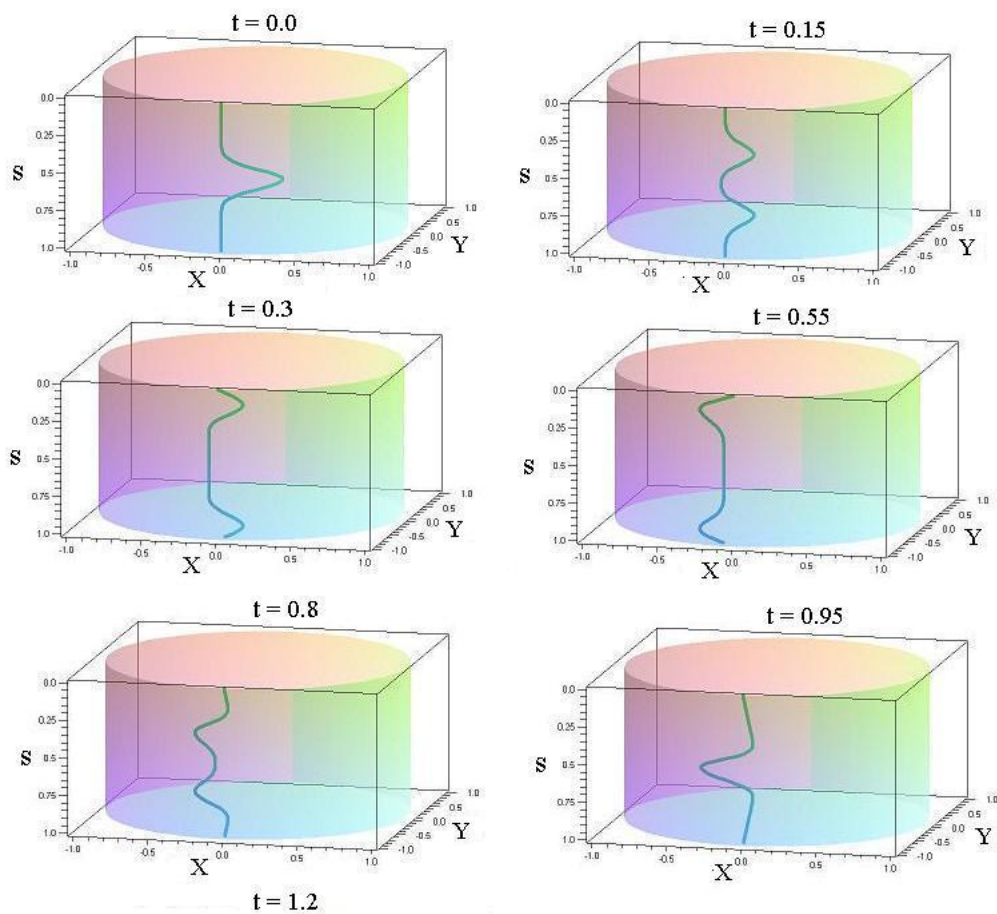


Fig. 2. Time snapshots of Pendulum Curtain with $g = 10$, $\kappa = 1$.

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