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REMARKS ON THE DIFFERENTIAL ALGEBRAIC APPROACH TO PARTICLE BEAM OPTICS BY M. BERZ*

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ABSTRACT

The underlying mathematical structure of the differential algebraic approach of M. Berz to particle beam optics is isomorphic to the familiar truncated polynomial algebra. Concrete examples of derivations in this algebra, consistent with the truncation operation, are given.

1 INTRODUCTION

The differential equations of beam optics

$$\begin{aligned} z' &= F(z, \delta), \\ z(s_i) &= z_i \quad (\delta - \text{parameters}), \end{aligned} \tag{1.1}$$

can be solved iteratively to any order in z_i [2-9]. The solution can be stated as a mapping $\mathcal{M}$ between the initial variables z_i and the final ones $z_f = z(s_f)$,

$$z_f = \mathcal{M}(z_i, \delta). \tag{1.2}$$

The derivatives

$$\frac{\partial^k \mathcal{M}}{\partial z_i^k}, \quad k = 1, 2, \ldots, n, \tag{1.3}$$

and

$$\frac{\partial \mathcal{M}}{\partial \delta} \tag{1.4}$$

are of interest as they yield the transfer matrix if $k = 1$, the aberrations if $k > 1$, and the sensitivities of a system to the external parameters δ. They can be quickly computed, without recourse to the definition of a derivative as a (computer inconvenient) limit,

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}. \tag{1.5}$$

To find all the derivatives, through the nth order, one evaluates the function $f(x)$ in an algebra $D(n, 1)$ (described in Section 2) which yields [1,5]

$$f(xe + d) = \left[f(x), f'(x), \ldots, f^{(n)}(x)\right], \tag{1.6}$$

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where

$$e = (\underset{\text{0th place}}{1}, 0, \ldots, 0) - \text{ unit element,} \tag{1.7}$$

and

$$d = (0, \underset{\text{1st place}}{1}, 0, \ldots, 0) - \text{differential in } D(n,1). \tag{1.8}$$

In case of a function of several independent variables $x_1, \ldots, x_\nu$ the formula (1.6) generalizes as follows

$$f(x_1 e + d_1, \ldots, x_\nu e + d_\nu) = (f, \nabla f, \ldots, \nabla^n f)(x_1, \ldots, x_\nu), \tag{1.9}$$

where

$$\nabla = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_\nu}\right), \tag{1.10}$$

and where the unit element e and the differentials d_k are

$$e = (\underset{\text{0th place}}{1}, 0, \ldots, 0), \tag{1.11}$$

$$d_1 = (0, \underset{\text{1st place}}{1}, 0, \ldots, 0), \tag{1.12}$$

$$\ldots\ldots\ldots\ldots$$

$$d_\nu = (0, 0, \ldots, 0, \underset{\nu\text{th place}}{1}, 0, \ldots, 0). \tag{1.13}$$

The dimensionality of the above elements is [1]

$$\dim(e) = \dim(d_k) = N(n,\nu) = \frac{(n+\nu)!}{n!\nu!}, \quad k = 1, \ldots, \nu. \tag{1.14}$$

The array (1.6), (1.9) can be easily implemented on a computer and evaluated in parallel. The task of computing derivatives is reduced to (computer convenient) arithmetic operations on the N-tupoles of real numbers which are described in Section 2. It turns out that the algebra $D(n,1)$ is a commutative algebra [9]. It is also a differential algebra [10] because it does admit derivations. This means that it is possible to find some linear operations ∂ acting on the N-tupoles, and obeying the Leibnitz rule

$$\partial(A \cdot B) = (\partial A) \cdot B + A \cdot \partial B. \tag{1.15}$$

Essentially this kind of approach to particle optics was proposed by Berz [1]. His formulation culminated in the computer code package – COSY INFINITY – which can handle aberrations of any order seemingly in any optical system [5]. The simplest, in our opinion, formulation of the basic assumptions and rules of this approach is based on the familiar truncated polynomial algebra [7,9].

The case of a real function $f(x)$ of a single real variable, and how to find its derivatives effectively through the nth order by evaluating it in the algebra

$D(n,1)$ will be shown. Examples of the derivations in this algebra will be constructed. More detailed treatment, also containing concrete examples of functions, can be found in [12].

After the Berz works it became clear that the differential algebraic techniques are useful and overcome the well known restrictions on computations of higher-order aberrations inherent in the TRANSPORT [13] or MAD codes [14]. In that respect the COSY INFINITY supersedes earlier codes like TRIO [15], GIOS-BEAMTRACE [16], COSY 5.0 [17] and HAMILTON [18]. It competes successfully with the more established MARYLIE 3.0 code [19], which becomes exceedingly complicated in higher orders.

2 THE TRUNCATED POLYNOMIAL ALGEBRA $D(n,1)$

Let us consider the set $D(R)$ of infinitely differentiable functions of a single, real variable $x \in R$. Taylor expansion of a function $a(x)$ from this set, through the order n,

$$a(x) = a_0 + a_1 \frac{x}{1!} + \cdots + a_n \frac{x^n}{n!} + o(x^n), \tag{2.1}$$

is fully characterized by the array A of real $n+1$ numbers

$$A = \{a_0, a_1, \ldots, a_n\} \in D(n,1). \tag{2.2}$$

Conversely, given A, one recovers an equivalence class $A = [a]$, of functions which can differ in the terms beyond the nth-order. These terms form an ideal $I_n(R)$ in $D(R)$ in the sense that:

1. a linear combination of terms $o(x^n)$ is again of order $o(x^n)$, viz.,

$$o(x^n) + o(x^n) = o(x^n), \tag{2.3}$$

2. the product of any function $a(x) \in D(R)$, with an element from $I_n(R)$, belongs to the ideal, viz.,

$$a(x)\, o(x^n) = o(x^n). \tag{2.4}$$

These properties are essential for mathematical correctness of the algebraic operations on the equivalence classes. Results of an addition and a multiplication do not depend on the particular choices of representatives of these equivalence classes when they are satisfied.

Any operation which is defined on the functions $a \in D(R)$ induces the corresponding operation on the coefficients $a_0, a_1, \ldots, a_n$ if the division onto the polynomial and the terms of higher orders is respected. One may tolerate some "spill" from the polynomial part into the ideal $I_n(R)$, but the reverse should be prevented. For instance, when multiplying $a(x)$ with x one loses the terms $a_n\,(x^{n+1}/n!)$ which goes now to the ideal. Differentiation, however, is dangerous in the sense that it brings unspecified term $a_{n+1}\,(x^n/n!)$ from the ideal into the "clean" polynomial area. Note that the operation $x\,(d/dx)$ preserves the ideal and nothing spills back to the polynomial part. The same is true for the operations $x^{\alpha}\,(d/dx)$, $\alpha = 1, 2, \ldots, n$. Higher α's render trivial operations destroying the polynomial part entirely.

One may write the function $a\,(x)$ as a scalar product, up to the higher-order terms

$$a\,(x) = (A, X) + o\,(x^n)\,, \tag{2.5}$$

where the vector X is composed of the basic monomials, normalized by the factorials

$$X = \left(1, \frac{x}{1!}, \cdots, \frac{x^n}{n!}\right). \tag{2.6}$$

A truncation operation T_n is introducted which preserves all the terms through the nth order:

$$T_n\,\{a\,(x)\} = (A, X)\,, \tag{2.7}$$

and

$$T_n\,\{I_n\,(R)\} = 0. \tag{2.8}$$

Hence, after the truncation, one is dealing with the nth-order polynomials. Note that the algebraic operations in $D\,(R)$ induce the corresponding operations in $D\,(n, 1)$:

1. Scalar multiplication

$$\lambda a\,(x) = \sum_{k=0}^{n} \lambda a_k \frac{x^k}{k!} + o\,(x^n)\,, \tag{2.9}$$

2. Addition

$$a\,(x) + b\,(x) = \sum_{k=0}^{n} (a_k + b_k)\,\frac{x^k}{k!} + o\,(x^n)\,, \tag{2.10}$$

3. Multiplication

$$\begin{aligned} a\,(x) \cdot b\,(x) &= [(A, X) + o\,(x^n)]\,[(B, X) + o\,(x^n)] \\ &= (A, X)\,(B, X) + o\,(x^n) \equiv (A \cdot B, X) + o\,(x^n) \\ &= c\,(x) = (C, X) + o\,(x^n) \end{aligned} \tag{2.11}$$

where

$$(C, X) = T_n\,\{(A, X)\,(B, X)\}\,. \tag{2.12}$$

The following arithmetic rules for $D\,(n, 1)$ are obtained:

1. Scalar multiplication

$$\lambda\,(a_0, a_1, \ldots, a_n) = (\lambda a_0, \lambda a_1, \ldots, \lambda a_n)\,, \tag{2.13}$$

2. Addition

$$(a_0, a_1, \ldots, a_n) + (b_0, b_1, \ldots, b_n) = (a_0 + b_0, a_1 + b_1, \ldots, a_n + b_n) \ , \qquad (2.14)$$

3. Multiplication

$$(a_0, a_1, \ldots, a_n)(b_0, b_1, \ldots, b_n) = (c_0, c_1, \ldots, c_n) , \qquad (2.15)$$

$$c_k = k! \sum_{\substack{0 \le i,j \le n \\ (i+j=k)}} \frac{a_i b_j}{i!j!}, k = 0, 1, \ldots, n. \qquad (2.16)$$

The multiplication is commutative, and is distributive across the addition:

$$A \cdot B = B \cdot A, \qquad (2.17)$$

$$A \cdot (B + C) = A \cdot B + A \cdot C. \qquad (2.18)$$

Hence, the set $D(n, 1)$ is a commutative algebra [10] which is the quotient algebra

$$D(n, 1) \sim D(R) / I_n(R) . \qquad (2.19)$$

It is also a differential algebra since it does admit derivations [11]. For example, the derivations on the algebra $D(R)$ of differentiable functions given by

$$\mathcal{D}_\alpha = x^\alpha \frac{d}{dx}, \quad \alpha = 1, 2, \ldots, n, \qquad (2.20)$$

generate the corresponding derivations ∂_α on the algebra $D(n, 1)$ as follows:

$$(\partial_\alpha A, X) = T_n \{(A, \mathcal{D}_\alpha X)\} , \qquad (2.21)$$

where $\mathcal{D}_\alpha$ acts on every component of the vector X.

To understand this, note first that the derivations $\mathcal{D}_\alpha$ satisfy the condition

$$\mathcal{D}_\alpha I_n(R) \subset I_n(R), \text{ or } T_n \{\mathcal{D}_\alpha I_n(R)\} = 0, \quad \alpha = 1, 2, \ldots, n. \qquad (2.22)$$

Since the derivations $\mathcal{D}_\alpha$ obey the Leibnitz rule, one has the equality

$$\mathcal{D}_\alpha (ab) = (\mathcal{D}_\alpha a) b + a \mathcal{D}_\alpha b \qquad (2.23)$$

where, due to the condition (2.22), one has

$$\begin{aligned} \mathcal{D}_\alpha a(x) &= (A, \mathcal{D}_\alpha X) + o(x^n) \\ &\equiv (\partial_\alpha A, X) + o(x^n) . \end{aligned} \qquad (2.24)$$

Applying the truncation operation T_n to both sides of the equality (2.23) and using the formulae (2.11) and (2.23), one gets, for any X, the equality

$$[\partial_\alpha (A \cdot B), X] = [(\partial_\alpha A) \cdot B, X] + (A \cdot \partial_\alpha B, X) . \qquad (2.25)$$

According to the main theorem of algebra, it is possible only when coefficients on both sides of this equation agree [10]. This implies that the Liebnitz rule is satisfied by ∂_α

$$\partial_\alpha (A \cdot B) = (\partial_\alpha A) \cdot B + A \cdot \partial_\alpha B, \quad \alpha = 1, 2, \ldots, n. \tag{2.26}$$

Hence, ∂_α are derivations in the algebra $D(n, 1)$.

Using the definition (2.21) and the explicit form (2.20) of the derivations $\mathcal{D}_\alpha$, one finds components of $\partial_\alpha A$

$$(\partial_\alpha A)_k = \begin{cases} k!/(k-\alpha)!\, a_{k-\alpha+1} & k \geq \alpha \\ 0 & k < \alpha \end{cases} \qquad k = 0, 1, \ldots, n. \tag{2.27}$$

It is clear that for $\alpha \geq n+1$ the derivations ∂_α trivialize to zero. More derivations on the algebra $D(n, 1)$ are obtained by taking linear combinations of ∂_α

$$\partial = \sum_{\alpha=1}^{n} \lambda_\alpha \partial_\alpha, \tag{2.28}$$

where λ_α are arbitrary real numbers.

Finally let us note that the usual derivative d/dx violates the condition (2.22), and thus does not generate a derivation on the algebra $D(n, 1)$; cf. [2], formulae (5), (6).

Some elements of the algebra $D(n, 1)$ are special. Apart from the zero and unit elements

$$\begin{aligned} 0 &= (0, 0, \ldots, 0), \\ e &= (1, 0, \ldots, 0), \end{aligned} \tag{2.29}$$

the differential elements are considered:

$$\begin{aligned} d_1 &= (0, 1, 0, \ldots, 0) \equiv d, && \text{1st differential}, \\ d_n &= (0, 0, \ldots, 0, 1), && n\text{th differential}. \end{aligned} \tag{2.30}$$

It follows from the multiplication rule, (2.15), that

$$d^k = k!\, d_k, \quad k = 1, 2, \ldots, n, \tag{2.31}$$

$$d^{n+1} = 0, \quad \text{nilpotency property}. \tag{2.32}$$

Any element $A \in D(n, 1)$ can then be decomposed as a linear combination of the unit element and the differentials:

$$\begin{aligned} A &= (a_0, a_1, \ldots, a_n) = (a_0, 0, \ldots, 0) + (0, a_1, 0, \ldots, 0) + \\ &\quad \cdots + (0, 0, \ldots, 0, a_n) = a_0 e + a_1 d_1 + \cdots + a_n d_n \\ &= a_0 e + a_1 \frac{d}{1!} + \cdots + a_n \frac{d^n}{n!} = a(d). \end{aligned} \tag{2.33}$$

The differentials can be consistently ordered as follows [1,2]:

$$\lambda_0 e > \lambda_1 d_1 > \cdots > \lambda_n d_n > 0, \tag{2.34}$$

for any positive numbers $\lambda_0, \lambda_1, \ldots, \lambda_n$. The first components, when not equal, decide which of the two elements is larger. Only when they coincide do we compare the second components, etc. The element λe can be viewed as an extension of the real number λ to the algebra $D(n,1)$.

One may also extend a function $f(x) \in D(R)$ to the algebra, as well. One replaces any constant c, appearing in f, by its extension ce, and the argument x is replaced by the element $xe + d \in D(n,1)$. Its formal Taylor expansion terminates because of the nilpotency of the differential and it yields [cf. (1.6)]

$$\begin{aligned} f(xe+d) &= f(xe) + f'(xe)\frac{d}{1!} + \cdots + f^{(n)}(xe)\frac{d^n}{n!} \\ &= f(x)e + f'(x)d_1 + \cdots + f^{(n)}(x)d_n \\ &= \left(f, f', \ldots, f^{(n)}\right)(x). \end{aligned} \tag{2.35}$$

The above extension is obviously very useful as it yields all the derivatives through the (computer convenient) arithmetic operations on $D(n,1)$. More general extensions are also possible by using higher order differentials.

Examples:

1. $$\exp(A) = \exp(a_0, a_1, \ldots, a_n) = \exp\left[(a_0, 0, \ldots, 0) + \underbrace{(0, a_1, \ldots, a_n)}_{b}\right]$$

$$= \exp(a_0 e)\exp(b) = \exp(a_0)\sum_{k=0}^{n}\frac{b^k}{k!}. \tag{2.36}$$

2. $$\begin{aligned} A^{-1} &= (a_0, a_1, \ldots, a_n)^{-1} = \frac{1}{a_0 e + b} \\ &= \frac{1}{a_0}e\left[1 - \frac{b}{a_0} + \left(\frac{b}{a_0}\right)^2 - \cdots + (-1)^{n+1}\left(\frac{b}{a_0}\right)^n\right], \quad a_0 \neq 0. \end{aligned} \tag{2.37}$$

3. $$\begin{aligned} \sqrt{A} &= \sqrt{a_0 e + b} = \sqrt{a_0}e\sqrt{1 + \frac{b}{a_0}} \\ &= \sqrt{a_0}e\left[1 + \sum_{k=1}^{n}(-1)^{k-1}\frac{1\cdot 3\cdots(2k-1)}{2^k k!}\left(\frac{b}{a_0}\right)^k\right], \quad a_0 > 0. \end{aligned} \tag{2.38}$$

In all these cases finite amounts of the algebraic operations are needed in order to compute the extended functions.

The whole scheme generalizes to any number of independent variables, at some expense of notational inconvenience, and yields the formula (1.9) [2,6,12].

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