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A DIFFERENTIATION INDEX FOR PARTIAL DIFFERENTIAL-ALGEBRAIC EQUATIONS*

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Abstract. A differentiation index for nonlinear partial differential-algebraic equations is presented. Determination of the differentiation index with respect to a direction in the space of independent variables uncovers all equations that must be satisfied by Cauchy data on the hyperplane orthogonal to that direction. This index is thus a generalization of the differentiation index of differential-algebraic equations. The motivation for this work is consistent initialization of partial differential-algebraic systems. The analysis is demonstrated through several examples, including some taken from fluid dynamics and chemical engineering.

Key words. index, consistent initialization, Cauchy data, partial differential equations, differentiation index, Navier–Stokes equations

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1. Introduction. The concept of the index has proven valuable in both the analysis and numerical solution of differential-algebraic equations (DAEs) [1, 2]. In particular, determination of the *differentiation index* of a DAE uncovers constraints that all solutions must satisfy. Algorithms have been developed that, based on a structural analysis that provides a lower bound on the differentiation index of a general DAE, assist in the tasks of consistent initialization [20, 21] and constraint-preserving numerical integration [18].

These algorithms have made possible a new generation of equation-based simulation packages that facilitate solution of DAE-based models of large-scale networks [5, 8]. These packages derive structurally low index models and solve them automatically, reducing the level of expertise required to set up and perform such simulations, and thereby making them more economically feasible in industrial settings [11, 16].

However, some networks cannot be described adequately by DAE, or lumped, models. In such networks, the dependence of variables on additional quantities besides time is important. Examples include spatial dependence of temperature and concentration within tubular chemical reactors, population balances over polymer chain length or crystal size, and concentration profiles with respect to film coordinates in nonequilibrium packed distillation column models. Such networks are naturally described by systems of partial differential-algebraic equations (PDAEs).

Some attempts have been made to define an index for PDAEs. These efforts have focused on a *perturbation index* for a class of one-dimensional problems [4], which is an extension of the perturbation index for DAEs [12]. The problems considered are the model equations together with initial and boundary data and domain dimensions. The perturbation index defined for such problems gives information on the expected smoothness of the solution and provides valuable insight into the behavior of finite

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element or finite difference discretizations of such systems.

In this paper, we will present the complementary notion of the *differentiation index* for general PDAEs. This index is defined for the PDAE itself, before specification of initial or boundary data. It is built on the generalization of initial data at a point for DAEs to Cauchy data on a hyperplane for PDAEs. Cauchy data are the multidimensional analogue of the initial or side conditions required to determine a unique solution of a system of DAEs [19]. Initial conditions and boundary conditions are examples of Cauchy data.

The question that motivates the work presented in this paper is simple: given a PDAE over n independent variables and a surface in $\mathbb{R}^{n-1}$, what equations must Cauchy data on that surface satisfy in order for those data to be consistent with the PDAE? In other words, what are the degrees of freedom for Cauchy data on that surface? Determination of the differentiation index of a PDAE will provide insight into the answer.

2. Review of the differentiation index of a DAE. The material in this section is necessarily brief. For a more complete treatment, see, for example, [1] or [2]. Consider the following general DAE:

$$\mathbf{F}\left(\dot{\mathbf{u}}, \mathbf{u}, t\right) = \mathbf{0}, \tag{2.1}$$

where $\dot{\mathbf{u}} = \frac{d\mathbf{u}}{dt} \in \mathbb{R}^m, \mathbf{u} \in \mathbb{R}^m, \mathbf{F} : G_1 \subset \mathbb{R}^{2m+1} \to \mathbb{R}^m, t \in I$, and I is a subinterval of $\mathbb{R}$. The system is assumed to be *solvable* [1]. The *differentiation index* ν (sometimes called the differential index) of this system is defined as the minimum number of times ν that all or some of the equations must be differentiated in order to determine $\dot{\mathbf{u}}$ as a continuous function of $\mathbf{u}$ and t [10].[1] A system is considered *high index* if $\nu \geq 2$. From here onward the term *index* will refer to the differentiation index.

Algebraic equations may be thought of as constraints on or invariants of the system. An index-0 DAE is simply a fully determined system of ODEs. In an index-1 DAE, the constraints typically appear as explicit algebraic equations. In high index systems, some of the constraints may be implicit in the equations.

Initial conditions are the values of $\mathbf{u}$ and $\dot{\mathbf{u}}$ at some time t_0, denoted $\mathbf{u}_0$ and $\dot{\mathbf{u}}_0$. Clearly, for the initial conditions to be *consistent* with the equations, they must satisfy

$$\mathbf{F}\left(\dot{\mathbf{u}}_0, \mathbf{u}_0, t_0\right) = \mathbf{0}. \tag{2.2}$$

If the system is index-0, and often if it is index-1, only m values of the unknowns $\mathbf{u}$ and $\dot{\mathbf{u}}$ are determined by the equations. Variables or their time derivatives that may be assigned arbitrary initial values and still allow consistent initialization are called *dynamic degrees of freedom* [21]. The number of dynamic degrees of freedom r that must be specified in order to determine a unique solution is less than or equal to the number of differential equations and also less than or equal to the number of differential variables. A particular set of r dynamic degrees of freedom to be arbitrarily specified is called *feasible* if the Jacobian of $\mathbf{F}$ with respect to the remaining variables is regular at $t = 0$ [21].

Consistent initial conditions must also satisfy any constraints that appear only implicitly. For high index or special index-1 systems [20], the result is that there are fewer dynamic degrees of freedom available than for a low index system of the

[1] Other definitions of the index of DAEs exist [3].

same size. Consistent initial conditions for high index systems are sometimes specified completely by the equations and implicit constraints, with no dynamic degrees of freedom.

Linear time invariant DAEs are the best understood class of DAE systems, and for them a very complete analysis exists. A general linear time invariant DAE has the form

$$\mathbf{A}\dot{\mathbf{u}} + \mathbf{B}\mathbf{u} - \mathbf{f}(t) = \mathbf{0}, \tag{2.3}$$

where $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m\times m}$, $\dot{\mathbf{u}}, \mathbf{u} \in \mathbb{R}^m$, $\mathbf{f}(t) : G_2 \subset \mathbb{R}^1 \to \mathbb{R}^m$, and again $t \in I$, with I a subinterval of $\mathbb{R}$.

Iff the *coefficient matrix pencil* $\mathbf{B} - \lambda\mathbf{A}$ is regular, then the system is solvable and may be transformed to an equivalent system of the following form [1]:

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{N} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{w}} \end{bmatrix} + \begin{bmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{w} \end{bmatrix} - \begin{bmatrix} \mathbf{g}_1(t) \\ \mathbf{g}_2(t) \end{bmatrix} = 0, \tag{2.4}$$

where $\dot{\mathbf{v}}, \mathbf{v} \in \mathbb{R}^q, \dot{\mathbf{w}}, \mathbf{w} \in \mathbb{R}^l, \mathbf{g}_1(t) : G_3 \subset \mathbb{R}^1 \to \mathbb{R}^q,\ \mathbf{g}_2(t) : G_4 \subset \mathbb{R}^1 \to \mathbb{R}^l$, and $q + l = m$. Here $\mathbf{C} \in \mathbb{R}^{q\times q}$, and $\mathbf{N} \in \mathbb{R}^{l\times l}$ is a matrix of nilpotency k, i.e., $\mathbf{N}^k = \mathbf{0}$; $\mathbf{N}^{k-1} \neq \mathbf{0}$. The variables $\mathbf{v}$ are called the differential variables, and $\mathbf{w}$ are the algebraic variables.

It can be shown [1] that the index of the system is equal to k, that $\mathbf{v}(t)$ is a solution of

$$\dot{\mathbf{v}} = -\mathbf{C}\mathbf{v} + \mathbf{g}_1(t), \tag{2.5}$$

and that $\mathbf{w}(t)$ is given by

$$\mathbf{w} = \sum_{i=0}^{k-1} (-1)^i\, \mathbf{N}^i \mathbf{g}_2^{(i)}(t). \tag{2.6}$$

The solution to (2.3) thus depends on up to $k-1$ derivatives of the forcing function $\mathbf{g}_2$. A unique solution is determined by only $m-l$ arbitrary constants, since no constants of integration appear in the evaluation of $\mathbf{w}$.

Example 0. Consider the following linear time invariant DAE:

$$\dot{u}_1 - u_2 = 0, \tag{2.7}$$

$$u_1 = f(t). \tag{2.8}$$

There is one explicit constraint on the solution (2.8). There is another constraint, given only implicitly, that is made explicit by differentiation with respect to the independent variable time:

$$\dot{u}_1 = f'(t). \tag{2.9}$$

Clearly,

$$u_2 = f'(t). \tag{2.10}$$

One more differentiation gives us the final constraint, this time on $\dot{u}_2$:

$$\dot{u}_2 = f''(t). \tag{2.11}$$

Consider the problem of determining consistent initial conditions for this system. The initial conditions must satisfy not only the original system (2.7)–(2.8) but also the implicit constraints (2.9)–(2.11). The system is index-2, and there are four equations that relate the four unknowns $\dot{u}_1(t_0), u_1(t_0), \dot{u}_2(t_0), u_2(t_0)$. Consistent initial conditions are the solution to this set of equations; there are no dynamic degrees of freedom.

For linear time-varying DAEs, the *derivative array equations* [10] provide the most useful insight into the index. Suppose that the system is

$$\mathbf{A}(t)\dot{\mathbf{u}} = \mathbf{f}(t) - \mathbf{B}(t)\mathbf{u}. \tag{2.12}$$

Provided that $\mathbf{A}$, $\mathbf{B}$, $\mathbf{u}$, and $\mathbf{f}$ are sufficiently smooth, repeatedly differentiating the system produces the following series of equations:

$$\begin{aligned} \mathbf{A}\dot{\mathbf{u}} &= \mathbf{f} - \mathbf{B}\mathbf{u}, \\ \left(\dot{\mathbf{A}} + \mathbf{B}\right)\dot{\mathbf{u}} + \mathbf{A}\ddot{\mathbf{u}} &= \dot{\mathbf{f}} - \dot{\mathbf{B}}\mathbf{u}, \\ \left(\ddot{\mathbf{A}} + 2\dot{\mathbf{B}}\right)\dot{\mathbf{u}} + \left(2\dot{\mathbf{A}} + \mathbf{B}\right)\ddot{\mathbf{u}} + \mathbf{A}\dddot{\mathbf{u}} &= \ddot{\mathbf{f}} - \ddot{\mathbf{B}}\mathbf{u}, \\ &\vdots \end{aligned} \tag{2.13}$$

The first j differentiations produce the following system:

$$\begin{bmatrix} \mathbf{A}^{(0)} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{A}^{(1)} + \mathbf{B}^{(0)} & \mathbf{A}^{(0)} & \cdots & \mathbf{0} \\ \mathbf{A}^{(2)} + 2\mathbf{B}^{(1)} & 2\mathbf{A}^{(1)} + \mathbf{B}^{(0)} & \ddots & \mathbf{0} \\ \vdots & \vdots & & \mathbf{A}^{(0)} \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(1)} \\ \mathbf{u}^{(2)} \\ \vdots \\ \mathbf{u}^{(j)} \end{bmatrix} = - \begin{bmatrix} \mathbf{B}^{(0)} \\ \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{B}^{(j-1)} \end{bmatrix} \mathbf{u} + \begin{bmatrix} \mathbf{f}^{(0)} \\ \mathbf{f}^{(1)} \\ \vdots \\ \mathbf{f}^{(j-1)} \end{bmatrix}, \tag{2.14}$$

which may be written more conveniently as

$$\mathcal{A}_j \mathbf{u}_j = -\mathcal{B}_j \mathbf{u} + \mathbf{f}_j. \tag{2.15}$$

This system is always singular, unless the original system consisted strictly of ODEs. However, the system might uniquely determine $\mathbf{u}^{(1)} = \dot{\mathbf{u}}$. The jth block row is produced by $j-1$ differentiations, so that if $\mathcal{A}_j$ determines $\dot{\mathbf{u}}$ as a unique function of $\mathbf{u}$ and t, the index of the original system is $j-1$. This property motivates the following definition [1].

DEFINITION 2.1. *The matrix $\mathcal{A}_j$ is smoothly* 1*-full if there is a smooth nonsingular* $\mathbf{R}(t)$ *such that*

$$\mathbf{R}\mathcal{A}_j = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{H} \end{bmatrix} \tag{2.16}$$

and the identity $\mathbf{I}$ *is* $m \times m$, *where* $\mathbf{A}, \mathbf{B}$ *are* $m \times m$. *There are no requirements on* $\mathbf{H}$.

Now consider t restricted to a subinterval I of $\mathbb{R}$. The index of any system that is not linear time-invariant is a local property and may change over I. If, however, $\mathcal{A}_j$ is smoothly 1-full over I, then the index ν over I is defined as the smallest integer k such that $\mathcal{A}_{k+1}$ is 1-full over I. This approach forms the basis for index analysis of nonlinear systems [1].

3. The differentiation index of a PDAE. A manifold in $\mathbb{R}^n$ is a surface of dimension $n-1$. At any point on the (assumed smooth and nondegenerate) surface, the manifold is characterized by its normal. A local change of coordinates may be made at that point, with the normal as one basis vector (the *exterior direction*) and all other basis vectors orthogonal to the normal (the *interior directions*). Derivatives taken in the direction of the normal are called *exterior derivatives*; those taken along any of the other basis vectors are called *interior derivatives* [13]. In the rest of the paper, we will deal with hyperplanes, so the change of coordinates to an exterior and zero or more interior directions will be a global transformation. Note that the value of a dependent variable over a hyperplane determines its interior derivatives on that hyperplane [15].

One interpretation of the index of a DAE is the number of differentiations required to produce a fully determined ODE. A possible approach to generalizing this interpretation to PDAEs would be to define the differentiation index as the number of differentiations with respect to a particular independent variable that are required to produce a fully determined system of PDEs. Such an approach is perfectly valid and may prove useful for some analyses, but it will not always provide the information about consistent Cauchy data that motivates this work. For example, the incompressible Navier–Stokes equations (section 5.3) are a system of PDEs that have implicit constraints on consistent initial data.

So, this work develops an index by focusing instead on Cauchy data. Cauchy data are the values of the dependent variables and the exterior derivatives of the variables over the entire hyperplane. As noted in the introduction, Cauchy data represent the generalization of initial data for DAEs to the multidimensional case.

Consider a PDAE system over $\mathbb{R}^n$. Without loss of generality, let the system be first order [13]. Call the independent variables $\mathbf{x} \in \mathbb{R}^n$, let the dependent variables be $\mathbf{u} \in \mathbb{R}^m$, and suppose the following PDAE holds over the rectangular domain $x_i \in I_i$, $i = 1 \ldots n$:

$$\mathbf{F}\left(\mathbf{u}_{x_{i=1\ldots n}}, \mathbf{u}, \mathbf{x}\right) = 0. \tag{3.1}$$

Here $\mathbf{u}_{x_i} = \frac{\partial \mathbf{u}}{\partial x_i} \in \mathbb{R}^m, \mathbf{u} \in \mathbb{R}^m, \mathbf{x} \in \mathbb{R}^n, \mathbf{F} : G_5 \subset \mathbb{R}^{2m+n} \to \mathbb{R}^m$, and I_i is a subinterval of $\mathbb{R}$, for $i = 1 \ldots n$. We assume that a solution $\mathbf{u}$ exists.

In order to make the parallel with the DAE case more clear, denote the partial derivative of $\mathbf{u}$ with respect to x_j by a dot, so $\mathbf{u}_{x_j} = \dot{\mathbf{u}}$. For all other $i \neq j$, partial differentiation will still be denoted by a subscripted independent variable. The dot denotes differentiation with respect to the direction exterior to the hyperplane $x_j =$ *constant*; all other partial derivatives are interior on that hyperplane. Using this notation, the general system (3.1) is written as

$$\mathbf{F}\left(\dot{\mathbf{u}}, \mathbf{u}_{x_{i=1\ldots n, i\neq j}}, \mathbf{u}, \mathbf{x}\right) = 0. \tag{3.2}$$

Note that $\mathbf{J}(\mathbf{F}, \dot{\mathbf{u}})$, the Jacobian of $\mathbf{F}$ with respect to $\mathbf{u}$, may be singular. Under the assumptions that a solution $\mathbf{u}$ exists and that both $\mathbf{u}$ and $\mathbf{F}$ are sufficiently differentiable, the differentiation index of this PDAE may be defined as follows.

DEFINITION 3.1. *The differentiation index with respect to x_j, or ν_{x_j}, is the smallest number of times $\mathbf{F}$ must be differentiated with respect to x_j in order to determine $\dot{\mathbf{u}}$ as a continuous function of $\mathbf{u}_{x_{i\neq j}}, \mathbf{u}, \mathbf{x}$.*

A formal index analysis built on the concept of a derivative array for PDAEs may be most easily constructed for linear systems. Such an analysis is not as straightforward as that for linear DAEs, however, because one must consider linear operator-valued coefficient matrices. This analysis may be extended fairly readily to a particular class of semilinear systems, of which linear systems are a special case, so this formal index analysis will be presented only once, for the more general class of systems.

Consider a PDAE system of the following form:

$$\mathbf{F}\left(\dot{\mathbf{u}}, \mathbf{u}_{x_{i=1\ldots n, i\neq j}}, \mathbf{u}, \mathbf{x}\right) = \sum_{i=1}^{n} \mathbf{A}_i(x_j)\mathbf{u}_{x_i} + \mathbf{C}(x_j)\mathbf{u} - \mathbf{f}(\mathbf{x}) = 0. \tag{3.3}$$

$\mathbf{A}_i(x_j), \mathbf{C}(x_j) : G_6 \subset \mathbb{R}^1 \to \mathbb{R}^{m\times m}$, and all other quantities are defined as in the general case (3.1). Such a system will hereafter be referred to as a linear x_j-varying PDAE.

The system may be rewritten as

$$\mathbf{A}(x_j)\dot{\mathbf{u}} + \mathbf{B}(x_j)\mathbf{u} - \mathbf{f}(\mathbf{x}) = 0, \tag{3.4}$$

where

$$\begin{aligned}
\mathbf{A}(x_j) &= \mathbf{A}_j(x_j),\\
\dot{\mathbf{u}} &= \mathbf{u}_{x_j},\\
\mathbf{B}(x_j) &= \mathbf{C}(x_j) + \sum_{i\neq j} \mathbf{A}_i(x_j) D_{x_i},\\
D_{x_i} &= \frac{\partial}{\partial x_i}.
\end{aligned}$$

This system (3.4) has the same form as the linear time-varying DAE (2.12).

However, here $\mathbf{B} \in P_{Ij}^{m\times m}$, the set of all m by m matrices whose elements belong to P_{Ij}. $P_{Ij} = \{L \mid Lu = \sum_{\boldsymbol{\tau}} l_{\boldsymbol{\tau}}(x_j) D_{\boldsymbol{\tau}} u, u \in \mathbb{R}\}$, where $\boldsymbol{\tau}$ is a multi-index with $\tau_i \in \mathbb{Z}^+$ and $\tau_j = 0$; $l_{\boldsymbol{\tau}}(x_j) : G \in \mathbb{R}^1 \to \mathbb{R}^1$ and is analytic for $x_j \in I_j$; I_j is a closed interval in $\mathbb{R}$; and $D_{\boldsymbol{\tau}} = \prod_{i=1}^{n} \left(\frac{\partial}{\partial x_i}\right)^{\tau_i}$. P_{Ij} is the set of all interior partial differential operators on any hyperplane ϕ orthogonal to x_j given by $x_j = c$, $c \in I_j$, with coefficients that vary smoothly in x_j over I_j. Any $p \in P_{Ij}$ is a linear operator on ϕ.

The operators $+$ and $\times$ are defined as follows for any two operators $a, b \in P_{Ij}$:

$$a + b = \sum_{\boldsymbol{\nu}} a_{\boldsymbol{\nu}} D_{\boldsymbol{\nu}} + \sum_{\boldsymbol{\nu}} b_{\boldsymbol{\nu}} D_{\boldsymbol{\nu}} = \sum_{\boldsymbol{\nu}} \left(a_{\boldsymbol{\nu}} + b_{\boldsymbol{\nu}}\right) D_{\boldsymbol{\nu}},$$

$$a \times b = \left(\sum_{\boldsymbol{\nu}} a_{\boldsymbol{\nu}} D_{\boldsymbol{\nu}}\right)\left(\sum_{\boldsymbol{\gamma}} b_{\boldsymbol{\gamma}} D_{\boldsymbol{\gamma}}\right) = \sum_{\boldsymbol{\nu}} \sum_{\boldsymbol{\gamma}} a_{\boldsymbol{\nu}} b_{\boldsymbol{\gamma}} D_{\boldsymbol{\nu}+\boldsymbol{\gamma}}.$$

LEMMA 3.2. *$\langle P_{Ij}^{m\times m}, +, \times\rangle$ is a ring.*

Proof. $\langle P_{Ij}, +\rangle$ is an abelian group. $\times$ is associative on P_{Ij} and is left and right distributive with $+$. Therefore $\langle P_{Ij}, +, \times\rangle$ is a ring. The set $P_{Ij}^{m\times m}$ of all square matrices whose elements belong to P_{Ij} forms a ring with the same operators [9]; thus $\langle P_{Ij}^{m\times m}, +, \times\rangle$ is a ring. □

Thus, many results from standard matrix algebra also hold for $P_{Ij}^{m\times m}$. For example, row operations may be used to permute rows, scale or add rows together, perform Gauss elimination, and evaluate determinants.

LEMMA 3.3. *For $\mathbf{A} \in P_{Ij}^{m\times m}$, if $|\mathbf{A}| \neq 0$, then $\exists\ \mathbf{R} \in P_{Ij}^{m\times m}$ such that $\mathbf{RA} = \mathbf{D}$, where $\mathbf{D} \in P_{Ij}^{m\times m}$ is a diagonal matrix with $d_{ii} \neq 0$.*

Proof. Because $\langle P_{Ij}^{m\times m}, +, \times\rangle$ is a ring, Gauss elimination may be used to produce first an upper triangular and then a diagonal matrix through row operations alone. Therefore, Gauss elimination gives a sequence of row operations $\mathbf{R} \in P_{Ij}^{m\times m}$ for which $\mathbf{RA} = \mathbf{D}$. If $|\mathbf{A}| \neq 0$, the elements of the diagonal matrix $\mathbf{D}$ will be strictly nonzero. ∎

In analogy with DAEs, the derivative array equations for the PDAE (3.4) may be calculated up to any order of differentiation with respect to x_j, as long as $\mathbf{A}(x_j)$, $\mathbf{B}(x_j)$, $\mathbf{f}$, and $\mathbf{u}$ are sufficiently differentiable. In the linear case, $\mathbf{A}^{(l)} = \mathbf{B}^{(l)} = \mathbf{0}$ if $l > 0$, so the derivative array equations with respect to x_j are

$$\begin{bmatrix} \mathbf{A} & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{B} & \mathbf{A} & \mathbf{0} & \dots \\ \mathbf{0} & \mathbf{B} & \mathbf{A} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(1)} \\ \cdot \\ \cdot \\ \mathbf{u}^{(k)} \end{bmatrix} = - \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \\ \cdot \\ \cdot \end{bmatrix} \mathbf{u} + \begin{bmatrix} \mathbf{f}^{(0)} \\ \cdot \\ \cdot \\ \mathbf{f}^{k-1} \end{bmatrix} \tag{3.5}$$

or

$$\mathcal{A}_k \mathbf{u}_k = -\mathcal{B}_k \mathbf{u} + \mathbf{f}_k. \tag{3.6}$$

The following result for linear PDAEs (3.3) will be useful later in the paper.

THEOREM 3.4. *$\nu_{x_i} \geq 1$ iff $|\mathbf{A}_i| = 0$.*

Proof. If $\nu_{x_i} \geq 1$, then by definition the system does not uniquely determine $\mathbf{u}_{x_i}$, and thus $|\mathbf{J}(\mathbf{F}, \mathbf{u}_{x_i})| = 0$. Since $\mathbf{J}(\mathbf{F}, \mathbf{u}_{x_i}) = \mathbf{A}_i$, we must have $|\mathbf{A}_i| = 0$. Similarly, if $|\mathbf{A}_i| = 0$, then $|\mathbf{J}(\mathbf{F}, \mathbf{u}_{x_i})| = 0$ and the system cannot be solved for unique $\mathbf{u}_{x_i}$, and by definition $\nu_{x_i} \geq 1$. ∎

In the linear x_j-varying case, the first k derivative array equations with respect to x_j are

$$\begin{bmatrix} \mathbf{A}^{(0)} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{A}^{(1)} + \mathbf{B}^{(0)} & \mathbf{A}^{(0)} & \dots & \mathbf{0} \\ \mathbf{A}^{(2)} + 2\mathbf{B}^{(1)} & 2\mathbf{A}^{(1)} + \mathbf{B}^{(0)} & \ddots & \mathbf{0} \\ \vdots & \vdots & & \mathbf{A}^{(0)} \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(1)} \\ \mathbf{u}^{(2)} \\ \vdots \\ \mathbf{u}^{(k)} \end{bmatrix} = - \begin{bmatrix} \mathbf{B}^{(0)} \\ \mathbf{B}^{(1)} \\ \vdots \\ \mathbf{B}^{(k-1)} \end{bmatrix} \mathbf{u} + \begin{bmatrix} \mathbf{f}^{(0)} \\ \mathbf{f}^{(1)} \\ \vdots \\ \mathbf{f}^{(k-1)} \end{bmatrix}. \tag{3.7}$$

While the derivative array equations have the same form as given for linear time-varying DAEs, $\mathbf{A}^{(i)} = (\frac{\partial}{\partial x_j})^i \mathbf{A} \in P_{Ij}^{m\times m}$ and $\mathbf{B}^{(i)} = (\frac{\partial}{\partial x_j})^i \mathbf{B} \in P_{Ij}^{m\times m}$.

The ring property of $P_{Ij}^{m\times m}$ allows the following definition.

DEFINITION 3.5. *The matrix $\mathcal{A}_k$ is smoothly 1-full on ϕ_{Ij} if there is a smooth nonsingular $\mathbf{R}(x_j)$ such that*

$$\mathbf{R}\mathcal{A}_k = \begin{bmatrix} \mathbf{D}(x_j) & \mathbf{0} \\ \mathbf{0} & \mathbf{H}(x_j) \end{bmatrix},$$

where $\mathbf{D}(x_j) \in P_j^{m\times m}$ is a nonsingular diagonal matrix and ϕ_{Ij} is the set of hyperrectangles orthogonal to the x_j-coordinate direction given by $\{\mathbf{x} \mid x_j = c, c \in I_j; x_{i=1\dots n, i\neq j} \in I_i\}$.

When $\mathcal{A}_k$ is smoothly 1-full on ϕ_{Ij}, the $k-1$ differentiations with respect to x_j that generate the derivative array equations give $\dot{\mathbf{u}}$ as an x_j-continuous function of $\mathbf{u}$ and $\mathbf{x}$ over all $\phi \in \phi_{Ij}$. As with DAEs, the solution of an index ν_{x_j} linear or linear

x_j-varying PDAE will depend on up to $\nu_{x_j} - 1$ derivatives with respect to x_j of the forcing function over ϕ_{Ij}.

THEOREM 3.6. *For a linear x_j-varying system, if k is the smallest integer such that $\mathcal{A}_k$ is smoothly* 1*-full over I_j, the maximum index ν_{x_j} on ϕ_{Ij} is $k-1$.*

Proof. Suppose that, on some hyperrectangle $x_j = c$, $c \in I_j$, the index ν_{x_j} is greater than $k-1$. Then $k-1$ differentiations do not determine $\dot{\mathbf{u}}$. But $\mathcal{A}_k$ is smoothly 1-full on I_j, so it does determine $\dot{\mathbf{u}}$ as a continuous function at $x_j = c$, and the index cannot be greater than $k-1$. $\square$

For more general semilinear and nonlinear systems, the derivative array equations may still be defined, again provided that the original system is sufficiently differentiable. However, they may not have the convenient matrix structure that exists for linear and linear x_j-varying systems. Even for simple linear systems, the full derivative array equations are often not calculated, as only a subset of the equations constrain Cauchy data when differentiated.[2]

Furthermore, nonlinear systems may develop discontinuous solutions even given smooth data and forcing functions. For such systems, the index is therefore a *local* property in $(\mathbf{u}, \mathbf{x})$-space, just as the differentiation index is a local property for nonlinear DAEs. Note that it is possible to specify discontinuous Cauchy data for a linear PDAE (such as a Riemann problem); there is no analogue of the Riemann problem for DAEs. In such a case, the index may locally fail to exist at the discontinuity, even for linear PDAEs with smooth forcing functions, while the index of a linear DAE with smooth forcing functions exists globally.

So in summary, suppose Cauchy data are to be specified on a hyperplane orthogonal to the x_j-coordinate direction given by $x_j = x_{j0} \in I_j$. Denote all derivatives with respect to the exterior direction x_j by a dot, i.e., $\dot{\mathbf{u}} = \mathbf{u}_{x_j}$. Cauchy data on this surface are the values of $\dot{\mathbf{u}}_0$ and $\mathbf{u}_0$ over the entire surface. In order for these data to be consistent with the original equation (3.1), clearly they must satisfy

$$\mathbf{F}\left(\dot{\mathbf{u}}_0, \mathbf{u}_{0x_{i\neq j}}, \mathbf{u}_0, x_{i\neq j}, x_{j0}\right) = 0. \tag{3.8}$$

Determination of ν_{x_j} will derive any other equations that restrict consistent Cauchy data, in a manner similar to how determination of the index of a DAE uncovers the complete set of equations that must be satisfied by consistent initial conditions.

Example 1. Consider the following system:

$$\begin{aligned} u_{x_1} - v_{x_2} &= 0, \\ v_{x_1} - u_{x_2} &= 0 \end{aligned} \tag{3.9}$$

over $0 \leq x_1, a \leq x_2 \leq b$. Suppose one wants to specify Cauchy data on the hyperplane given by $x_1 = 0$. Clearly such data must satisfy

$$\begin{aligned} \dot{u} - v_{x_2} &= 0, \\ \dot{v} - u_{x_2} &= 0 \end{aligned} \tag{3.10}$$

on $(x_1 = 0)$. No additional independent equations relating $\dot{u}$ and $\dot{v}$ may be derived through differentiation with respect to x_1; the system determines $\dot{u}$ and $\dot{v}$, so its index with respect to x_1 is 0. Two degrees of freedom exist for specification of Cauchy data on $(x_1 = 0)$.

[2]In the following examples, typically only this subset of the equations will be differentiated.

This system is the wave equation, written as a first order system. The question of Cauchy data on $(x_1 = 0)$ corresponds to the initial conditions. For the wave equation, initial conditions are typically provided as values of u and v over the initial hyperplane. Alternative specifications of Cauchy data, involving ODEs or PDEs, will be considered in the next section.

Example 2. Consider the following system:

$$\begin{aligned} u_{x_1} - v &= 0, \\ u_{x_2} &= f_1(x_1). \end{aligned} \tag{3.11}$$

Suppose we wish to specify Cauchy data on $(x_1 = 0)$. Such data must of course satisfy the original equations, here rewritten using a dot to again denote differentiation along the exterior direction:

$$\begin{aligned} \dot{u} - v &= 0, \\ u_{x_2} &= f_1(x_1). \end{aligned} \tag{3.12}$$

Differentiating the second equation with respect to x_1 produces another independent equation involving $\dot{u}$,

$$\dot{u}_{x_2} = \frac{d}{dx_1} f_1(x_1). \tag{3.13}$$

Differentiating this new equation and the first equation in (3.12) gives two additional equations in the two new unknowns $\ddot{u}$ and $\dot{v}$:

$$\begin{aligned} \ddot{u} - \dot{v} &= 0, \\ \ddot{u}_{x_2} &= \frac{d^2}{dx_1^2} f_1(x_1). \end{aligned} \tag{3.14}$$

Assuming that $f_1(x_1)$ is twice differentiable, two differentiations with respect to x_1 give u_{x_1} and v_{x_1} as continuous functions of u, v, and $\mathbf{x}$; thus ν_{x_1}, the index of this system with respect to x_1, is 2. The system (3.12)–(3.14) is fully determined in the variables $\ddot{u}, \dot{u}, u, \dot{v}$, and v; no degrees of freedom are available for the specification of Cauchy data on the hyperplane $(x_1 = 0)$.

Now, suppose we wish instead to specify Cauchy data on $(x_2 = 0)$. The exterior direction to this hyperplane is x_2 and the system may be rewritten for clarity as

$$\begin{aligned} u_{x_1} - v &= 0, \\ \dot{u} &= f_1(x_1). \end{aligned} \tag{3.15}$$

Differentiation of the first equation yields

$$\dot{u}_{x_1} - \dot{v} = 0, \tag{3.16}$$

which gives $\dot{u}$ and $\dot{v}$ as functions of u, v, and $\mathbf{x}$. No additional independent equations may be derived that relate the variables $\dot{u}, u, \dot{v}$, and v. Therefore $\nu_{x_2} = 1$ and there is one degree of freedom available for specification of Cauchy data on the hyperplane. Note, however, that neither $\dot{u}$ nor $\dot{v}$ may be specified; only u or v may be set independently on the hyperplane.

To verify the preceding results, note that the solution of the PDAE system above on the semi-infinite domain $0 \leq x_1, -a \leq x_2 \leq a$ is determined by a single function $g(x_1)$ specified at some point $c : -a \leq c \leq a$:

$$\begin{aligned} u(x_1, x_2) &= x_2 f_1(x_1) + g(x_1), \\ v(x_1, x_2) &= x_2 \frac{d}{dx_1} \left(f_1(x_1) + g(x_1) \right). \end{aligned} \tag{3.17}$$

Thus the solution on the hyperplane $(x_1 = 0)$ is given by $f(0)$ and $g(0)$; no other degrees of freedom remain (as indicated by the index analysis). The conditions for consistency with the equations fully determine all Cauchy data on that hyperplane.

Example 3. The hyperplane on which Cauchy data are analyzed for consistency with the equations need not be orthogonal to one of the original coordinate axes. If the index with respect to a noncoordinate direction is needed, the coordinates may be transformed so that one of the new coordinate vectors lies along the direction of interest, and all other coordinate vectors are orthogonal to the direction of interest.

Consider the index of the one-way wave equation

$$cu_{x_1} + u_{x_2} = 0 \tag{3.18}$$

with respect to the direction $(x_1, x_2) = (1, -1)$. Define a new coordinate system by

$$\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \tag{3.19}$$

so that the direction of interest is now in the y direction and the z direction is orthogonal to the y direction. Transforming to the new coordinate system, the equation becomes

$$(c-1)\dot{u} + (c+1)u_z = 0. \tag{3.20}$$

The index with respect to y is zero, unless $c = 1$. In this case, the index becomes 1, and Cauchy data on $y = y_0$ must also satisfy

$$\dot{u}_z = 0. \tag{3.21}$$

When $c \neq 1$, the index is zero and either $\dot{u}$ or u may be specified arbitrarily on the hyperplane. In the case $c = 1$, neither may be specified independently. However, there is a *lower dimensionality degree of freedom.* That is, the system (3.20)–(3.21) constrains both $\dot{u}$ and u over the hyperplane $(y = y_0)$, so that neither may be specified arbitrarily *over the entire surface.* The value of each may be given arbitrarily *at a single point on the surface*, and that value determines the Cauchy data.

Note that the surface $(y = y_0)$ is a characteristic surface of the one-way wave equation when $c = 0$. The differentiation index and characteristics are related by the following theorem.

THEOREM 3.7. *A hyperplane $\phi(\mathbf{x}) = 0$ is a characteristic surface of a linear system iff $\nu_{\nabla\phi} \geq 1$.*

Proof. Consider, without loss of generality, a linear system of first order

$$\sum_{i=1}^{n} \mathbf{A}_i \mathbf{u}_{x_i} = \mathbf{f}(\mathbf{u}, \mathbf{x}) \tag{3.22}$$

and a hyperplane given by

$$\phi(\mathbf{x}) = 0, \quad \phi_{\mathbf{x}} = [\phi_{x_1}\ \phi_{x_2}\ \ldots\ \phi_{x_n}] \neq 0. \tag{3.23}$$

Consider a coordinate change from $\mathbf{x}$ to $\mathbf{z}$, where $z_n = \phi(\mathbf{x})$, and z_i, $i = 1 \ldots (n-1)$, denotes distance in the direction of basis vector $\mathbf{b}_i$. Let the basis vectors for the new coordinate system be orthogonal so that $\mathbf{b}_i \cdot \nabla\phi = \mathbf{b}_i \cdot \mathbf{b}_{j\neq i} = 0$. In the new coordinates, the system becomes

$$\mathbf{B}_n \mathbf{u}_{z_n} + \sum_{i=1}^{n-1} \mathbf{B}_i \mathbf{u}_{z_i} = \mathbf{f}(\mathbf{u}, \mathbf{x}(\mathbf{z})), \tag{3.24}$$

where

$$\begin{aligned} \mathbf{B}_n &= \sum_{j=1}^{n} \mathbf{A}_i \phi_{x_i}, \\ \mathbf{B}_i &= \sum_{j=1}^{n} \mathbf{A}_j \frac{\partial z_i}{\partial x_j}, \quad i = 1 \ldots n-1. \end{aligned} \tag{3.25}$$

Note that $\mathbf{u}_{z_n}$ is the exterior derivative, and all other derivatives are interior on the surface.

If the system has $\nu_{\nabla\phi} \geq 1$, then by Theorem 3.4 $|\mathbf{B}_n| = 0$. If $|\mathbf{B}_n| = 0$, the surface is a characteristic surface [19]. Conversely, if the surface is characteristic, then by definition $|\mathbf{B}_n| = 0$ and thus $\nu_{\nabla\phi} \geq 1$. $\square$

Remark. For a linear system that includes one or more algebraic equations, every hyperplane is a characteristic surface.

4. Dynamic degrees of freedom. Index analysis of PDAEs with respect to a direction x_j requires derivation of all independent equations that constrain allowable Cauchy data on a hyperplane ϕ orthogonal to that direction. The consistent Cauchy data problem for the original first-order PDAE (3.2) consists in part of the original m equations in the $2m$ variables $\dot{\mathbf{u}}$ and $\mathbf{u}$. Again note that interior derivatives of $\mathbf{u}$ on ϕ and the value of $\mathbf{u}$ itself over ϕ are not independent; the interior derivatives of $\mathbf{u}$ are simply functions of $\mathbf{u}$ on ϕ.

For a linear system (3.4) with constant coefficient matrices, assume that $[\mathbf{A} : \mathbf{B}]$ has full rank. This implies that the coefficients in the derivative array equations $[\mathcal{A}_k : \mathcal{B}_k]$ have full rank for any k. Now suppose that the index of the system with respect to x_j is $k-1$, so that $\mathcal{A}_k$ is smoothly 1-full. Using Gauss elimination on the derivative array equations, the number of elements of $\mathbf{u}$ that are determined by algebraic or interior PDEs on ϕ may be shown to be η, where $\eta = \dim(\mathcal{N}(\mathcal{A}_k))$. Because the kth derivative array equations are 1-full, all m exterior partial derivatives $\dot{\mathbf{u}}$ are also determined by algebraic or interior PDEs. For a semilinear, quasi-linear, or nonlinear system, algebraic manipulation of all or of a subset of the derivative array equations may be employed on a case-by-case basis to determine what variables are given by algebraic or interior PDEs over ϕ. Note that this analysis does not provide any information regarding the well-posedness of the resulting interior PDEs.

Let $r = m - \eta$. The definition of dynamic degrees of freedom for DAEs [21] then generalizes naturally to PDAEs.

DEFINITION 4.1. *Variables $\mathbf{u}$ or their exterior derivatives $\dot{\mathbf{u}}$ which can be assigned arbitrary distributions over ϕ and still allow solution of* (3.2) *are called dynamic degrees of freedom on ϕ; r dynamic degrees of freedom on ϕ must be specified to fully determine Cauchy data on ϕ.*

A DAE initialization problem always produces an algebraic system. However, with PDAEs, a consistent Cauchy data problem may itself be another PDAE, in more dependent variables over one fewer independent variable than the original system. Determination of a unique solution may require additional data in the form of side or boundary conditions.

Example 4. Consider the equations that consistent Cauchy data must obey on a characteristic manifold of the one-way wave equation (3.20)–(3.21). With two equations in u and $\dot{u}$, there are no dynamic degrees of freedom on $(y = y_0)$.

Let $p = u$ and $q = \dot{u}$, so that the consistent Cauchy data problem is written as

$$\begin{aligned} p_z &= 0, \\ q_z &= 0. \end{aligned} \tag{4.1}$$

For the original system of one dependent variable over two independent variables, our consistent Cauchy data problem is a system of two dependent variables over a single independent variable.

It is a simple, index-0 DAE, which has no implicit constraints that relate p and q. Two dynamic degrees of freedom on $(y = y_0, z = z_0)$ are required in order to specify a unique solution. Thus determination of consistent Cauchy data requires no dynamic degrees of freedom over the initial hyperplane $(y = y_0)$ but requires two side conditions on the lower dimensional hyperplane $(y = y_0, z = z_0)$.

5. Larger examples. In the following examples, all equations, forcing functions, and dependent variables are assumed to possess all required partial derivatives.

5.1. An illustrative system. Consider again the simple system (3.11) presented in section 3. Recall that, for Cauchy data on the hyperplane $(x_2 = 0)$, a value of either $v(x_1, 0)$ or $u(x_1, 0)$ completely determined the data. Let us consider each case in more detail. The exterior direction is x_2, so $u_{x_2} = \dot{u}$ and $v_{x_2} = \dot{v}$. The equations that must be satisfied over the hyperplane include the original equations

$$\begin{aligned} u_{x_1} - v &= 0, \\ \dot{u} &= f_1(x_1), \end{aligned} \tag{5.1}$$

and the additional independent equation derived during index analysis,

$$\dot{u}_{x_1} - \dot{v} = 0. \tag{5.2}$$

Here $r = 1$; one dynamic degree of freedom on $(x_2 = 0)$ is required to fully determine Cauchy data.

First, consider specification of v over the hyperplane, so that

$$v = h_1(x_1) \tag{5.3}$$

is appended to the system (5.1)–(5.2). These four equations in the four variables $\dot{u}$, u, $\dot{v}$, and v form the PDAE (here a DAE) that will be used to determine the Cauchy data on $(x_2 = 0)$.

Because Cauchy data on the 1-dimensional hyperplane in $\mathbb{R}^2$ are determined by a DAE, additional 0-dimensional Cauchy data may be required for specification of a unique solution. It is thus necessary to perform index analysis on this interior system (5.1)–(5.3) to determine what restrictions exist on 0-dimensional Cauchy data.

For clarity, let $a = u$, $b = v$, $c = \dot{u} = u_{x_2}$, and $d = \dot{v} = v_{x_2}$, so that the equations (5.1)–(5.3) become

$$\begin{aligned} a_{x_1} - b &= 0, \\ c_{x_1} - d &= 0, \\ c &= f_1(x_1), \\ b &= h_1(x_1). \end{aligned} \tag{5.4}$$

We now consider a 0-dimensional subsurface $(x_2 = 0, x_1 = k_1)$ on which added data are to be specified. Using the standard notation for DAEs, the system is

$$\begin{aligned} \dot{a} - b &= 0, \\ \dot{c} - d &= 0, \\ c &= f_1(x_1), \\ b &= h_1(x_1). \end{aligned} \tag{5.5}$$

Differentiation of the last three equations gives

$$\begin{aligned} \ddot{c} - \dot{d} &= 0, \\ \dot{c} &= \frac{d}{dx_1} f_1(x_1), \\ \dot{b} &= \frac{d}{dx_1} h_1(x_1). \end{aligned} \tag{5.6}$$

The second equation above may be differentiated again without producing any new variables, so also

$$\ddot{c} = \frac{d^2}{dx_1^2} f_1(x_1). \tag{5.7}$$

Two differentiations were required to derive these eight equations in the nine unknowns $\dot{a}$, a, $\dot{b}$, b, $\ddot{c}$, $\dot{c}$, c, $\dot{d}$, and d. The index of the DAE is two, and under the assumption that $h_1(x_1)$ is once differentiable and $f_1(x_1)$ is twice differentiable with respect to x_1, one dynamic degree of freedom on $(x_2 = 0, x_1 = k_1)$ is required to determine uniquely consistent Cauchy data on $(x_2 = 0)$.

The case is different if u rather than v is specified. Appending

$$u = h_2(x_1) \tag{5.8}$$

as the dynamic degree of freedom on $(x_2 = 0)$ to the system (5.1) produces a different DAE on the hyperplane. Using the same new variables a, b, c, and d, the data must now satisfy

$$\begin{aligned} \dot{a} - b &= 0, \\ \dot{c} - d &= 0, \\ c &= f_1(x_1), \\ a &= h_2(x_1). \end{aligned} \tag{5.9}$$

Differentiating the entire system yields

$$\begin{aligned} \ddot{a} - \dot{b} &= 0, \\ \ddot{c} - \dot{d} &= 0, \\ \dot{c} &= \frac{d}{dx_1} f_1(x_1), \\ \dot{a} &= \frac{d}{dx_1} h_2(x_1). \end{aligned} \tag{5.10}$$

Differentiating the last two equations again produces two new equations without introducing any new unknowns.

$$\begin{aligned} \ddot{c} &= \frac{d^2}{dx_1^2} f_1(x_1), \\ \ddot{a} &= \frac{d^2}{dx_1^2} h_2(x_1). \end{aligned} \tag{5.11}$$

Two differentiations were required to derive these 10 equations in the 10 unknowns $\ddot{a}$, $\dot{a}$, a, $\ddot{c}$, $\dot{c}$, c, $\dot{b}$, b, $\dot{d}$, and d. The index of the consistent Cauchy data problem that resulted from specifying u rather than v over the hyperplane $(x_2 = 0)$ is again two, but in this case $r = 0$ and no dynamic degrees of freedom on $(x_2 = 0, x_1 = k_1)$, or lower-dimensional data, are required to determine unique Cauchy data on $(x_2 = 0)$. Here both $f_1(x_1)$ and $h_2(x_1)$ must be twice differentiable with respect to x_1.

This result makes sense, when one considers the original system. If v is specified over $(x_2 = 0)$, the first equation in the original system (5.1) then determines u up to a constant of integration. The value of u at some point on $(x_2 = 0)$ fixes this constant of integration and fully specifies unique Cauchy data on that surface. If u is specified instead, the first equation gives v directly and no additional information is required.

Determination of consistent Cauchy data on $(x_2 = 0)$ thus requires specification of one dynamic degree of freedom on $(x_2 = 0)$. If v is specified, an additional dynamic degree of freedom on $(x_2 = 0, x_1 = k_1)$ is required to fully determine Cauchy data on $(x_2 = 0)$. If u is specified, no dynamic degrees of freedom are needed on lower dimensional hyperplanes.

Now, consider the equations that Cauchy data on the hyperplane $(x_1 = 0)$ must satisfy. Again using a dot to denote exterior derivatives, the system is

$$\begin{aligned} \dot{u} - v &= 0, \\ u_{x_2} &= f_1(x_1). \end{aligned} \tag{5.12}$$

Differentiating the second equation produces no new variables, but produces an independent equation:

$$\dot{u}_{x_2} = \frac{d}{dx_1} f_1(x_1). \tag{5.13}$$

Differentiating the first equation and the second one more time produces two new equations in two new variables, which include $\dot{v}$:

$$\begin{aligned} \ddot{u} - \dot{v} &= 0, \\ \ddot{u}_{x_2} &= \frac{d^2}{dx_1^2} f_1(x_1). \end{aligned} \tag{5.14}$$

Again under the assumption that all required derivatives exist, the index of the system with respect to x_1 is 2. There are five equations that relate the five unknowns $u, \dot{u}, \ddot{u}, v, \dot{v}$, so no dynamic degrees of freedom on $(x_1 = 0)$ may be specified arbitrarily.

The consistent Cauchy data problem is again not strictly algebraic, so lower dimensional data may be required to determine a unique solution. Let $a = u$, $b = v$, $c = \dot{u} = u_{x_1}$, $d = \ddot{u} = u_{x_1x_1}$, and $e = \dot{v} = v_{x_1}$, and consider the hyperplane $(x_1 = 0, x_2 = k_2)$. Using a dot to now denote differentiation in the x_2 direction, the system under consideration (5.12)–(5.14) is

$$\begin{aligned} c - b &= 0, \\ \dot{a} &= f_1(x_1), \\ d - e &= 0, \\ \dot{c} &= \frac{d}{dx_1} f_1(x_1), \\ \dot{d} &= \frac{d^2}{dx_1^2} f_1(x_1). \end{aligned} \tag{5.15}$$

Differentiating the algebraic equations produces two additional equations.

$$\begin{aligned} \dot{c} - \dot{b} &= 0, \\ \dot{d} - \dot{e} &= 0. \end{aligned} \tag{5.16}$$

Thus there are 7 equations in 10 unknowns, and 3 dynamic degrees of freedom on $(x_1 = 0, x_2 = k_2)$ are required. Five equations determine the values of $\dot{a}, \dot{b}, \dot{c}, \dot{d}$, and $\dot{e}$. Feasible specification is a, and either b or c, and either d or e.

However, note that specification of d or e is used to determine $u_{x_1x_1}$ and v_{x_1}, neither of which occurs in the original equations. Three dynamic degrees of freedom on $(x_1 = 0, x_2 = k_2)$ must be specified to determine unique Cauchy data for the system (5.12)–(5.14) derived during index analysis on $(x_1 = 0)$, but only two are required to determine unique Cauchy data for the original variables u, u_{x_1}, and v.

Unique Cauchy data on $(x_1 = 0)$ for the original variables requires specification of u and either u_{x_1} or v at a single point $(x_1 = 0, x_2 = k_2)$. This result again makes sense when one considers the original system. The second equation in (5.12) determines u up to a constant of integration over $(x_1 = 0)$. Equation (5.13) specifies u_{x_1} up to another constant of integration over $(x_1 = 0)$, and the first equation in (5.12) relates u_{x_1} and v on that same hyperplane. Specification of u fixes the first constant, and specification of either u_{x_1} or v fixes the second.

5.2. Pressure-swing adsorption. Consider a pressure-swing adsorption system that consists of an inert carrier gas and a single adsorbate. Under assumptions of isothermal operation, negligible axial dispersion and pressure drop, plug flow, and perfect gas behavior, the adsorbate concentration on the solid q, mole fractions of adsorbate and inert in the gas phase a and b, and flow velocity u are related by the following system of equations over time t and axial position in the absorber z [14]. A, B, C, D, E, and F are parameters.

$$\begin{aligned} Ea_t + Bq_t + (ua)_z + Aa &= 0, \\ Bq_t + u_z + A &= 0, \\ a + b &= 1, \\ q - \frac{Ca^F}{1 + Da^F} &= 0. \end{aligned} \tag{5.17}$$

Now, consider the equations that Cauchy data on the hyperplane $(t = 0)$ must satisfy. The exterior derivative is with respect to t, so using our previously established notation, the system may be written as

$$
\begin{aligned}
E\dot{a} + B\dot{q} + (ua)_z + Aa &= 0,\\
B\dot{q} + u_z + A &= 0,\\
a + b &= 1,\\
q + (Dq - C)\, a^F &= 0.
\end{aligned} \tag{5.18}
$$

Data on $(t = 0)$ must also satisfy

$$
\begin{aligned}
E\ddot{a} + B\ddot{q} + \dot{u}_z a + u_z\dot{a} + \dot{u}a_z + u\dot{a}_z + A\dot{a} &= 0,\\
B\ddot{q} + \dot{u}_z &= 0,\\
\dot{a} + \dot{b} &= 0,\\
\dot{q} + Da^F\dot{q} + (Dq - C)\, Fa^{F-1}\dot{a} &= 0.
\end{aligned} \tag{5.19}
$$

Differentiating the fourth equation in this system (5.19) with respect to t produces another independent equation without introducing any new variables, so the data must also satisfy

$$
\ddot{q} + 2FDa^{F-1}\dot{a}\dot{q} + Da^F\ddot{q} + (Dq - C)\left((F-1)\, Fa^{F-2}\dot{a}^2 + Fa^{F-1}\ddot{a}\right) = 0. \tag{5.20}
$$

Two differentiations were required to derive these 9 independent equations in the 10 dependent variables $q, \dot{q}, \ddot{q}, a, \dot{a}, \ddot{a}, b, \dot{b}, u, \dot{u}$. The index of this system with respect to t is thus 2. There is only one dynamic degree of freedom on $(t = 0)$.

One feasible specification of the dynamic degrees of freedom is q over $(t = 0)$. The detailed derivation is somewhat tedious and is therefore omitted, but if q is specified over $(t = 0)$, the resulting DAE is index 1 and has four dynamic degrees of freedom on $(t = 0, z = c_1)$. However, only one of these is required to determine the original variables; $q(0, z)$ together with either q_t, a_t, u_z, or u at a point $(t = 0, z = c_1)$ completely specifies unique Cauchy data for the original variables on the initial hyperplane.

5.3. The Navier–Stokes equations. Consider the two-dimensional, incompressible formulation of the Navier–Stokes equations:

$$
\begin{aligned}
u_t + uu_{x_1} + p_{x_1} + vu_{x_2} - \nu u_{x_1x_1} - \nu u_{x_2x_2} &= 0,\\
v_t + uv_{x_1} + vv_{x_2} + p_{x_2} - \nu v_{x_1x_1} - \nu v_{x_2x_2} &= 0,\\
u_{x_1} + v_{x_2} &= 0.
\end{aligned} \tag{5.21}
$$

Consider the initial hyperplane, orthogonal to t at $t = 0$. The exterior direction is along the t-axis; x_1 and x_2 are interior directions. The system may be rewritten as

$$
\begin{aligned}
\dot{u} + uu_{x_1} + p_{x_1} + vu_{x_2} - \nu u_{x_1x_1} - \nu u_{x_2x_2} &= 0,\\
\dot{v} + uv_{x_1} + vv_{x_2} + p_{x_2} - \nu v_{x_1x_1} - \nu v_{x_2x_2} &= 0,\\
u_{x_1} + v_{x_2} &= 0.
\end{aligned} \tag{5.22}
$$

Differentiating the third equation with respect to the exterior direction produces another independent equation:

$$
\dot{u}_{x_1} + \dot{v}_{x_2} = 0. \tag{5.23}
$$

The first two equations in the original system, and the differentiated continuity equation, may be differentiated again to produce three independent equations in three new variables (which include $\dot{p}$).

$$\begin{aligned} \ddot{u} + \dot{u}u_{x_1} + u\dot{u}_{x_1} + \dot{p}_{x_1} + \dot{v}u_{x_2} + v\dot{u}_{x_2} - \nu\left(\dot{u}_{x_1x_1} + \dot{u}_{x_2x_2}\right) &= 0, \\ \ddot{v} + \dot{u}v_{x_1} + u\dot{v}_{x_1} + \dot{p}_{x_2} + \dot{v}v_{x_2} + v\dot{v}_{x_2} - \nu\left(\dot{v}_{x_1x_1} + \dot{v}_{x_2x_2}\right) &= 0, \\ \ddot{u}_{x_1} + \ddot{v}_{x_2} &= 0. \end{aligned} \tag{5.24}$$

Two differentiations with respect to t were required to uniquely determine the exterior derivatives of all variables, so the index of the Navier–Stokes equations with respect to time is 2. On the initial hyperplane, there are seven independent equations (5.22)–(5.24) that relate the eight variables $\ddot{u}, \dot{u}, u, \ddot{v}, \dot{v}, v, \dot{p}, p$, so $r = 1$ and only one dynamic degree of freedom on $(t = 0)$ exists for the specification of Cauchy data.

Typical initial conditions for the Navier–Stokes equations include specification of both u and v as dynamic degrees of freedom on $t = 0$, often $u = v = 0$ [7]. It is easy to verify that the second specification is redundant, as indicated by the index analysis. Consider the original equations (5.22) and the implicit constraint (5.23), which involve only the original variables, together with algebraic specification of u on the initial hyperplane:

$$\begin{aligned} \dot{u} + uu_{x_1} + p_{x_1} + vu_{x_2} - \nu u_{x_1x_1} - \nu u_{x_2x_2} &= 0, \\ \dot{v} + uv_{x_1} + vv_{x_2} + p_{x_2} - \nu v_{x_1x_1} - \nu v_{x_2x_2} &= 0, \\ u_{x_1} + v_{x_2} &= 0, \\ \dot{u}_{x_1} + \dot{v}_{x_2} &= 0, \\ u &= 0. \end{aligned} \tag{5.25}$$

Consistent Cauchy data, which are values of u, $\dot{u}$, v, $\dot{v}$, and p over the entire domain at $t = 0$, are a solution to this 5×5 elliptic system. The solution is uniquely determined when boundary conditions for the elliptic system are specified.

Algebraic manipulation produces the following simplified system:

$$\begin{aligned} \dot{u} + p_{x_1} &= 0, \\ \dot{v} + p_{x_2} - \nu v_{x_1x_1} &= 0, \\ v_{x_2} &= 0, \\ p_{x_1x_1} + p_{x_2x_2} &= 0, \\ u &= 0. \end{aligned} \tag{5.26}$$

This system is not strictly algebraic, so as in the previous examples, lower-dimensionality degrees of freedom may be explored. Let $a = u$, $b = u_t$, $c = v$, $d = v_t$, $e = p$, and consider now the hyperplane $(t = 0, x_1 = c_1)$. The exterior direction is now x_1, so the system may be written as

$$b + \dot{e} = 0, \tag{5.27}$$

$$d + e_{x_2} - \nu\ddot{c} = 0, \tag{5.28}$$

$$c_{x_2} = 0, \tag{5.29}$$

$$\ddot{e} + e_{x_2x_2} = 0, \tag{5.30}$$

$$a = 0. \tag{5.31}$$

Proceeding with determination of the index of this system with respect to x_1, differentiation of all equations save the fourth produces four additional independent equations:

$$\dot{b} + \ddot{e} = 0, \tag{5.32}$$
$$\dot{d} + \dot{e}_{x_2} - \nu \dddot{c} = 0, \tag{5.33}$$
$$\dot{c}_{x_2} = 0, \tag{5.34}$$
$$\dot{a} = 0. \tag{5.35}$$

The third equation may be differentiated twice more without introducing any new variables, so consistent data on $(t = 0, x_1 = c_1)$ must also satisfy

$$\ddot{c}_{x_2} = 0 \tag{5.36}$$

and

$$\dddot{c}_{x_2} = 0. \tag{5.37}$$

Three differentiations were required to produce these 11 independent equations in the 13 variables $a, \dot{a}, b, \dot{b}, c, \dot{c}, \ddot{c}, \dddot{c}, d, \dot{d}, e, \dot{e}, \ddot{e}$, so the index with respect to x_1 of this system (not of the original Navier–Stokes equations) is three. Two dynamic degrees of freedom are required on $(t = 0, x_1 = c_1)$.

Block decomposition of the system shows that six equations (5.31), (5.35), (5.29), (5.34), (5.36), (5.37) may be solved for the six unknowns a, $\dot{a}$, c, $\dot{c}$, $\ddot{c}$, $\dddot{c}$; two equations (5.27), (5.33) relate b, $\dot{d}$, $\dot{e}$; and three equations (5.28), (5.30), (5.32) relate $\dot{b}$, d, e, $\ddot{e}$. One specification of either b, $\dot{d}$, or $\dot{e}$, and another of either $\dot{b}$, d, e, or $\ddot{e}$, are required to determine unique Cauchy data if all specifications are to be made on a single surface orthogonal to x_1 and t. None of the variables a, $\dot{a}$, c, $\dot{c}$, $\ddot{d}$, and $\ddot{c}$ may be specified independently on $(t = 0, x_1 = c_1)$.

The first set of two equations, plus a dynamic degree of freedom assignment from the first group of three variables, is used to determine $\dot{e}$. This corresponds to a Neumann condition on pressure for Laplace's equation in (5.26). The second group is used to determine e, which corresponds to a Dirichlet condition on pressure.

It is well known that specification of p (here e) and p_{x_1} (here $\dot{e}$) on the same line $(x_1 = c_1)$, together with Laplace's equation for p, produces an ill-posed problem [6]. Rather, either p or p_{x_1} are required on two separate hyperplanes orthogonal to the x_1-axis. Clearly, then, our index analysis provides only restrictions on allowable Cauchy data on a given surface, rather than complete information on proper boundary conditions for all problems.

Consider now the subsurface $(t = 0, x_2 = c_2)$. The exterior direction of interest is now x_2, so the system is

$$\begin{aligned} b + e_{x_1} &= 0, \\ d + \dot{e} - \nu c_{x_1 x_1} &= 0, \\ \dot{c} &= 0, \\ e_{x_1 x_1} + \ddot{e} &= 0, \\ a &= 0. \end{aligned} \tag{5.38}$$

The first, second, and last equations may be differentiated without producing any new variables, so we must also have

$$\begin{aligned} \dot{b} + \dot{e}_{x_1} &= 0, \\ \dot{d} + \ddot{e} - \nu \dot{c}_{x_1 x_1} &= 0, \\ \dot{a} &= 0 \end{aligned} \tag{5.39}$$

on $(t = 0, x_2 = c_2)$.

This is a system of eight equations in the eleven unknowns a, $\dot{a}$, b, $\dot{b}$, c, $\dot{c}$, d, $\dot{d}$, e, $\dot{e}$, $\ddot{e}$. Three equations give the values of a, $\dot{a}$, and c. Three equations relate the variables b, $\dot{d}$, e, $\ddot{e}$, and two equations relate $\dot{b}$, c, d, $\dot{e}$. Feasible specification is thus one variable from the second group and two from the third. Again, the first group corresponds to a Dirichlet condition on pressure. The second group includes a condition on v (here c) and a Neumann condition on pressure.

Index analysis rules out some specifications as infeasible and in general provides only an upper bound on the number of degrees of freedom available on a particular surface. Consider planes of the form $(t = 0, x_2 = c_i)$. If v is specified over one such plane, it cannot be specified on any others. The third equation in (5.26) fixes it on all other parallel planes. Physically, this is due to the incompressibility condition and specification of $u = 0$ over the initial hypersurface. Because the fluid is incompressible and flow in the x_1 direction (u) at $t = 0$ is zero, flow in the x_2 direction (v) must be constant along lines $x_1 =$ constant. Mathematically, this appears as the third equation in the simplified original system (5.26) that says that, at $t = 0$, v does not vary with x_2. So, while index analysis indicates that three dynamic degrees of freedom are available on two parallel hyperplanes $(t = 0, x_2 = c_i)$ and $(t = 0, x_2 = c_j)$, specification of v on one takes up that degree of freedom on both.

Index analysis of the incompressible Navier–Stokes equations demonstrates that only one dependent variable may be independently specified over $(t = 0)$. If that specification is $u = 0$, added information on 1-dimensional hyperplanes within $(t = 0)$ is required to determine unique, consistent Cauchy data on $(t = 0)$. On hyperplanes of the form $(t = 0, x_1 = c_1)$, the only allowable dynamic degrees of freedom are combinations of p and p_{x_1}, while on hyperplanes of the form $(t = 0, x_2 = c_2)$, the only allowable dynamic degrees of freedom are combinations of p, p_{x_2}, and v. Depending on how these degrees of freedom are specified, additional data on 0-dimensional hyperplanes may be required to complete determination of unique Cauchy data on $(t = 0)$. The example also demonstrates that, while index analysis can provide useful information about allowable boundary conditions for an elliptic Cauchy data problem, it does not provide all the information needed to form a well-posed problem.

6. Conclusion.

A generalization of the differentiation index of a DAE that applies to PDAEs is presented. This generalized index is calculated with respect to a direction in the independent variable space of the equations. The index with respect to an arbitrary direction may be calculated by transforming the independent variables to a new coordinate system. Classical PDEs, such as the Navier–Stokes equations, as well as more general PDAEs may have a high index with respect to one or more directions in the independent variable space.

This index analysis makes explicit all equations that must be satisfied by Cauchy data on a hyperplane orthogonal to the direction of interest. These equations may be simple algebraic equations, DAEs, or PDAEs. In either of the latter two cases, additional data or side conditions may be required on subsurfaces of the original hyperplane. This index analysis may be used to determine restrictions on this additional data.

The question that motivated this work, and thus the most obvious application of this analysis, is that of consistent initialization of PDAEs for dynamic simulation. In this case the PDAE is assumed to be well-posed as a time evolution problem; that is, no information is carried backward in time along characteristics to the initial hyperplane ($t = 0$). Marching solution techniques, whether built using the method of lines or the Rothe method, require data on the initial hyperplane. In general, such methods require data on the hyperplane $x_j = x_{j0}$, where x_j is the evolution variable.

The index with respect to time may also prove important for numerical solution using the method of lines, in the same way that the differentiation index of DAEs has proven valuable in construction of robust, automated integration methods that preserve all solution invariants [1, 8, 18]. It is possible that, by treating a PDAE as an abstract Cauchy problem in t and using the index of the PDAE with respect to t, some or all of these DAE algorithms may be applied in a straightforward manner to PDAEs.

Finally, there is the question of whether or not the index of a given method of lines discretization is equal to the index of the original PDAE with respect to the evolution variable. When the discretization scheme is taken as consisting of two parts, the approximation of interior partial differential operators by relationships between parameters (values at nodes, coefficients in a series, etc.) and the enforcement of boundary conditions through those parameters, there are several examples where different implementations of the same boundary conditions produce DAEs of differing indexes. At present, the authors have been unable to find an example of an interior partial differential operator approximation that alters the index according to the definition presented in this paper. An a priori determination of whether a particular method of lines discretization scheme preserves the index of a PDAE is beyond the scope of this paper and will be addressed separately [17].

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