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ON THE CONSISTENCY ANALYSIS OF FINITE DIFFERENCE APPROXIMATIONS

Abstract. Finite difference schemes are widely used in applied mathematics to numerically solve partial differential equations. However, for a given solution scheme, it is usually difficult to generally evaluate the quality of their underlying finite difference approximation with respect to the inheritance of algebraic properties of the differential problem under consideration. In this contribution, we present an appropriate quality criterion of strong consistency for finite difference approximations to systems of nonlinear partial differential equations. This property strengthens the standard requirement of consistency of difference equations with the differential ones. On this foundation, we use a verification algorithm for strong consistency, which is based on the computation of difference Gröbner bases. This allows for the evaluation and construction of solution schemes, which preserve some fundamental algebraic properties of the system at the discrete level. We demonstrate our presented concept by simulating a Kármán vortex street for two-dimensional incompressible viscous flow described by the Navier–Stokes equations.

§1. Introduction

Solving partial differential equations (PDEs) belongs to the most fundamental and practically important research challenges in mathematics and in the computational sciences. Such equations are typically solved numerically since obtaining their explicit solution is usually very difficult in practice or even impossible. One of the classical and nowadays well-established and popular approaches is the finite difference method [14, 22, 26] which exploits a local Taylor expansion to replace a differential equation by the

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difference one. This raises the question how to preserve fundamental properties of the underlying PDEs at the discrete level. From a geometric point of view, the most important properties are symmetries and conservation laws. Importance of conservation laws in mathematical physics could not be underestimated, since many fundamental properties for nonlinear PDEs (like existence and uniqueness of solutions) are typically based on conservation laws. From an algebraic perspective, basic objects which should be preserved are algebraic relations between equations and their differential (difference) consequences. The problem here occurs because finite difference approximations of derivations do not satisfy the Leibniz rule.

The fundamental requirement of a finite difference scheme (FDS) is its convergence to a solution of the corresponding differential problem as the grid spacings go to zero. According to the Lax-Richtmyer equivalence theorem [30,32] proved for a linear scalar PDE it has been adopted that the convergence is provided if a given finite-difference approximation (FDA) to the PDE is consistent and stable. The consistency implies a reduction of the FDA to the original PDE when the grid spacings go to zero, and it is obvious that the consistency is necessary for convergence. The theorem states that a FDS for an initial value (Cauchy) problem providing the existence and uniqueness of the solution converges if and only if its FDA is consistent and numerically stable.

For a system of PDEs the s(trong) consistency [8,12] of its FDA means not only the consistency of elements in FDA with the PDEs (w(eak) consistency) but also the consistency of any difference-algebraic relation of the elements in the FDA with a certain differential-algebraic consequence of the PDEs.

In this paper, we describe algorithmic methods to generate FDAs to PDEs on orthogonal and uniform grids, and to verify s-consistency of the obtained FDAs. The main algorithmic tool for the case of linear PDEs is the difference elimination provided by Gröbner bases [8, 11, 13, 21] for a certain elimination ranking. Given a system of polynomially-nonlinear PDEs and its FDA, the s-consistency analysis is based on a computation of a difference standard (Gröbner) basis and the construction of a differential Thomas decomposition [3, 24] for the PDE system. This paper is an extension of the methodology of [2, 8–10, 12]. As a relevant example in practice, we apply the procedure of the strong consistent FDA generation to the two-dimensional Navier-Stokes equations for the unsteady motion of an incompressible fluid of constant viscosity. For these equations, we consider two fully conservative FDAs (one s-consistent and one w-consistent). We use the FDAs for the numerical simulation on exact solutions and consider a Kármán vortex street to analyze the influence of the consistency on the numerical quality of these schemes.

§2. FDAs to PDEs and the Thomas decomposition

We consider a PDE systems of the form

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

where $f_1, \ldots, f_p$ are elements of the differential polynomial ring [19, 23]

$$\mathcal{R} := \mathcal{K}[u^1, \ldots, u^m]$$

over a differential coefficient field $\mathcal{K}$. To apply the algorithms described in the following and related software, the field $\mathcal{K}$ can be either the field of constants or the field $\mathbb{Q}(\mathbf{x})$ of rational functions in the independent variables $\mathbf{x} := \{x_1, \ldots, x_n\}$ with rational coefficients. The differential polynomial ring $\mathcal{R}$ contains polynomials in the dependent variables $\mathbf{u} := \{u^1, \ldots, u^m\}$ and their partial derivatives as the action of the operator power products of the derivation operators $\delta_1 := \partial_{x_1}, \ldots, \delta_n := \partial_{x_n}$ on the dependent variables.

To approximate the differential system (1) by a difference system, we use an orthogonal and uniform (i.e. regular Cartesian) computational grid, which is given by the set of points $(k_1h_1, \ldots, k_nh_n) \in \mathbb{R}^n$. In this context, $\mathbf{h} := (h_1, \ldots, h_n)$, $h_i > 0$ is the grid spacing set, and the grid points are enumerated by $(k_1, \ldots, k_n) \in \mathbb{Z}^n$. If the actual solution to the problem (1) is the vector-valued function $\mathbf{u}(\mathbf{x})$, its approximation in the grid nodes is given by the vector-valued grid function $\widetilde{\mathbf{u}}_{k_1,\cdots,k_n} := \widetilde{\mathbf{u}}(k_1h_1, \ldots, k_nh_n)$.

The coefficients on the grid as rational functions in $\{k_1h_1, \ldots, k_nh_n\}$ are elements of the difference field [21] with mutually commuting differences $\{\sigma_1, \ldots, \sigma_n\}$ acting on a function $\phi(\mathbf{x})$ as forward shift operators

$$\sigma_i \circ \phi(x_1, \ldots, x_n) = \phi(x_1, \ldots, x_i + h_i, \ldots, x_n), \quad h_i > 0\,. \tag{2}$$

The monoid generated by σ will be denoted by Θ, i.e. $\Theta := \{\, \sigma_1^{i_1} \circ \cdots \circ \sigma_n^{i_n} \mid i_1, \ldots, i_n \in \mathbb{N}_{\geq 0} \,\}$.

The standard technique to obtain a FDA to (1) is the replacement of the derivatives occurring in (1) by finite differences.

In [9], another approach to the generation of FDAs is suggested, which is based on the finite volume method and difference elimination. As it was shown for the classical Falkowich-Kármán equation in gas dynamics, this method may derive a FDA which reveals better numerical behavior then those obtained by the standard technique. In this contribution, we consider a FDA to the PDE system (1) as a finite set of difference polynomials

$$\widetilde{f}_1 = \cdots = \widetilde{f}_q = 0, \quad \widetilde{F} := \{\widetilde{f}_1, \ldots, \widetilde{f}_q\} \subset \widetilde{\mathcal{R}}\,.^{1} \tag{3}$$

Definition 1. *[8]* We shall say that a differential (resp. difference) polynomial $f \in \mathcal{R}$ (resp. $\widetilde{f} \in \widetilde{\mathcal{R}}$) is a differential-algebraic (resp. difference-algebraic) consequence of F (resp. $\widetilde{F}$), if f (resp. $\widetilde{f}$) vanishes on every possible common solutions of (1) (resp. (3)). We shall denote the set of all such consequences by $[\![F]\!]$ (resp. by $[\![\widetilde{F}]\!]$).

Algebraically, $[\![F]\!]$ is the radical of the differential ideal generated by F (cf. [19]) and $[\![\widetilde{F}]\!]$ is the perfect difference ideal generated by $\widetilde{F}$ (see Def. 9).

Definition 2. *[8]* Let $S^{=}$ and $S^{\neq}$ be finite sets of differential polynomials such that $S^{=} \neq \varnothing$ contains equations $(\forall s \in S^{=})\ [s = 0]$ whereas $S^{\neq}$ contains inequations $(\forall s \in S^{\neq})\ [s \neq 0]$. Then the pair $\left(S^{=}, S^{\neq}\right)$ of sets $S^{=}$ and $S^{\neq}$ is called differential system.

Let $\mathfrak{Sol}\,(S^{=}/S^{\neq})$ denote the solution set of the system $\left(S^{=}, S^{\neq}\right)$, i.e. the set of common solutions of differential equations $\{\, s = 0 \mid s \in S^{=}\}$ that do not annihilate elements $s \in S^{\neq}$.

Theorem 1. [3, 24, 31] *Any differential system $\left(S^{=}, S^{\neq}\right)$ is decomposable into a finite set of involutive differential subsystems $(S_i^{=}, S_i^{\neq})$ with a disjoint set of solutions:*

$$(S^{=}/S^{\neq}) \Longrightarrow \bigcup_i \,(S_i^{=}/S_i^{\neq})\,, \quad \mathfrak{Sol}\,(S^{=}/S^{\neq}) = \biguplus_i \mathfrak{Sol}\,(S_i^{=}/S_i^{\neq})\,. \tag{4}$$

Remark 1. Each output involutive subsystem $(S_i^{=}/S_i^{\neq})$ in (4) contains all its so-called integrability conditions. Let q be the maximal order of partial derivatives occurring in $S_i^{=}$. Then differential polynomial $p \in [\![S_i^{=}]\!]$ is an integrability condition for $S_i^{=}$ if the differential order of p is $\leq q$ and p cannot be obtained from the set $S_i^{=}$ pure algebraically, i.e. without differentiation of its elements [2].

[1]Please note, that $q = p$ is not a necessary condition.

[2]We refer to [27] for a more rigorous definition of integrability conditions and for the algebraic and geometric characterization of involutive differential equations. Computation of integrability conditions provides a tool to construct partial solutions to PDEs (cf. [29]).

We illustrate the differential Thomas decomposition by the following example taken from [7, 8].

Example 1. Consider the differential system $(S^{=}, \varnothing)$ with

$$S^{=} = \{(u_y + v)u_x + 4v\,u_y - 2v^2,\ (u_y + 2v)u_x + 5v\,u_y - 2v^2\}$$

of two quadratically-nonlinear first-order PDEs with two dependent and two independent variables. Its Thomas decomposition for a ranking satisfying $u_x \succ u_y \succ v_x \succ v_y \succ u \succ v$ is given by

$$\left(\begin{array}{ll} (u_y + v)u_x + 4v\,u_y - 2v^2 & \\ u_y^2 - 3u_y + 2v^2 & , v \\ v_x + v_y & \end{array}\right) \cup \left(\begin{array}{ll} u_x & , u_y \\ v & \end{array}\right) \cup \left(\begin{array}{ll} u_y & , \varnothing \\ v & \end{array}\right).$$

§3. Difference Gröbner and standard bases

Given an admissible ordering $\succ$, every difference polynomial $\widetilde{f}$ has the leading monomial $\mathrm{lm}(\widetilde{f}) \in \mathcal{M}$ with the leading coefficient $\mathrm{lc}(\widetilde{f})$. Now we consider the notions of a difference ideal [21] and its standard basis. The last notion is in the full analogy to that in differential algebra [23].

Definition 3. *[21]* A set $\mathcal{I} \subset \widetilde{\mathcal{R}}$ is a *difference polynomial ideal* or *σ-ideal*, if

$$(\,\forall\, a, b \in \mathcal{I}\,)\ (\,\forall\, c \in \widetilde{\mathcal{R}}\,), \quad (\,\forall\, \theta \in \Theta\,)\ [\, a + b \in \mathcal{I},\ a \cdot c \in \mathcal{I},\ \theta \circ a \in \mathcal{I}\,].$$

If $\widetilde{F} \subset \widetilde{\mathcal{R}}$, the smallest σ-ideal containing $\widetilde{F}$ is said to be generated by $\widetilde{F}$ and denoted by $[\widetilde{F}]$.

If for $v, w \in \mathcal{M}$ the equality $w = t \cdot \theta \circ v$ holds with $\theta \in \Theta$ and $t \in \mathcal{M}$, then we shall say that v divides w and write $v \mid w$. It is easy to see that this divisibility relation yields a partial order.

Definition 4. *[8]* Given a σ-ideal $\mathcal{I}$ and an admissible monomial ordering $\succ$, a subset $\widetilde{G} \subset \mathcal{I}$ is its *(difference) standard basis*, if $[\widetilde{G}] = \mathcal{I}$ and

$$(\,\forall\, \widetilde{f} \in \mathcal{I}\,)(\,\exists\, \widetilde{g} \in \widetilde{G}\,)\ \ [\,\mathrm{lm}(\widetilde{g}) \mid \mathrm{lm}(\widetilde{f})\,]\,.$$

If the standard basis is finite it is called a *Gröbner basis*.

Definition 5. *[8]* A polynomial $\widetilde{p} \in \widetilde{\mathcal{R}}$ is said to be *head reducible* modulo $\widetilde{q} \in \widetilde{\mathcal{R}}$ to $\widetilde{r}$, if $\widetilde{r} = \widetilde{p} - m \cdot \theta \circ \widetilde{q}$ and $m \in \mathcal{M}$, $\theta \in \Theta$ are such that

$\mathrm{lm}(\widetilde{p}) = m \cdot \theta \circ \mathrm{lm}(\widetilde{q})$ holds. In this case the transformation from $\widetilde{p}$ to $\widetilde{r}$ is an elementary reduction and denoted by

$$\widetilde{p} \underset{\widetilde{q}}{\longrightarrow} \widetilde{r}.$$

Given a set $\widetilde{F} \subset \widetilde{\mathcal{R}}$, $\widetilde{p}$ is *head reducible* modulo $\widetilde{F}$, if there is $\widetilde{f} \in \widetilde{F}$ such that $\widetilde{p}$ is *head reducible* modulo $\widetilde{f}$[3]. A polynomial $\widetilde{p}$ is *head reducible* to $\widetilde{r}$ modulo $\widetilde{F}$, if there is a chain of elementary reductions

$$\widetilde{p} \underset{\widetilde{F}}{\longrightarrow} \widetilde{p}_1 \underset{\widetilde{F}}{\longrightarrow} \widetilde{p}_2 \underset{\widetilde{F}}{\longrightarrow} \cdots \underset{\widetilde{F}}{\longrightarrow} \widetilde{r}\,. \tag{5}$$

Similarly, one can define a tail reduction. If $\widetilde{r}$ in (5) and each of its monomials is not reducible modulo $\widetilde{F}$, then we shall say that $\widetilde{r}$ is in the *normal form* modulo $\widetilde{F}$ and write $\widetilde{r} = \mathrm{NF}(\widetilde{p}, \widetilde{F})$. A polynomial set $\widetilde{F}$ with more then one element is *interreduced*, if

$$(\,\forall \widetilde{f} \in \widetilde{F}\,)\;[\,\widetilde{f} = \mathrm{NF}(\widetilde{f}, \widetilde{F} \setminus \{\widetilde{f}\})\,]\,. \tag{6}$$

Admissibility of $\succ$, as in commutative algebra, provides termination of the chain (5) for any $\widetilde{p}$ and $\widetilde{F}$. In doing so, $\mathrm{NF}(\widetilde{p}, \widetilde{F})$ can be computed by the difference version of a multivariate polynomial division algorithm [4,6]. If $\widetilde{G}$ is a standard basis of $[\widetilde{G}]$, then from Def. 4 and Def. 5 follows, that $\widetilde{f} \in [\widetilde{G}] \Longleftrightarrow \mathrm{NF}(\widetilde{f}, \widetilde{G}) = 0$.

Thus, if an ideal has a finite standard (Gröbner) basis, then its construction solves the ideal membership problem as well as in commutative [4,6] and differential [23,34] algebra. The algorithmic characterization of standard bases, and their construction in difference polynomial rings is done in terms of difference S-polynomials.

Definition 6. [8] Given an admissible ordering, and normalized difference polynomials $\widetilde{p}$ and $\widetilde{q}$, the polynomial $S(\widetilde{p}, \widetilde{q}) := m_1 \cdot \theta_1 \circ \widetilde{p} - m_2 \cdot \theta_2 \circ \widetilde{q}$ is called *S-polynomial* associated to $\widetilde{p}$ and $\widetilde{q}$[4], if $m_1 \cdot \theta_1 \circ \mathrm{lm}(\widetilde{p}) = m_2 \cdot \theta_2 \circ \mathrm{lm}(\widetilde{q})$ with co-prime $m_1 \cdot \theta_1$ and $m_2 \cdot \theta_2$.

Theorem 2. [8] *Given an ideal $\mathcal{I} \subset \widetilde{\mathcal{R}}$ and an admissible ordering $\succ$, a set of polynomials $\widetilde{G} \subset \mathcal{I}$ is a standard basis of $\mathcal{I}$, if and only if*

$$\mathrm{NF}(S(\widetilde{p}, \widetilde{q}), \widetilde{G}) = 0$$

[3] Denotation: $\widetilde{p} \underset{\widetilde{F}}{\longrightarrow}$.

[4] For $\widetilde{p} = \widetilde{q}$ we shall say that S-polynomial is associated with $\widetilde{p}$.

for all S-polynomials associated with polynomials in $\widetilde{G}$.

Let $\mathcal{I} = [\widetilde{F}]$ be a σ-ideal generated by a finite set $\widetilde{F} \subset \widetilde{\mathcal{R}}$ of difference polynomials. Then for a fixed admissible monomial ordering the difference analogue of the simplest version of Buchberger's algorithm (cf. [4, 6, 23]), if it terminates, returns a standard basis $\widetilde{G}$ of $\mathcal{I}$. The algorithm always terminates when the input polynomials are linear. In this case one can use the freely available [25] Maple package LDA [13]. If the input difference polynomials are not linear, the algorithm may not terminate.

§4. Consistency of FDA

Definition 7. [12] We shall say that a difference equation $\widetilde{f}(\mathbf{u}) = 0$ defined on the orthogonal and uniform grid with the grid spacing set $\mathbf{h} := (h_1, \ldots, h_n)$ *implies the differential equation* $f(\mathbf{u}) = 0$ and write $\widetilde{f} \rhd f$ if the Taylor expansion about a grid point yields

$$\widetilde{f}(\mathbf{u}) \xrightarrow[\forall i\, h_i \to 0]{} f(\mathbf{u}) + O(\mathbf{h})$$

where $O(\mathbf{h})$ denotes terms that reduce to zero when $h_i \to 0$ $(i = 1, \ldots, n)$.

Definition 8. [12] Given a PDE system (1) and its FDA (3), we shall say that (3) is *weakly consistent* or *w-consistent* with (1), if

$$(\,\forall \widetilde{f} \in \widetilde{F}\,)\ (\,\exists f \in F\,)\ [\,\widetilde{f} \rhd f\,].$$

In [12] it was shown that for a linear PDE systems this definition of consistency is not satisfactory in view of the inheritance of the properties of the differential systems by their discretization. Instead, we introduced another concept of consistency for linear FDAs which is extended to non-linear systems of PDEs as follows.

Definition 9. [21] A *perfect difference ideal* generated by a set $\widetilde{F} \in \widetilde{\mathcal{R}}$ and denoted by $[\![\widetilde{F}]\!]$ is the smallest difference ideal containing $\widetilde{F}$ and such that for any $\widetilde{f} \in \mathcal{R}$, $\theta_1, \ldots, \theta_r \in \Theta$ and $k_1, \ldots, k_r \in \mathbb{N}_{\geq 0}$

$$(\theta_1 \circ \widetilde{f})^{k_1} \cdots (\theta_r \circ \widetilde{f})^{k_r} \in [\![\widetilde{F}]\!] \Longrightarrow \widetilde{f} \in [\![\widetilde{F}]\!]\,.$$

It is clear that $[\widetilde{F}] \subseteq [\![\widetilde{F}]\!]$. In difference algebra perfect ideals play the same role as radical ideals in commutative [6] and differential [16] algebra, for example, in the Nullstellensatz [33]. By this reason we shall consider the perfect ideal $[\![\widetilde{F}]\!]$ generated by the difference polynomials in the FDA (3) as the set of its difference-algebraic consequences. Respectively, the set of differential-algebraic consequences of a PDE system is the radical differential ideal generated by the set F in (1).

Definition 10. [8] A FDA (3) to a PDE system (1) is *strongly consistent* or *s-consistent*, if

$$(\,\forall \widetilde{f} \in [\![\widetilde{F}]\!]\,)\;(\,\exists f \in [\![F]\!]\,)\;[\,\widetilde{f} \rhd f\,]\,. \tag{7}$$

Theorem 3. [8] *A difference approximation* (3) *to a differential system* (1) *is s-consistent, if and only if a reduced standard basis* $\widetilde{G} \subset \widetilde{\mathcal{R}}$ *of the difference ideal* $[\widetilde{F}]$ *satisfies*

$$(\,\forall \widetilde{g} \in \widetilde{G}\,)\;(\,\exists g \in [\![F]\!]\,)\;[\,\widetilde{g} \rhd g\,]\,.$$

It should be noted that condition (7) does not exploit the equality of cardinalities for sets of differential and difference equations as we assumed here. The equality of cardinalities is also not used in the proof of Theorem 3. Therefore, both Definition 10 and Theorem 3 are relevant to the case when the FDA has a number of equations different from that in the PDE system. Examples of such discretizations for linear PDE systems are considered in [12].

Remark 2. If a system of PDEs is linear, then its FDA is also linear. In this case one can also apply the algorithm ***JanetBasis*** of [12] and its Maple implementation Janet [5] for PDE systems and LDA [25] for the FDA, respectively.

Remark 3. The differentiation operator satisfies the product rule $(ab)' = a'b + ab'$. However, for its finite difference approximation D in general $D(ab) \neq D(a)b + a\,\mathrm{D}(b)$ holds. It is one of the main reasons why it is hard to construct strong consistent schemes.

§5. Generation of FDAs

In this section we extend the computer algebra-assisted approach [9] to the generation of FDAs to PDEs of polynomial-nonlinear type. Given PDEs and a regular Cartesian grid, the extended version of this approach produces FDAs by performing the following steps.

(1) In the case of a PDE system, complete it to involution. Generally, the completion is provided by the differential Thomas decomposition. The role of this step is twofold.
   (a) The completion means computation of the hidden integrability conditions (see Remark 1) and their incorporation into the PDE system. Thereby, an appropriate discretization of the involutive system may preserve all integrability conditions at the discrete level. In so doing, FDAs to equations in computational fluid and gas dynamics may be fully conservative [28].
   (b) The completion provides the s-consistency check of the obtained FDAs (Sec. (4)).
(2) If (some of) the PDEs admit the conservation law form, then rewrite such equations into this form. Then there are two options to discretize the obtained differential PDEs.
   (a) Replacement of the partial derivatives in the PDEs obtained at the previous step by finite differences to provide w-consistency for their discrete equation(s) in the case of a single PDE and s-consistency in the case of a PDE system. However, some conservation laws may be violated at the discrete level. Then all differential conservation laws have to be regained when the grid spacings go to zero.
   (b) Conversion of the differential conservation laws into their integral form. The integral form may admit (cf. [9]) non-smooth and even discontinuous solutions which are of special interest in computational fluid and gas dynamics [14, 22, 32]. In addition, the use of integral conservation laws provides more opportunities for the construction of FDAs that are both fully conservative and s-consistent. In addition, for nonlinear PDEs this may lead to FDAs whose degree of nonlinearity may be higher than that of the PDEs. An example of such a situation with a quadratically nonlinear PDE and a cubically nonlinear FDA was demonstrated in [9] for the classical Falkowich-Kármán equation in gas dynamics. In doing so, the cubically nonlinear FDA is fully conservative and the related FDS possesses a stable and uniform convergence to a shock-wave solution, unlike all known quadratically nonlinear FDAs.

   In the presence of integral equations, the following steps have to be done.

- Choice of an integration contour on the grid and addition to the output of the previous step. Consider the exact integral relations between derivatives of the dependent variables that occur in the integral conservation laws. The number of added integral relations should be sufficient for the difference elimination of all partial derivatives.
- Discretization of the obtained equations on the solution grid using methods of numerical integration.
- Elimination of the derivatives of the dependent variables from the obtained difference equations by construction of a difference Gröbner basis for an appropriate elimination order. This gives a FDA as the subset of the Gröbner basis which does not contain derivatives.

§6. Application to the Navier–Stokes equations

In this section we apply the above described approach to the two-dimensional Navier–Stokes equations for the unsteady motion of an incompressible viscous liquid of constant viscosity. In the dimensionless form these equations are given by

$$\left\{\begin{array}{ll} f_1 := & u_x + v_y = 0\,, \\ f_2 := & u_t + uu_x + vu_y + p_x - \frac{1}{\mathrm{Re}}\,\Delta\, u = 0\,, \\ f_3 := & v_t + uv_x + vv_y + p_y - \frac{1}{\mathrm{Re}}\,\Delta\, v = 0\,. \end{array}\right. \tag{8}$$

Here $\mathbf{u} = (u, v)$ is the velocity field, p is the pressure, the constant Re is the Reynolds number, f_1 is the continuity equation, f_2 and f_3 are the proper Navier–Stokes equations.

If one chooses an elimination ranking $\succ$ on partial derivatives compatible with $p \succ u \succ v$ and $\partial_t \succ \partial_x \succ \partial_y$ such that

$$u_t \succ v_t \succ p_x \succ p_y \succ u_x \succ u_y \succ v_x \succ v_y\,,$$

then (8) has the only integrability condition (see Remark 1) which is the well-known pressure Poisson equation [15]

$$f_4 := (f_1)_t - (f_2)_x = \,\Delta\, p + u_x^2 + 2v_x u_y + v_y^2\,. \tag{9}$$

The inclusion of (9) in (8),

$$\left\{\begin{array}{ll} f_1 = & \underline{u_x} + v_y = 0\,, \\ f_2 = & \underline{u_t} + uu_x + vu_y + p_x - \frac{1}{\mathrm{Re}}\,\Delta\, u = 0\,, \\ f_3 = & \underline{v_t} + uv_x + vv_y + p_y - \frac{1}{\mathrm{Re}}\,\Delta\, v = 0\,, \\ f_4 = & \underline{\Delta\, p} + u_x^2 + 2v_x u_y + v_y^2 = 0 \end{array}\right. \tag{10}$$

yields an involutive system (cf. [10]). The underlined terms in Eq. (10) are leaders.

It is easy to rewrite the equations in system (10) as conservation laws in the differential form

$$\left\{\begin{array}{ll} f_1 = & \mathrm{div}(u,\, v) = 0\,, \\ f_2 = & u_t + \mathrm{div}\left(u^2 + p - \frac{1}{\mathrm{Re}}u_x,\, vu - \frac{1}{\mathrm{Re}}u_y\right) = 0\,, \\ f_3 = & v_t + \mathrm{div}\left(uv - \frac{1}{\mathrm{Re}}v_x,\, v^2 + p - \frac{1}{\mathrm{Re}}v_y\right) = 0\,, \\ f_4 = & \mathrm{div}\left(uu_x + vu_y + p_x,\, uv_x + vv_y + p_y\right) = 0 \end{array}\right. \tag{11}$$

where $\mathrm{div}(a,b) := a_x + b_y$.
The following FDA with a 5×5 stencil was constructed in ([10], Eq. 13) and analyzed in [1,8]. Application of Theorem 3 shows that the FDA (12) is s-consistent and fully conservative:

$$\left\{\begin{array}{l} \widetilde{f}_1 := \frac{u^n_{j+1\,k} - u^n_{j-1\,k}}{2h} + \frac{v^n_{j\,k+1} - v^n_{j\,k-1}}{2h} = 0\,, \\ \widetilde{f}_2 := \frac{u^{n+1}_{j\,k} - u^n_{j\,k}}{\tau} + \frac{{u^2}^n_{j+1\,k} - {u^2}^n_{j-1\,k}}{2h} + \frac{{uv}^n_{j\,k+1} - {uv}^n_{j\,k-1}}{2h} \\ \qquad + \frac{p^n_{j+1\,k} - p^n_{j-1\,k}}{2h} - \frac{1}{\mathrm{Re}}\left(\frac{u^n_{j+2\,k} - 2u^n_{j\,k} + u^n_{j-2\,k}}{4h^2} + \frac{u^n_{j\,k+2} - 2u^n_{j\,k} + u^n_{j\,k-2}}{4h^2}\right) = 0\,, \\ \widetilde{f}_3 := \frac{v^{n+1}_{j\,k} - v^n_{j\,k}}{\tau} + \frac{{uv}^n_{j+1\,k} - {uv}^n_{j-1\,k}}{2h} + \frac{{v^2}^n_{j\,k+1} - {v^2}^n_{j\,k-1}}{2h} \\ \qquad + \frac{p^n_{j\,k+1} - p^n_{j\,k-1}}{2h} - \frac{1}{\mathrm{Re}}\left(\frac{v^n_{j+2\,k} - 2v^n_{j\,k} + v^n_{j-2\,k}}{4h^2} + \frac{v^n_{j\,k+2} - 2v^n_{j\,k} + v^n_{j\,k-2}}{4h^2}\right) = 0\,, \\ \widetilde{f}_4 := \frac{{u^2}^n_{j+2\,k} - 2{u^2}^n_{j\,k} + {u^2}^n_{j-2\,k}}{4h^2} + 2\frac{{uv}^n_{j+1\,k+1} - {uv}^n_{j+1\,k-1} - {uv}^n_{j-1\,k+1} + {uv}^n_{j-1\,k-1}}{4h^2} \\ \qquad + \frac{{v^2}^n_{j\,k+2} - 2{v^2}^n_{j\,k} + {v^2}^n_{j\,k-2}}{4h^2} + \frac{p^n_{j+2\,k} - 2p^n_{j\,k} + p^n_{j-2\,k}}{4h^2} + \frac{p^n_{j\,k+2} - 2p^n_{j\,k} + p^n_{j\,k-2}}{4h^2} = 0\,. \end{array}\right. \tag{12}$$

From the numerical standpoint it is tempting to replace the approximations (12) with the more compact FDA with a 3×3 stencil as follows:

$$
\begin{cases}
\widetilde{e}_1 := \dfrac{u^n_{j+1\,k} - u^n_{j-1\,k}}{2h} + \dfrac{v^n_{j\,k+1} - v^n_{j\,k-1}}{2h} = 0\,, \\[2ex]
\widetilde{e}_2 := \dfrac{u^{n+1}_{j\,k} - u^n_{j\,k}}{\tau} + \dfrac{{u^2}^n_{j+1\,k} - {u^2}^n_{j-1\,k}}{2h} + \dfrac{{uv}^n_{j\,k+1} - {uv}^n_{j\,k-1}}{2h} + \dfrac{p^n_{j+1\,k} - p^n_{j-1\,k}}{2h} \\
\quad - \dfrac{1}{\mathrm{Re}} \left(\dfrac{u^n_{j+1\,k} - 2u^n_{j\,k} + u^n_{j-1\,k}}{h^2} + \dfrac{u^n_{j\,k+1} - 2u^n_{j\,k} + u^n_{j\,k-1}}{h^2} \right) = 0, \\[2ex]
\widetilde{e}_3 := \dfrac{v^{n+1}_{j\,k} - v^n_{j\,k}}{\tau} + \dfrac{{uv}^n_{j+1\,k} - {uv}^n_{j-1\,k}}{2h} + \dfrac{{v^2}^n_{j\,k+1} - {v^2}^n_{j\,k-1}}{2h} + \dfrac{p^n_{j\,k+1} - p^n_{j\,k-1}}{2h} \\
\quad - \dfrac{1}{\mathrm{Re}} \left(\dfrac{v^n_{j+1\,k} - 2v^n_{j\,k} + v^n_{j-1\,k}}{h^2} + \dfrac{v^n_{j\,k+1} - 2v^n_{j\,k} + v^n_{j\,k-1}}{h^2} \right) = 0, \\[2ex]
\widetilde{e}_4 := \dfrac{{u^2}^n_{j+1\,k} - 2{u^2}^n_{j\,k} + {u^2}^n_{j-1\,k}}{h^2} \\
\quad + 2\dfrac{{uv}^n_{j+1\,k+1} - {uv}^n_{j+1\,k-1} - {uv}^n_{j-1\,k+1} + {uv}^n_{j-1\,k-1}}{4h^2} \\
\quad + \dfrac{{v^2}^n_{j\,k+1} - 2{v^2}^n_{j\,k} + {v^2}^n_{j\,k-1}}{h^2} + \dfrac{p^n_{j+1\,k} - 2p^n_{j\,k} + p^n_{j-1\,k}}{h^2} \\
\quad + \dfrac{p^n_{j\,k+1} - 2p^n_{j\,k} + p^n_{j\,k-1}}{h^2} = 0.
\end{cases}
\tag{13}
$$

The difference polynomial system $\widetilde{F} := \{\widetilde{e}_1, \widetilde{e}_2, \widetilde{e}_3, \widetilde{e}_4\}$ is w-consistent with (8). However, it is not s-consistent (cf. [2, 8, 10]). This can be shown by analysing the equality

$$
\begin{aligned}
&{\widetilde{e}_2}{}^n_{j+1,k} 2h - {\widetilde{e}_1}{}^{n+1}_{j,k} \tau - {\widetilde{e}_2}{}^n_{j-1,k} 2h + {\widetilde{e}_3}{}^n_{j,k+1} 2h - {\widetilde{e}_3}{}^n_{j,k-1} 2h + {\widetilde{e}_1}{}^n_{j,k} \tau \\
&\quad + \tfrac{4}{\mathrm{Re}} \left({\widetilde{e}_1}{}^n_{j+1,k} + {\widetilde{e}_1}{}^n_{j,k+1} - 4{\widetilde{e}_1}{}^n_{j,k} + {\widetilde{e}_1}{}^n_{j-1,k} + {\widetilde{e}_1}{}^n_{j,k-1} \right) - {\widetilde{e}_4}{}^n_{j,k} h^2 \\
&= {u^2}^n_{j+2,\,k} - {u^2}^n_{j+1,\,k} - {u^2}^n_{j-1,\,k} + {u^2}^n_{j-2,\,k} \\
&\quad + {v^2}^n_{j,\,k+2} - {v^2}^n_{j,\,k+1} - {v^2}^n_{j,\,k-1} + {v^2}^n_{j,\,k-2} \\
&\quad + p^n_{j+2,\,k} + p^n_{j,\,k+2} - p^n_{j+1,\,k} - p^n_{j,\,k+1} - p^n_{j-1,\,k} - p^n_{j,\,k-1} + p^n_{j-2,\,k} + p^n_{j,\,k-2}\,,
\end{aligned}
\tag{14}
$$

which is a difference-algebraic consequence (see Def. 1) of $\widetilde{F}$. Divided by $3\,h^2$, it implies

$$
g := \Delta\, p + 2uu_{xx} + 2vv_{yy} + 2u_x^2 + 2v_y^2\,. \tag{15}
$$

The differential polynomial g in (15) is not a differential-algebraic consequence of (8). This can also be verified using the well known exact solution [18] to the Navier–Stokes equations (8)

$$\begin{cases} u = -e^{-\frac{2t}{\mathrm{Re}}}\cos(x)\sin(y)\,, \\ v = e^{-\frac{2t}{\mathrm{Re}}}\sin(x)\cos(y)\,, \\ p = -\frac{1}{4}e^{-\frac{4t}{\mathrm{Re}}}(\cos(2x)+\cos(2y))\,, \end{cases} \tag{16}$$

whose substitution into the right-hand side of (15) shows that g does not vanish whereas, by Def. 1, (16) must be a solution to any differential-algebraic consequence of (8). Therefore, the FDA (13) is not s-consistent.

§7. Numerical Simulations

In this section we present some numerical simulations to experimentally compare the two above presented FDAs (12) and (13).[5]

For that, we suppose that the Navier–Stokes system (10) is defined for $t \geq 0$ in the rectangular domain $\mathbf{\Omega} = [0, M_x] \times [0, M_y]$, provide initial conditions for $t = 0$, and no-slip boundary conditions for $t > 0$ at $(x, y) \in \partial\mathbf{\Omega}$. Let $\mathbf{\Omega}$ be discretized in the (x, y)-directions by means of $(m + 1) \cdot (M_y/M_x m + 1)$ equidistant points $x_j = jh$ and $y_k = kh$, for $j = 0, \ldots, m$, $k = 0, \ldots, M_y/M_x m$, and $h = M_x/m$.

We simulate a Kármán vortex street by solving the Navier–Stokes system (10) numerically over time using the two above presented FDAs (12) and (13). The relative error of the configuration vector norm $\|(p, u, v)\|$ is measured over time.[6] The temporal evolution is illustrated in Fig. (2) for the different FDAs and varying spatial resolutions $m \in \{250, 500, 1\,000\}$ ($M_x = 1.92$, $M_y = 1.08$). The superior behavior of the s-consistent FDA (12) compared to the s-inconsistent FDA (13) can clearly be observed. As expected, stability can be improved by increasing m. Since in our experiments we are essentially interested in comparing different discretizations of u, v, and p on the space domain, the value of the time step was always chosen in order to provide stability. Using $\mathrm{Re} = 220$ we can observed the characteristic repeating pattern of the swirling vortices as illustrated in Fig. (1).

---

[5] The simulations have been carried out on a 2.7GHz Intel® Core i7 computer with 16GB DDR3 SDRAM.

[6] For each of the FDAs (12) and (13) a ground truth is computed using $m = 25,000$, which leads to almost identical results. The relative error for each scheme is determined relatively to the corresponding ground truth.

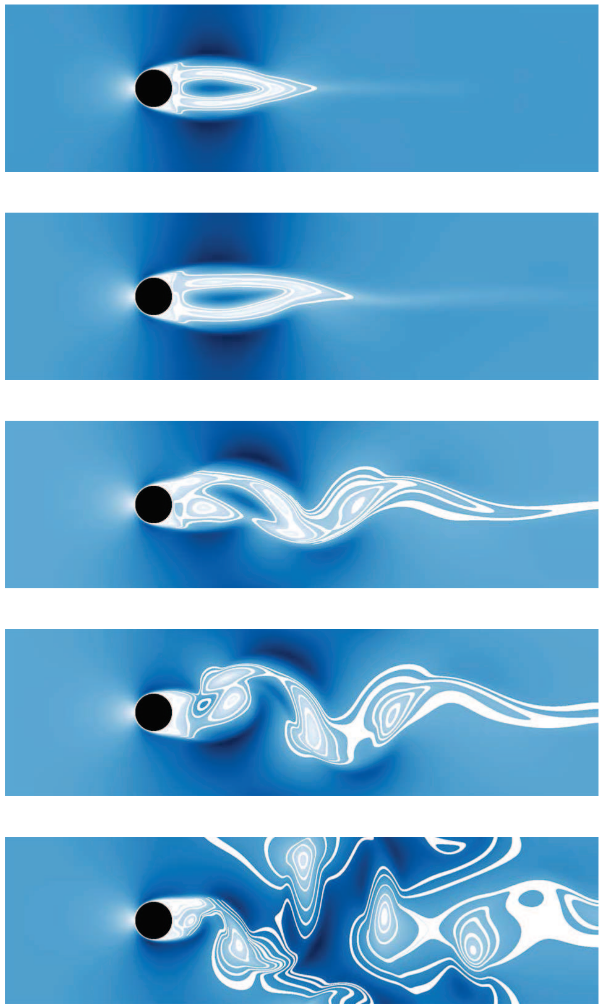

Figure 1. Simulation of the Kármán vortex street computed with the FDA (12) and $m = 1\,000$. The characteristic repeating pattern of swirling vortices can be observed, cf. [17].

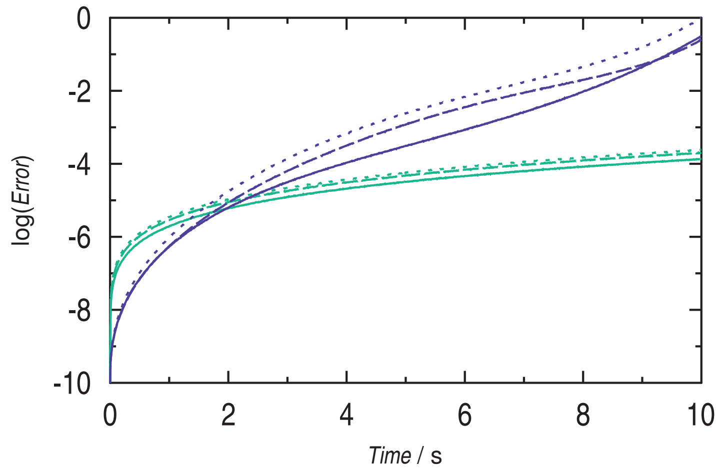

Figure 2. Temporal evolution of the relative error of the Kármán vortex street simulation using different FDA (12) (green curves) and FDA (13) (blue curve). Different spatial resolutions are used: $m = 250$ (dotted curves), $m = 500$ (dashed curves), and $m = 1\,000$ (solid curves).

§8. Conclusion

In this paper, we considered algorithmic aspects of the generation of FDAs to systems of polynomially-nonlinear PDEs on regular Cartesian solution grids. One of the major quality criteria to a FDA is its strong consistency which implies the preservation of fundamental algebraic properties of the system at the discrete level. Its algorithmic verification relies on the completion of the PDE system to involution as well as on the technique of difference Gröbner (standard) bases. This technique plays also the important role in the algorithmic generation of fully conservative FDAs using their representation in the form of integral conservation laws. This allows for the critical evaluation of different FDAs as we demonstrated in the context of the Navier–Stokes equations.

In summary, we think, that the presented computer algebra assisted methods for the algorithmic generation of difference approximations and the verification of their algebraic properties are enormously helpful for the construction and evaluation of appropriate discretizations to physical problems, so that our approach lays the ground for a fruitful discussion.

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