Consistency of Finite Difference Approximations for Linear PDE Systems and its Algorithmic Verification

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Abstract

In this paper we consider finite difference approximations for numerical solving of systems of partial differential equations of the form $f_1 = \cdots = f_p = 0$, where $F := \{f_1, \ldots, f_p\}$ is a set of linear partial differential polynomials over the field of rational functions with rational coefficients. For orthogonal and uniform solution grids we strengthen the generally accepted concept of equation-wise consistency (e-consistency) of the difference equations $\tilde{f}_1 = \cdots = \tilde{f}_p = 0$ as approximation of the differential ones. Instead, we introduce a notion of consistency of the set of all linear consequences of the difference polynomial set $\tilde{F} := \{\tilde{f}, \ldots, \tilde{f}_p\}$ with the linear subset of the differential ideal $\langle F \rangle$. The last consistency, which we call s-consistency (strong consistency), admits algorithmic verification via a Gröbner basis of the difference ideal $\langle \tilde{F} \rangle$. Some related illustrative examples of finite difference approximations, including those which are e-consistent and s-inconsistent, are given.

1 Introduction

Since, apart from very special cases, partial differential equations (PDEs) can only be solved numerically, the construction of their numerical solutions is a fundamental task in science and engineering. Among three classical numerical methods that are widely used for numerical solving of PDEs the finite difference method[1] is the oldest one and is based upon the application of a local Taylor expansion to approximate the differential equations by difference ones [1, 2] defined on the chosen computational grid. The difference equations that approximate differential equations in the system of PDEs form its finite difference approximation (FDA) which together with discrete approximation of initial or/and boundary conditions is called finite-difference scheme (FDS).

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[1]The other two methods are the finite element method and the finite volume method.

A good FDA has to mimic or inherit the algebraic structure of a differential system. In particular it has to reproduce such fundamental properties of the continuous equations as symmetries and conservation laws [3, 4]. Provided with appropriate initial or/and boundary conditions in their discrete form, the main requirement to the FDS is its *convergence*. The last means that the numerical solution approaches to the true solution to the PDE system as the grid spacings go to zero. Further important properties of FDS are *consistency* and *stability*. The former means that the difference equations in FDA are reduced to the original PDEs when the grid spacings vanish,[2] whereas the latter means that the error in the solution remains bounded under small perturbation in the numerical data. Consistency is necessary for convergence. In accordance to the Lax-Richtmyer equivalence theorem [1, 2] proved first for (scalar) linear PDEs and extended to some nonlinear equations [5], a consistent FDA to a PDE with the well-posed initial value (Cauchy) problem converges if and only if it is stable. Thus, the consistency check is an important step in analysis of difference schemes.

In this paper for a FDA to a linear PDE system on uniform and orthogonal grids we suggest another concept of consistency called strong consistency (s-consistency) which means consistency of the set of all linear difference consequences of the FDA with the set of linear differential consequences of the PDE system. This concept improves the concept of equation-wise consistency (e-consistency) of a FDA with a PDE system and also admits an algorithmic check. This check is done via construction of a Gröbner basis for the difference ideal generated by the FDA to linear differential polynomials in the PDE system. We show that every s-consistent FDA is e-consistent and the converse is not true. It means that an s-consistent FDA reproduces at the discrete level more algebraic properties of the PDE system than one which is e-consistent and s-inconsistent. For the algorithmic check of s-consistency we use the involutive algorithm [6, 7] which apart from the construction of a Gröbner basis allows also to verify easily well-posedness of the initial value problem for an analytic system of PDEs [8, 9] as a prerequisite of convergence for its FDS.

The structure of the paper is as follows. In Sect. 2 we shortly describe the mathematical objects with which we deal in the paper. In Sect. 3 for the uniform and orthogonal grids with equally spaced nodes we define s-consistency of a FDA to a system of PDEs and relate it with the underlying consistency properties of a difference Gröbner basis of the ideal generated by the polynomials in the FDA. The algorithmic verification of s-consistency is presented in Sect. 4. Then we illustrate the concepts and methods of the paper by some examples (Sect. 5). In Sect. 6 we consider peculiarities of consistency for the grids with different spacings and conclude in Sect. 7.

[2]In Section 3 we give a more precise definition of consistency.

2 Preliminaries

Let $\mathbf{x} := \{x_1, \ldots, x_n\}$ be the set of n real (independent) variables and $\mathbb{K} := \mathbb{Q}(\mathbf{x})$ be the field of rational functions with rational coefficients. $\mathbb{K}$ is both a differential and a difference field [10], respectively, for the set $\{\partial_1, \ldots, \partial_n\}$ of derivation operators and the set $\{\sigma_1, \ldots, \sigma_n\}$ of the differences acting on the functions $\phi \in \mathbb{K}$ as the right-shift operators $\sigma_i \circ \phi(x_1, \ldots, x_n) = \phi(x_1, \ldots, x_i + h_i, \ldots, x_n)$. Here the shift parameters h_i can take positive real values.

We shall use the same notation $\mathbb{K}[u^{(1)}, \ldots, u^{(m)}]$ for both differential and difference polynomial rings over $\mathbb{K}$ and denote them by $\mathcal{R}$ resp. $\tilde{\mathcal{R}}$. The differential (resp. difference) indeterminates $u^{(1)}, \ldots, u^{(m)}$ will be considered for differential (resp. difference) equations as dependent variables, and sometimes we shall use also the vector notation $\mathbf{u} := (u^{(1)}, \ldots, u^{(m)})$. The subset of the differential ring $\mathcal{R}$ containing linear polynomials will be denoted by $\mathcal{R}_L$, and the linear subset of the difference ring by $\tilde{\mathcal{R}}_L$.

Hereafter we consider PDE systems of the form

$$f_1 = \cdots = f_p = 0, \quad F := \{f_1, \ldots, f_p\} \subset \mathcal{R}_L\,. \tag{1}$$

To approximate the differential system (1) by a difference one we shall use an orthogonal and uniform computational grid (mesh) as the set of points $(k_1 h_1, \ldots, k_n h_n)$ in $\mathbb{R}^n$. Here $\mathbf{h} := (h_1, \ldots, h_n)$ $(h_i > 0)$ is the tuple of mesh steps (grid spacings) and the integer-valued vector $\mathbf{k} := (k_1, \ldots, k_n) \in \mathbb{Z}^n$ numerates the grid points. If the actual solution to the problem (1) is given by $\mathbf{u}(\mathbf{x})$ then its approximation in the grid node will be given by the grid (vector) function $\mathbf{u}_{k_1,\ldots,k_n} = \mathbf{u}(k_1 h_1, \ldots, k_n h_n)$.

In the finite difference method derivatives in (1) are approximated by finite differences. This can be done in many ways. For example, the first-order derivative can be approximated by the forward difference

$$\partial_{x_j} u^{(i)} = \Delta_j(u^{(i)}) + O(h_j),$$

where

$$\Delta_j(u^{(i)}) := \frac{u^{(i)}_{k_1,\ldots,k_j+1,\ldots,k_n} - u^{(i)}_{k_1,\ldots,k_j,\ldots,k_n}}{h_j} \tag{2}$$

or by the centered difference

$$\partial_{x_j} u^{(i)} = \frac{u^{(i)}_{k_1,\ldots,k_j+1,\ldots,k_n} - u^{(i)}_{k_1,\ldots,k_j-1,\ldots,k_n}}{2h_j} + O(h_j^2)\,. \tag{3}$$

By substituting finite differences for derivatives into system (1) and applying appropriate right-shift operators from the monoid generated by $\{\sigma_1, \ldots, \sigma_n\}$ to remove negative shifts in indices which may come out of expressions like (3) we obtain a FDA to (1) of the form

$$\tilde{f}_1 = \cdots = \tilde{f}_p = 0, \quad \tilde{F} := \{\tilde{f}_1, \ldots, \tilde{f}_p\} \subset \tilde{\mathcal{R}}_L\,. \tag{4}$$

In [11] another approach to generation of FDA was suggested. It is based on the finite volume method and on difference elimination. That approach is algorithmic and for nonlinear equations it can construct FDAs that cannot be obtained by the straightforward substitution of finite differences for derivatives into the differential equations. An example of such approximation was constructed in [11] for the Falkovich-Karman differential equation describing transonic flow in gas dynamics. Whereas the underlying differential equation is quadratically nonlinear, the obtained difference approximation is cubically nonlinear. Due to this fact the corresponding FDS reveals better numerical behavior than known quadratically nonlinear schemes.

3 Consistency

Here and in the next two sections we consider orthogonal and uniform grids with equisized mesh steps $h_1 = \cdots = h_n = h$. First, we give the generally accepted definition [1, 2] of consistency of a single differential equation with its difference approximation.

Definition 1. *Given a PDE $f = 0$ and a FDA $\tilde{f} = 0$, the FDA is said to be* consistent *with the PDE if for any smooth, i.e. sufficiently differentiable for the context, vector-function $\mathbf{u}(\mathbf{x})$*

$$f(\mathbf{u}) - \tilde{f}(\mathbf{u}) \to 0 \quad \text{as} \quad h \to 0,$$

the convergence being pointwise at each point $\mathbf{x}$.

Definition 1 allows to verify easily the consistency of $\tilde{f}$ with f by using the Taylor expansion of $\tilde{f}$ about a grid point which is non-singular for its coefficients. As a simple example consider the advection (or one-way wave) equation

$$f(u) = 0, \quad f(u) := u_x + \nu u_y \quad (\nu = \text{const}), \tag{5}$$

which is the simplest hyperbolic PDE. Its discretization by using the forward differences (2) for the derivatives gives

$$\tilde{f}(u) := \frac{u_{i+1,j} - u_{i,j}}{h} + \nu \frac{u_{i,j+1} - u_{i,j}}{h}\,. \tag{6}$$

The Taylor expansion about the grid point $(x = ih, y = jh)$ yields

$$\begin{aligned} u_{i+1,j} &= u_{i,j} + hu_x + \tfrac{h^2}{2} u_{xx} + O(h^3)\,, \\ u_{i,j+1} &= u_{i,j} + hu_y + \tfrac{h^2}{2} u_{yy} + O(h^3)\,, \end{aligned}$$

and thus

$$f(u) - \tilde{f}(u) = -\frac{h}{2}\,(u_{xx} + \nu u_{yy}) + O(h^2) \xrightarrow[h \to 0]{} 0\,.$$

This shows the consistency of (6) with (5).

If one considers a system of PDEs and performs its equation-wise discretization, as it is usually done in practice, then a natural generalization of Definition 1 to systems of equations is as follows.

Definition 2. *Given a PDE system (1) and its difference approximation (4), we shall say that (4) is* equation-wise consistent *or* e-consistent *with (1) if every difference equation in (4) is consistent with the corresponding differential equation in (1).*

In fact, in the literature only e-consistency of FDA to systems of PDEs is considered. However e-consistency may not be satisfactory in view of inheritance of properties of the differential systems at the discrete level.

We are now going to introduce another concept of consistency for difference approximations to PDE systems which strengthens Definition 2 and provides consistency of the (infinite) subset of $\tilde{\mathcal{R}}_L$ of all linear difference consequences of the discrete system (4) with the subset of $\mathcal{R}_L$ of all linear differential consequences of the PDE system (1).

To formulate the new concept we need the following definition.

Definition 3. *We shall say that a* difference equation $\tilde{f}(\mathbf{u}) = 0$ implies the differential equation $f(\mathbf{u}) = 0$ *and write* $\tilde{f} \rhd f$ *when the Taylor expansion about a grid point yields*

$$\tilde{f}(\mathbf{u}) \xrightarrow[h\to 0]{} f(\mathbf{u})h^k + O(h^{k+1}),\ \ k \in \mathbb{Z}_{\geq 0}\,. \tag{7}$$

It is clear that in this terminology, Definition 1 means $\tilde{f} \rhd f$. Now we give our main definition.

Definition 4. *Given a PDE system (1) and its difference approximation (4), we shall say that (4) is* strongly consistent *or* s-consistent *with (1) if*

$$\forall \tilde{f} \in \langle \tilde{F} \rangle \cap \tilde{\mathcal{R}}_L \ \exists f \in \langle F \rangle \cap \mathcal{R}_L \ \ : \ \ \tilde{f} \rhd f\,. \tag{8}$$

Comparing Definitions 2 and 4 one sees that s-consistency implies e-consistency. The converse is not true as shown by explicit examples in Sect. 5.

The s-consistency admits an algorithmic verification which is based on the following statement.

Theorem 1. *A difference approximation (4) to a differential system (1) is s-consistent if and only if any reduced Gröbner basis* $\tilde{G} \subset \tilde{\mathcal{R}}_L$ *of the difference ideal* $\langle \tilde{F} \rangle$ *satisfies*

$$\forall \tilde{g} \in \tilde{G} \ \exists g \in \langle F \rangle \cap \mathcal{R}_L \ \ : \ \ \tilde{g} \rhd g\,. \tag{9}$$

Proof. Let $\succ$ be a difference ranking [10] and $\tilde{G}$ be a reduced difference Gröbner basis [10, 12] of $\langle \tilde{F} \rangle$ for this ranking satisfying the condition (9). Denote by G the set of differential polynomials that are implied by the elements in $\tilde{G}$. Consider a linear difference polynomial $\tilde{f} \in \langle \tilde{F} \rangle \cap \tilde{\mathcal{R}}_L$ and its standard representation (cf. [13]) w.r.t. $\tilde{G}$ and $\succ$ as a finite sum of the form

$$\begin{cases} \tilde{f} = \sum_{\tilde{g}\in\tilde{G}} \sum_{\mu} a_\mu \sigma^\mu \circ \tilde{g}, \quad a_\mu \in \mathbb{K}\,, \\ \forall \tilde{g},\, \mu \ : \ \sigma^\mu \circ \mathrm{ld}(\tilde{g}) \preceq \mathrm{ld}(\tilde{f})\,. \end{cases} \tag{10}$$

Here $\mathrm{ld}(q)$ denotes the *leader* [10] of a difference polynomial q, and we use the multiindex notation

$$\mu := (\mu_1, \ldots, \mu_n) \in \mathbb{Z}^n_{\geq 0},\ \ \sigma^\mu := \sigma_1^{\mu_1} \circ \cdots \circ \sigma_n^{\mu_n}\,.$$

Choose now a grid point, nonsingular for the sum in (10), and consider its Taylor expansion (in grid spacing h) about this point. The shift operators σ_j $(j = 1, \ldots, n)$ which occur in σ^μ and in $\tilde{g} \in \tilde{G}$ are expanded in the Taylor series

$$\sigma_j = \sum_{k \geq 0} h^k \partial_j^k \tag{11}$$

along with the shifted rational functions in the independent variables.

The representation (10) guarantees that the highest ranking partial derivatives which occur in the leading order in h and come from different elements of the Gröbner basis cannot cancel. Thereby, due to the condition (9), in the leading order in h, the Taylor expansion of $\tilde{f}$ will contain a finite sum of the form

$$f := \sum_{g \in G} \sum_{\mu} b_\mu \partial^\mu \circ g, \quad b_\mu \in \mathbb{K}\,, \tag{12}$$

and hence $\tilde{f} \rhd f \in \langle F \rangle \cap \mathcal{R}_L$.

Since $\tilde{G} \subset \langle \tilde{F} \rangle \cap \tilde{\mathcal{R}}_L$, the converse is trivially true. □

Corollary 1. *Let a FDA $\tilde{F} \subset \tilde{\mathcal{R}}_L$ be s-consistent with a set $F \subset \mathcal{R}_L$, then*

$$\forall \tilde{p} \in \langle \tilde{F} \rangle\ \exists p \in \langle F \rangle\ \ :\ \ \tilde{p} \rhd p\,. \tag{13}$$

Proof. Consider a difference polynomial $\tilde{q} \in \tilde{\mathcal{R}}$ as a grid function. If one applies the Taylor expansion (11) of the shift operators about a grid point, then in the limit $h \to 0$ this polynomial takes the form

$$\tilde{q} = h^k q + O(h^{k+1}), \quad k \in \mathbb{Z}_{\geq 0},$$

where $q \in \mathcal{R}$ is a differential polynomial.

If now we multiply both sides of the representation (10) by a polynomial $\tilde{q}$, apply a finite number of the shift operators σ_i to the product and apply the Taylor expansion about a grid point to the result, then in the leading order in h we obtain the differential polynomial which results from the linear differential polynomial of the form (12) by its multiplication by q and applying finitely many derivations ∂_j.

Clearly, before doing the Taylor expansion one can also multiply the r.h.s. in (10) and apply the shift operations to the product several times. Afterwards, the leading (in h) order of the expansion will yield the differential polynomial generated by elements in the differential polynomial set G that is implied by the Gröbner basis of $\langle \tilde{F} \rangle$. □

If one uses a minimal difference involutive basis [7, 9], then the representation (10) is unique with operators σ^μ being products of multiplicative differences.

It should be also noted that the condition (8) does not exploit the equality $\operatorname{card} F = \operatorname{card} \tilde{F}$ of the cardinalities for sets of differential and difference equations as is assumed in Definition 2. The equality of cardinalities is not used in the proof of Theorem 1 either. Therefore, both Definition 4 and Theorem 1 are relevant to the case when the FDA has different number of equations than the PDE system.

4 Algorithmic Check

Given a finite set $F \subset \mathcal{R}_L$ of linear differential polynomials and its FDA $\tilde{F} \subset \tilde{\mathcal{R}}_L$, one can algorithmically verify whether $\tilde{F}$ is s-consistent with F. For a difference polynomial $\tilde{f} \in \tilde{\mathcal{R}}_L$ its consistency (e-consistency) with a differential polynomial $f \in \mathcal{R}_L$, i.e. condition $\tilde{f} \rhd f$, can be algorithmically verified by performing the Taylor expansion of $\tilde{f}$ in the grid spacing h. The condition $g \in \langle F \rangle \cap \mathcal{R}_L$ can also be algorithmically verified by construction of a Gröbner basis of the differential ideal $\langle F \rangle$.

The following algorithm verifies s-consistency of a finite set $\tilde{F} \subset \tilde{\mathcal{R}}_L$ of linear difference polynomials as FDA to a finite set $F \subset \mathcal{R}_L$ of linear partial differential polynomials. The algorithm uses Janet bases [7, 8] for both differential and difference ideals, though reduced Gröbner bases or other involutive bases can also be used.

Algorithm: *ConsistencyCheck* $(F, \tilde{F})$

1: **choose** differential resp. difference ranking $\succ_1$, $\succ_2$
2: $J :=$***JanetBasis*** $(F, \succ_1)$
3: $\tilde{J} :=$***JanetBasis*** $(\tilde{F}, \succ_2)$
4: $S :=$ **true**
5: **while** $\tilde{J} \neq \emptyset$ and $S =$ **true do**
6:     **choose** $\tilde{g} \in \tilde{J}$
7:     $\tilde{J} := \tilde{J} \setminus \{\tilde{g}\}$
8:     **compute** g such that $\tilde{g} \rhd g$
9:     **if** $\boldsymbol{NF}_{\mathcal{J}}(g, J) \neq 0$ **then**
10:         $S :=$ **false**
11:     **fi**
12: **od**
13: **return** S

The subalgorithm ***JanetBasis*** invoked in lines 2 and 3 computes the differential and difference Janet basis, respectively. The subalgorithm $\boldsymbol{NF}_{\mathcal{J}}$ on line 9 computes the differential involutive normal form [8] of a linear differential polynomial g modulo J, and thereby checks whether $g \in \langle J \rangle \cap \mathcal{R}_L$. The subscript $\mathcal{J}$ indicates that the normal form is computed for Janet division.

Correctness of the algorithm ***ConsistencyCheck*** follows from Theorem 1 and from the fact that the Janet bases are Gröbner ones. Its *termination* is an obvious consequence of the finiteness of the set $\tilde{J}$, termination of the subalgorithms and the Taylor expansion step of line 8.

Algorithm: *JanetBasis* $(F, \succ)$

Input: $F \subset \mathcal{R}_L$ (resp. $\tilde{\mathcal{R}}_L$), a finite set; $\succ$, a ranking
Output: J, a Janet basis of $\langle F \rangle$
1: **choose** $f \in F$ with lowest $\mathrm{ld}(f)$ w.r.t. $\succ$
2: $J := \{f\}$; $Q := F \setminus \{f\}$
3: **while** $Q \neq \emptyset$ **do**
4: $\quad h := 0$
5: $\quad$ **while** $Q \neq \emptyset$ and $h = 0$ **do**
6: $\qquad$ **choose** $q \in Q$ with lowest $\mathrm{ld}(q)$ w.r.t. $\succ$
7: $\qquad Q := Q \setminus \{q\}$; $h := \boldsymbol{NF}_{\mathcal{J}}(q, J)$
8: $\quad$ **od**
9: $\quad$ **if** $h \neq 0$ **then**
10: $\qquad$ **for all** $\{g \in J \mid \mathrm{ld}(g) \succ \mathrm{ld}(h)\}$ **do**
11: $\qquad\quad J := J \setminus \{g\}$
12: $\qquad\quad Q := Q \cup \{g\} \setminus \{\vartheta \circ g \mid \vartheta \in NM_{\mathcal{J}}(g, J)\}$
13: $\qquad$ **od**
14: $\qquad J := J \cup \{h\}$; $Q := Q \cup \{\vartheta \circ h \mid \vartheta \in NM_{\mathcal{J}}(h, J)\}$
15: $\quad$ **fi**
16: **od**
17: **return** J

For completeness of this paper we present also the ***JanetBasis*** algorithm in its simplest form. The algorithm computes the minimal Janet basis for both differential and difference ideals generated by the input set. The operator ϑ in lines 12 and 14 is either derivation or difference, and the set $NM_{\mathcal{J}}$ contains the Janet nonmultiplicative derivations (differences) for the polynomial g (line 12) and h (line 14). In its improved version this algorithm allows to compute the reduced Gröbner basis in the course of the Janet basis computation, that is, without performing extra reductions to produce the former from the latter.

The algorithm ***JanetBasis*** has been implemented in Maple for differential and difference ideals in the form of the packages called Janet [14] and LDA (Linear Difference Algebra) [15]. Besides the main procedure, which computes involutive bases w.r.t. Janet or Janet-like division [16], commands that return the normal form of a linear differential or difference polynomial modulo an ideal and many tools for dealing with linear differential or difference operators are included; syzygies, Hilbert polynomials and series can be computed, and the set of standard monomials modulo an ideal (together with a Stanley decomposition) can be determined.

5 Examples

In this section we demonstrate the notion of strong consistency on some examples. The computations were carried out in a few seconds with the packages Janet and LDA in Maple 13 on an AMD Opteron machine. Alternatively, the Gröbner package in Maple in connection with the Ore algebra package [12] can be used to get the same results.

In the below examples difference approximations to the initial PDE systems are e-consistent by construction. We show, however, that $s-consistency$ does not always hold for those approximations.

Example 1. *Consider the overdetermined linear PDE system*

$$u_x + yu_z + u = 0, \quad u_y + xu_w = 0 \tag{14}$$

for one unknown function u of four independent variables x, y, z, w. The minimal Janet basis J for the differential ideal in $\mathcal{R}$ generated by the left hand sides of (14) w.r.t. the degrevlex ranking with

$$\partial_x \succ \partial_y \succ \partial_z \succ \partial_w \tag{15}$$

contains an additional integrability condition and is completely given by

$$u_x + yu_w + u, \quad u_y + xu_w, \quad u_z - u_w. \tag{16}$$

It coincides with the reduced Gröbner basis for this ideal. First we choose forward differences (2) to discretize the original PDEs (14)

$$\Delta_1(u) + jh\Delta_3(u) + u_{i,j,k,l} = 0, \quad \Delta_2(u) + ih\Delta_4(u) = 0$$

at the grid point $x = ih, y = jh, z = kh, w = lh$. The minimal Janet basis $\tilde{J}_1$ (w.r.t. degrevlex with $\sigma_1 \succ \sigma_2 \succ \sigma_3 \succ \sigma_4$) for the difference ideal generated by these two linear difference polynomials $\tilde{f}_1$, $\tilde{f}_2$ coincides with the reduced Gröbner basis and consists of these polynomials (with leading terms $u_{i+1,j,k,l}$ respectively $u_{i,j+1,k,l}$) and three additional elements with leading terms $u_{i,j,k,l+2}$, $u_{i,j,k+1,l+1}$, $u_{i,j,k+2,l}$. For every difference polynomial $\tilde{f} \in \tilde{J}_1$ there exists $f \in \langle J \rangle \cap \mathcal{R}_L$ such that $\tilde{f} \rhd f$, as can be checked by applying reduction modulo J to the Taylor expansion of $\tilde{f}$ about a grid point. Moreover, the set $\langle J \rangle \cap \mathcal{R}_L$ of differential polynomials implied by $\tilde{J}_1$ contains, in addition to equations (14), $yu_z - yu_w$, $u_z - u_w$ and $xu_z - xu_w$ which also show that the integrability condition $u_z - u_w$ is recovered as limit for $h \to 0$ from the discretization.

The discretization $\Delta_3(u) - \Delta_4(u)$ of $u_z - u_w$ has non-zero normal form modulo $\tilde{J}_1$. We add this difference polynomial as another generator for the *difference ideal in $\tilde{\mathcal{R}}$. The minimal Janet basis $\tilde{J}_2$ for this larger ideal is given by*

$$\Delta_1(u) + u_{i,j,k,l}, \quad \Delta_2(u), \quad \Delta_3(u), \quad \Delta_4(u). \tag{17}$$

Now it is easy to check that the chosen discretization of (16) using forward differences is not s-consistent. We tried also some other discretizations of the differential Janet basis (16) and all of them were $s-inconsistent$. We conclude that it may be a non-trivial task to find a difference approximation of a Gröbner basis for an overdetermined set of partial differential polynomials that is strongly consistent.

Finally, we mention that the minimal Janet basis $\tilde{J}_3$ for the difference ideal generated by $\tilde{f}_1$, $\tilde{f}_2$ w.r.t. the elimination ranking with $\sigma_1 \succ \sigma_2 \succ \sigma_3 \succ \sigma_4$ contains the difference polynomial $\Delta_4^2 - ih^2\Delta_4^3$ whose limit u_{ww} for $h \to 0$ is not an element of $\langle J \rangle \cap \mathcal{R}_L$. Moreover, if we add $\Delta_3(u) - \Delta_4(u)$ as another generator as above, the minimal Janet basis w.r.t. this elimination ranking equals (17).

Example 2. *Consider the linear PDE system of two equations*

$$u_{xxy} + v_x = 0, \quad u_{xyy} + v_y = 0 \tag{18}$$

for two unknown functions $u^{(1)} = u$, $u^{(2)} = v$ of two independent variables x, y. The left hand sides in (18) form a minimal Janet basis J (and reduced Gröbner basis) w.r.t. the ranking (15) for the ideal they generate. Using forward differences first to discretize (18) we get

$$\Delta_1^2\Delta_2(u) + \Delta_1(v) = 0, \quad \Delta_1\Delta_2^2(u) + \Delta_2(v) = 0. \tag{19}$$

The left hand sides form a Gröbner basis for the difference ideal in $\tilde{\mathcal{R}}$ they generate. It is easily verified by the consistency check (Sect. 4) that (19) is s-consistent with (18).

We now modify the discretization (19) slightly by using two-step forward differences

$$\Delta_{2,1}(v) := \frac{v_{i+2,j} - v_{i,j}}{2h}\,, \quad \Delta_{2,2}(v) := \frac{v_{i,j+2} - v_{i,j}}{2h}\,,$$

i.e. the centered difference (3) w.r.t. the point $(x = (i+1)h, y = (j+1)h)$ instead of the one-step forward differences (2) for the second summands in (19). Thus, we consider

$$\Delta_1^2\Delta_2(u) + \Delta_{2,1}(v) = 0, \quad \Delta_1\Delta_2^2(u) + \Delta_{2,2}(v) = 0. \tag{20}$$

In this case, the left hand sides D_1, D_2 in (20) do not form a Gröbner basis for the ideal they generate, but the non-zero polynomial

$$\Delta_2(D_1) - \Delta_1(D_2) = (\Delta_2\Delta_{2,1} - \Delta_1\Delta_{2,2})(v)$$

has to be included as well. The Taylor expansion of this difference polynomial about a grid point has limit $v_{xyy} - v_{xxy}$ for $h \to 0$, which is not an element *of $\langle J\rangle \cap \mathcal{R}_L$. Hence, the difference approximation (20) is not s-consistent with (18).*

However, the following three FDA are strongly consistent with (18): two-step forward difference for ∂_x and one-step forward difference for ∂_y:

$$\Delta_{2,1}^2\Delta_2(u)+\Delta_{2,1}(v),\quad \Delta_{2,1}\Delta_2^2(u)+\Delta_2(v);$$

shifted centered difference for ∂_x (i.e. $\sigma_1(\sigma_1-\sigma_1^{-1})/(2h)$) and forward difference for ∂_y:

$$\Delta_{2,1}^2\Delta_2(u)+\sigma_1\Delta_{2,1}(v),\quad \Delta_{2,1}\Delta_2^2(u)+\sigma_1\Delta_2(v);$$

shifted centered differences for both ∂_x and ∂_y:

$$\Delta_{2,1}^2\Delta_{2,2}(u)+\sigma_1\sigma_2\Delta_{2,1}(v),\quad \Delta_{2,1}\Delta_{2,2}^2(u)+\sigma_1\sigma_2\Delta_{2,2}(v).$$

These three difference systems form reduced Gröbner bases for the difference ideals they generate, and the consistency check gives an affirmative answer in each case.

Example 3. *The linear PDE system*

$$f_1 := u_{xz}+yu=0,\quad f_2 := u_{yw}+zu=0 \tag{21}$$

for one unknown function u of four independent variables x, y, z, w has minimal Janet basis w.r.t. the ranking (15)

$$yu_y-zu_z,\quad u_x-u_w,\quad u_{zw}+yu.$$

We have the following two integrability conditions (see [9]) for f_1, f_2:

$$\begin{aligned}&(\partial_{yyww}+2z\partial_{yw}+z^2)f_1\\ &\qquad -(\partial_{xyzw}+z\partial_{xz}+y\partial_{yw}-\partial_x+2\partial_w+yz)f_2=0,\\ &(\partial_{xyzw}+z\partial_{xz}+y\partial_{yw}+2\partial_x-\partial_w+yz)f_1\\ &\qquad -(\partial_{xxzz}+2y\partial_{xz}+y^2)f_2=0.\end{aligned}$$

They form a reduced Gröbner basis for the ideal of all linear partial differential relations satisfied by f_1, f_2, as can be checked by a syzygy computation with the Janet package. A more compact way to write these integrability conditions is as follows:

$$\begin{aligned}((\partial_x\partial_z+y)(\partial_y\partial_w+z)-\partial_w+\partial_x)f_1-(\partial_x\partial_z+y)^2f_2 &= 0,\\ (\partial_y\partial_w+z)^2f_1-((\partial_y\partial_w+z)(\partial_x\partial_z+y)+\partial_w-\partial_x)f_2 &= 0.\end{aligned}$$

First we use forward differences (2) to discretize (21) at the grid point $x=ih, y=jh, z=kh, w=lh$:

$$\tilde{f}_1 := (\Delta_1\Delta_3)(u)+jhu_{i,j,k,l},\quad \tilde{f}_2 := (\Delta_2\Delta_4)(u)+khu_{i,j,k,l}.$$

The minimal Janet basis (and reduced Gröbner basis) w.r.t. degrevlex (with $\sigma_1 \succ \sigma_2 \succ \sigma_3 \succ \sigma_4$) for the difference ideal generated by $\tilde{f}_1$ and $\tilde{f}_2$ is

$$\Delta_1(u) - jh^2 u_{i,j,k,l},\ u_{i,j+1,k,l},\ u_{i,j,k+1,l},\ \Delta_4(u) - kh^2 u_{i,j,k,l}.$$

It is easily verified using the consistency check of Sect.4 that the FDA $\tilde{f}_1$, $\tilde{f}_2$ is not s-consistent.

Let us exchange $f_1 = 0$ in (21) by another linear PDE: $f_3 := u_{xy} + zu = 0$. It is a consequence of (21):

$$f_3 = -(\partial_y^2 \partial_w + z\partial_y) f_1 + (\partial_x \partial_y \partial_z + y\partial_y + 2) f_2.$$

However, the PDE system

$$f_2 = 0, \quad f_3 = 0 \tag{22}$$

is not equivalent to (21). It admits the following strongly consistent FDA:

$$\tilde{f}_2 := (\Delta_2 \Delta_4)(u) + khu_{i,j,k,l}, \quad \tilde{f}_3 := (\Delta_1 \Delta_2)(u) + khu_{i,j,k,l}.$$

In fact, the minimal Janet basis for (22) is $\{u_x - u_w, u_{yw} + zu\}$, and the reduced Gröbner basis for the difference ideal generated by $\tilde{f}_2$, $\tilde{f}_3$ is

$$(\Delta_1 - \Delta_4)(u), \quad (\Delta_2 \Delta_4)(u) + khu_{i,j,k,l},$$

which is easily checked to be s-consistent with (22). We note that if we discretize the integrability condition

$$(\partial_{xy} + z) f_2 - (\partial_{yw} + z) f_3 = 0 \tag{23}$$

for (22) with forward differences, we get

$$(\Delta_1 \Delta_2 + kh)\tilde{f}_2 - (\Delta_2 \Delta_4 + kh)\tilde{f}_3 = 0,$$

i.e. the discretization of (23) is satisfied.

In contrast to the previous PDE system we consider now

$$f_1 = 0, \quad f_3 = 0. \tag{24}$$

It is not equivalent to (21) either. In this case, if we discretize with forward differences,

$$\tilde{f}_1 := (\Delta_1 \Delta_3)(u) + jhu_{i,j,k,l}, \quad \tilde{f}_3 := (\Delta_1 \Delta_2)(u) + khu_{i,j,k,l},$$

we obtain an FDA which is not s-consistent with (24). In fact, the minimal Janet basis for the difference ideal is $\{u\}$ having only the zero solution.

We could have predicted this collapse of solutions by examining the following integrability condition: $(\partial_{xy} + z) f_1 - (\partial_{xz} + y) f_3 = 0$.

We discretize it with forward differences:

$$\begin{aligned}
& (\Delta_1\Delta_2 + kh)\tilde{f}_1 - (\Delta_1\Delta_3 + jh)\tilde{f}_3 \\
= \;& \Delta_1\Delta_2(jhu) - jh\Delta_1\Delta_2(u) + kh\Delta_1\Delta_3(u) - \Delta_1\Delta_3(khu) \\
= \;& h\Delta_1((k\Delta_3 - \Delta_3 k)(u) - (j\Delta_2 - \Delta_2 j)(u)) \\
= \;& \frac{1}{h}(u_{i+1,j+1,k,l} - u_{i,j+1,k,l} - u_{i+1,j,k+1,l} + u_{i,j,k+1,l}).
\end{aligned}$$

This discretization has limit $u_{xz} - u_{xy}$ for $h \to 0$, whose normal form modulo the Janet basis for (24) is $(z-y)u$, i.e., $u = 0$ is implied.

One can check that the FDA $\{\tilde{f}_1, \tilde{f}_2, \tilde{f}_3\}$ is not s-consistent with

$$f_1 = 0, \quad f_2 = 0, \quad f_3 = 0; \tag{25}$$

the discretizations of the two integrability conditions of order four given in the beginning of this example have a non-zero limit for $h \to 0$ modulo the Janet basis for (25).

6 Grid with Different Spacings

For an orthogonal and uniform grid with the spacings $\mathbf{h} := (h_1, \ldots, h_n)$ Definition 1 of consistency for a FDA with a PDE can be reformulated as the condition

$$f(\mathbf{u}) - \tilde{f}(\mathbf{u}) \to 0 \;\text{ as }\; |\mathbf{h}| \to 0 \quad (i = 1, \ldots, n), \tag{26}$$

where $|\mathbf{h}| \to 0$ means $h_1, \ldots, h_n \to 0$.

In some cases, however, one has to restrict the manner in which $|\mathbf{h}| \to 0$. Consider again the advection equation (5) and its difference approximation in the Lax-Friedrichs form [2]

$$\tilde{f} = \frac{2u_{i+1,j+1} - u_{i,j+2} - u_{i,j}}{2h_1} + \nu \frac{u_{i,j+2} - u_{i,j}}{2h_2}\,. \tag{27}$$

The Taylor expansion of $\tilde{f}$ about the point $x = h_1 i, y = h_2(j+1)$ reads

$$\begin{aligned}
\tilde{f} &= u_x + \nu u_y + \tfrac{h_1}{2}u_{xx} - \tfrac{h_2^2}{2h_1}u_{yy} + \nu\tfrac{h_2^2}{6}u_{yyy} + \tfrac{1}{6}\nu u_{xxx}h_1^2 \\
&+ \tfrac{1}{6}\nu u_{xxx}h_1^2 - \tfrac{h_2^4}{24h_1}u_{xxxx} + \nu\tfrac{h_2^4}{120}u_{xxxxx} + O(h_1^3 + \tfrac{h_2^6}{h_1} + h_2^6).
\end{aligned}$$

It shows that the consistency with (5) holds only if $h_1 \to 0$ and $h_2^2/h_1 \to 0$ (cf. [2]).

Respectively, Definition 2 of e-consistency for systems of linear PDEs discretized on the general orthogonal and uniform grids has the following form.

Definition 5. *A difference approximation (4) to (1) is* e-consistent *if there is a passage to the limit $|\mathbf{h}| \to 0$ which provides consistency of every difference equation in (4) with the corresponding differential equation in (1) by doing the Taylor expansion about a grid point.*

The search for such a passage by analyzing the multivariate Taylor expansion of every equation in the difference system (4) generally can be problematic and computationally cumbersome. We shall not consider this problem and adopt Definition 3 to the grid under consideration.

Definition 6. *A difference approximation to a PDE system is* s-consistent *with this system if there is a passage to the limit* $|\mathbf{h}| \to 0$ *such that the following holds:*

$$\forall \tilde{f} \in \langle \tilde{F} \rangle \cap \tilde{\mathcal{R}}_L \; \exists f \in \langle F \rangle \cap \mathcal{R}_L \; : \; \tilde{f} \rhd f \, . \tag{28}$$

Now instead of straightforward reformulation of Theorem 1 for the grid with different spacings we restate it as follows.

Theorem 2. *A passage to the limit* $|\mathbf{h}| \to 0$ *providing the fulfillment of condition (28) exists if and only if there is a passage to the limit for a reduced Gröbner basis* $\tilde{G} \subset \tilde{\mathcal{R}}_L$ *of the difference ideal* $\langle \tilde{F} \rangle$ *such that*

$$\forall \tilde{g} \in \tilde{G} \; \exists g \in \langle F \rangle \cap \mathcal{R}_L \; : \; \tilde{g} \rhd g \, ,$$

and for every such passage the condition (28) is satisfied.

Proof. It can be easily seen from the proof of Theorem 1 that the same reasoning is applicable in this case, too. □

7 Conclusion

We have shown that for a uniform and orthogonal solution grid a Gröbner basis of the difference ideal generated by a discretized linear system of PDEs contains important information on quality of the discretization, namely, on consistency of its linear difference consequences with the linear consequences of the PDE system. This property that we call s(strong)-consistency is superior to the in practice commonly used concept of consistency of the difference equations with their differential counterparts.

Even rather simple examples in Sect. 5 demonstrate that for overdetermined systems of PDEs the problem of constructing their s-consistent discretization may be a nontrivial problem. The algorithmic consistency check (Sect. 4) does not give answer how to construct a strongly consistent FDA for such systems. The algorithmic approach to generation of FDA suggested in [11] provides a more regular procedure for constructing a good FDA, since it exploits the conservation law form of the PDE system, when it admits such form, and preserves this form at the discrete level. Since conservation laws, if they are not explicitly incorporated into the PDE system, can always be expressed (linearly in the case of linear PDEs) in terms of integrability conditions (cf. [9], ch.2), the completion of the system to involution (or construction of its differential Gröbner basis) is an important step of its preprocessing before numerical solving. It is well known that conservation laws need special care in numerical solving of PDEs [3]. Thus, the last equation in (16) being the integrability condition for system (14) has the conservation law form.

Our algorithmic check of s-consistency is based on completion to involution (or construction of a Gröbner basis which is a formally integrable PDEs system [9] in the differential case) for both differential and difference systems. In addition to the consistency verification, if the initial differential system of the form $F \subset \mathcal{R}_L$ is involutive for an orderly (Riquier) ranking, then it admits formal well-posing of the initial value problem in the domain where none of the leading coefficients and none of the coefficient denominators vanish (cf. [8, 9, 17]). In view of the Lax-Richtmyer theorem [1, 2] this provides the necessary condition for convergence of a numerical solution to the exact one when the grid spacings go to zero. Another necessary condition for convergence is stability. For many discretizations the latter may hold only under certain restrictions on the grid spacings. For example, difference approximations (6) and (27) are stable only if $|\nu h_1/h_2| \leq 1$ (Courant-Friedrichs-Levy stability condition [1, 2]).

For grids with unequal spacings the consistency verification may be more difficult because of the restrictions on the passage to the limit in (26) and respectively in checking s-consistency conditions (28). However, such situation arises not very often in practice when any passage to zero in (26) (resp. in (28)) is acceptable.

Extension of the results in the paper to nonlinear PDEs has such a principle obstacle as nonexistence of Gröbner bases (except in very restricted cases) for differential ideals generated by nonlinear differential polynomials, cf. [18]. And even in the case of their existence their computation is only possible by hand since there is no software computing such Gröbner bases. Nevertheless, consideration of difference $S-$polynomials and the condition of their reducibility to zero modulo the set of polynomials in the difference approximation may be useful for verification of its consistency. This was demonstrated recently in [19] where the method of paper [11] was applied to the generation of FDA to two-dimensional Navier-Stokes equations, and for one of the constructed approximations its inconsistency was detected.

While nonlinear differential systems can be disjointly decomposed into algebraically simple and involutive subsystems [20], investigating whether nonlinear difference systems can be treated in a similar way is a new important research topic.

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References

[1] J.W.Thomas. *Numerical Partial Differential Equations: Finite Difference Methods*, 2nd Edition. Springer-Verlag, New York, 1998.

[2] J.C.Strikwerda. *Finite Difference Schemes and Partial Differential Equations*, 2nd Edition. SIAM, Philadelphia, 2004.

[3] J.W.Thomas. *Numerical Partial Differential Equations: Conservation Laws and Elliptic Equations*. Springer-Verlag, New York, 1999.

[4] V.Dorodnitsyn. *The group properties of difference equations*, Moscow, Fizmatlit, 2001 (in Russian).

[5] E.E.Rosinger. *Nonlinear equivalence, reduction of PDEs to ODEs and fast convergent numerical methods*. Pitman, London, 1983.

[6] V.P.Gerdt. *Involutive Algorithms for Computing Gröbner Bases*. Computational Commutative and Non-Commutative Algebraic Geometry. IOS Press, Amsterdam, 2005, pp. 199–225. arXiv:math.AC/0501111.

[7] V.P.Gerdt. *Gröbner Bases Applied to Systems of Linear Difference Equations*. Physics of Particles and Nuclei Letters Vol.5, No.3, 2008, 425–436. arXiv:cs.SC/0611041

[8] V.P.Gerdt. *Completion of Linear Differential Systems to Involution*, Computer Algebra in Scientific Computing / CASC 1999, Springer, Berlin, 1999, pp. 115–137. arXiv:math.AP/9909114.

[9] W.M.Seiler. *Involution: The Formal Theory of Differential Equations and its Applications in Computer Algebra*. Algorithms and Computation in Mathematics 24, Springer, 2010.

[10] A.Levin. *Difference Algebra*. Algebra and Applications 8, Springer, 2008.

[11] V.P.Gerdt, Yu.A.Blinkov and V.V.Mozzhilkin. *Gröbner Bases and Generation of Difference Schemes for Partial Differential Equations*. Symmetry, Integrability and Geometry: Methods and Applications (SIGMA) 2, 051, 2006, 26 pages. arXiv:math.RA/0605334

[12] F.Chyzak. *Gröbner Bases, Symbolic Summation and Symbolic Integration*. In: Gröbner Bases and Applications, B.Buchberger and F.Winkler (Eds.), Cambridge University Press, 1998.

[13] T.Becker and V.Weispfenning. *Gröbner Bases: A Computational Approach to Commutative Algebra*. Graduate Texts in Mathematics 141, Springer, New York, 1993.

[14] Yu.A.Blinkov, C.F.Cid, V.P.Gerdt, W.Plesken and D.Robertz. *The MAPLE Package Janet: I. Polynomial Systems. II. Linear Partial Differential Equations.* Proc. 6th Int.Workshop on Computer Algebra in Scientific Computing, Passau, 2003. Cf. also `http://wwwb.math.rwth-aachen.de/Janet`

[15] V.P.Gerdt and D.Robertz. *A Maple Package for Computing Gröbner Bases for Linear Recurrence Relations.* Nuclear Instruments and Methods in Physics Research 559(1), 2006, 215–219. arXiv:cs.SC/0509070. Cf. also `http://wwwb.math.rwth-aachen.de/Janet`

[16] V.P.Gerdt and Yu.A.Blinkov. *Janet-like Monomial Division.* Computer Algebra in Scientific Computing / CASC 2005, LNCS 3781, Springer-Verlag, Berlin, 2005, pp. 174–183; *Janet-like Gröbner Bases*, ibid., pp. 184–195.

[17] A.G.Khovanskii and S.P.Chulkov. *Hilbert polynomial for a system of linear partial differential equations.* Research Report in Mathematics, No.4, Stockholm University, 2005.

[18] A.Zobnin. *Admissible orderings and Finiteness Criteria for Differential Standard Bases.* Proceedings of ISSAC'2005, ACM Press, 2005, pp. 365–372.

[19] V.P.Gerdt and Yu.A.Blinkov. *Involution and Difference Schemes for the Navier-Stokes Equations.* Computer Algebra in Scientific Computing / CASC 2009, LNCS 5743, Springer-Verlag, Berlin, 2009, pp. 94–105.

[20] T.Bächler, V.P.Gerdt, M.Lange-Hegermann and D.Robertz. *Thomas Decomposition: I. Algebraic Systems; II. Differential Systems.* Submitted to Computer Algebra in Scientific Computing / CASC 2010 (September 5–12, 2010, Tsakhkadzor, Armenia).