

ALGEBRAIC FOUNDATIONS FOR FINITE DIFFERENCE SCHEMES

CHRISTIAN DINGLER AND VIKTOR LEVANDOVSKYY

ABSTRACT. In this paper we present a very general way to generate finite difference schemes of arbitrary partial differential equations analytically. This approach uses the concept of polynomial rings and Gröbner bases. A criterion for the existence of a scheme for a partial differential equation with some arbitrary approximation rules is given.

1. INTRODUCTION

It is well known that in general one cannot solve an arbitrary partial differential equation symbolically. In this case numerical schemes are used. Instead of the function - in the sense of a clearly defined map - one receives approximations of finitely many function values in a certain interval (more details in [2],[4]). For instance, let us take a look at the well known advection equation as example for a Cauchy problem of an unknown real-valued function $u = u(x, t)$ in two real arguments x and t :

$$u_t + au_x = 0$$

with the initial boundary condition

$$u(x, 0) = u_0(x)$$

for some function u_0 . The Cauchy-Kowalewska theorem guarantees that in a neighborhood of the boundary there exists exactly one analytic function that solves the problem above.

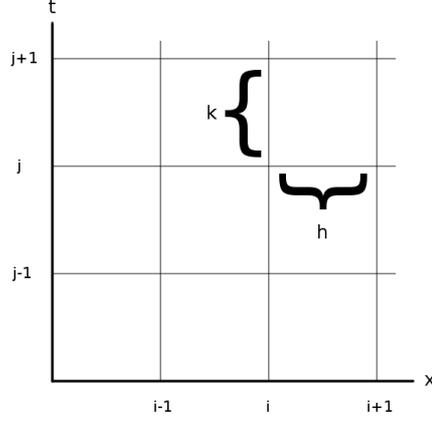
With $(h, k) = (\Delta x, \Delta t) \in \mathbb{R}^+ \times \mathbb{R}^+$ introduce the notation

$$u_i^j = u(ih, jk)$$

to approximate the unknown values of the function u in the several points $(ih, jk) \in \mathbb{R} \times \mathbb{R}^+$ for all $(i, j) \in \mathbb{Z} \times \mathbb{N}$ by those u_i^j . Figure 1 illustrates this idea of discretization by means of a rectangular and uniform mesh.

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FIGURE 1. Rectangular and uniform mesh in (x, t) -plane

Then the substitution of the occurring derivatives u_t and u_x by suitable difference quotients in the specific point (ih, jk) via

$$(u_t)_i^j = \frac{u_i^{j+1} - \frac{1}{2}(u_{i+1}^j + u_{i-1}^j)}{k}$$

respectively

$$(u_x)_i^j = \frac{u_{i+1}^j - u_{i-1}^j}{2h}$$

leads to

$$\frac{u_i^{j+1} - \frac{1}{2}(u_{i+1}^j + u_{i-1}^j)}{k} + a \frac{u_{i+1}^j - u_{i-1}^j}{2h} = 0$$

or equivalently we can derive a recurrent formula to compute u_i^{j+1} from u_{i+1}^j and u_{i-1}^j :

$$u_i^{j+1} = \frac{1}{2}(u_{i+1}^j + u_{i-1}^j) - \frac{ak}{2h}(u_{i+1}^j - u_{i-1}^j)$$

Figure 2 shows the *stencil* of the grid points, i.e. the formal relation visualized in the mesh.

Recent approaches as in [3] propose a formulation of such schemes completely in terms of partial difference operators T_x, T_t with

$$T_x \circ u(x, t) = u(x + h, t)$$

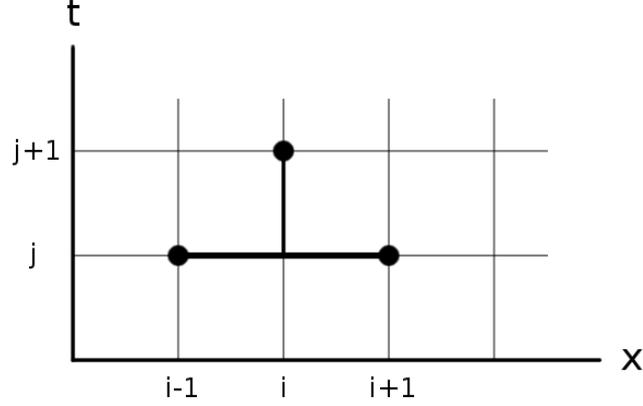


FIGURE 2. Stencil of Lax-Friedrich-scheme

respectively

$$T_t \circ u(x, t) = u(x, t + k)$$

Then the above scheme can be abbreviated as

$$\left(T_t T_x - \left(\frac{1}{2} (T_x^2 + 1) - \frac{ak}{2h} (T_x^2 - 1) \right) \right) \circ u(x, t) = 0$$

This Lax-Friedrich-scheme is known to be numerically stable when finding the values u_i^j iteratively (cf. [4]).

2. SETTING

Continuous world. The problem of generating difference schemes requires the partial differential equation and the corresponding approximations on the input. Let u be an unknown function and consider the set

$$S = \left\{ \sum_{\gamma \in \Gamma_\alpha} \left(c_{\alpha\gamma} \cdot \prod_{\beta \in B_\gamma} u_{x^\beta} \right) \mid \alpha \in \Psi \right\}$$

which is any *finite* set of partial differential equations involving u . For further explanation we introduce the notation

$$u_{x^\beta} := \frac{\partial^\beta}{\partial x^\beta} u := \frac{\partial^{|\beta|}}{\partial x_1^{\beta_1} \dots \partial x_i^{\beta_i}} u$$

and assume all $c_{\alpha\gamma}$ to be invertible. We allow in this case even the occurrence of non-linear terms with respect to the u_{x^β} .

First consider one equation, i.e. $|S| = 1$, since in the case of several differential equations one has to generate the several schemes independently from each other and in this paper we shall restrict ourselves to

case of one partial differential equation if not indicated otherwise. The occurring derivatives u_{x^β} of u in the set S will be collected in the set

$$\Lambda = \{u_{x^{\alpha_1}}, \dots, u_{x^{\alpha_l}}\} = \bigcup_{\alpha \in \Psi} \bigcup_{\gamma \in \Gamma_\alpha} \bigcup_{\beta \in B_\gamma} \{u_{x^\beta}\}$$

Now we define the suitable ring in which we will work and formulate some requirements that show the desired properties of this ring.

Consider a numerical field \mathbb{F} of transcendence degree zero over the field of rational numbers \mathbb{Q} , i.e. the field extension \mathbb{F}/\mathbb{Q} is purely algebraic over \mathbb{Q} . This ensures that all occurring objects are computable in practice. We allow the "coefficients" $c_{\alpha\gamma}$ in S to be functions, e.g. $c_{\alpha\gamma} \in C_1$, where $C_1 = C^\infty$ is possible.

The occurring derivatives shall be the variables in the ring to be defined below

$$\Lambda = \{u_{x^{\alpha_1}}, \dots, u_{x^{\alpha_l}}\} =: \{z_1, \dots, z_l\}$$

The final ring, called D_0 , associated to S is defined as

$$D_0 = \mathbb{F} \otimes_{\mathbb{F}} C_1[\Lambda] = \mathbb{F} \otimes_{\mathbb{F}} C_1[u_{x^{\alpha_1}}, \dots, u_{x^{\alpha_l}}]$$

This notation is set up for a suitable frame of the continuous world. It assures that all the occurring parameters are invertible and no problems arise when performing term operations. Remember in this context that no discretization or approximation was needed so far.

Remark 2.1. D_0 is not necessarily a differential ring but indeed a subring of a differential ring and it is a finitely generated \mathbb{F} -algebra (differential rings in general are not finitely generated).

In this special case $C_1 = C^\infty(\mathbb{F}, \mathbb{F})$ of all invertible infinitely differentiable functions $\mathbb{F} \rightarrow \mathbb{F}$ one sees that $(C_1, (\partial_{x_i})_i)$ is a *differential field* since it is closed under the action of the operators ∂_{x_i} for all i .

Discrete world. We now formulate the specific notions for the discrete aspects in an analogous manner to the issues in the continuous world.

As in 1 the discretization is described by means of a finite difference scheme, focuses on approximations of the values of a function and is the basis for recurrent solution formulas. Often for a function

$$u : \mathbb{F}^{n+1} \rightarrow \mathbb{F}$$

$$(x_1, \dots, x_n, t) \mapsto u(x_1, \dots, x_n, t)$$

an *uniform* grid (i.e. Δx_i and Δt are constant) in the space of the function arguments (x_1, \dots, x_n, t) is used. To make this point we formally describe the set of all grid points that can occur in the process of

discretization for a given set $\{u_{x^\theta} | \theta \in \Theta\}$ of arbitrary partial derivatives

$$D_1 = \mathbb{F} \left[\left\{ (u_{x^\theta})^\delta \mid \theta \in \Theta, \delta \in \mathbb{Z}^{n+1} \right\} \right]$$

Clearly, D_1 is an infinite set.

We want to model an arbitrary shifting process on the i -th argument x_i of a function u in the point $(x_1, \dots, x_i, \dots, x_n, t)$ with a shift operator

$$T_{x_i} \circ u(x_1, \dots, x_i, \dots, x_n, t) = u(x_1, \dots, x_i + \Delta x_i, \dots, x_n, t)$$

by considering and allowing only those points that are on the unbounded and infinite grid

$$\Omega := (\mathbb{Z}\Delta x_1 \times \dots \times \mathbb{Z}\Delta x_n \times \mathbb{Z}\Delta t) \cap \mathbb{R}^{n+1}$$

In general the arguments of the considered functions u are in the \mathbb{R} -space \mathbb{R}^{n+1} that is obviously no finitely generated \mathbb{Z} -module. So the definition of Ω provides that it is naturally isomorphic as a \mathbb{Z} -module:

$$\mathbb{Z}^{n+1} \cong \Omega$$

and hence the shifted points are again in the grid and it makes sense to work with the shift operators T_i on \mathbb{Z}^{n+1} (rather than with the T_{x_i} on \mathbb{R}^{n+1}):

$$T_i : x_{\delta_i} \mapsto x_{\delta_i+1}$$

with $\delta \in \mathbb{Z}^{n+1}$ and $x_{\delta_i} = \delta_i \Delta x_i$ and $t_{\delta_{n+1}} = \delta_{n+1} \Delta t$.

The philosophy of this setting can obviously been seen if we introduce the notation

$$\left(\frac{\partial^\alpha}{\partial x^\alpha} u \right) (x_{\delta_1}, \dots, x_{\delta_n}, t_{\delta_{n+1}}) \stackrel{\text{approx}}{\approx} (u_{x^\alpha})^\delta$$

for the approximated values of a function u_{x^α} .

This convention and notation provides some advantages with respect to the infinitely many grid points and gives the possibility to calculate on a sufficiently large grid, such that the boundary conditions can be ignored when dealing with an arbitrarily chosen generic point and its neighbored points.

With this in mind one can define *shift operators* in each direction (*forward* and *backward*) T_1, \dots, T_n, T_{n+1} on D_1 . Let $\gamma \in \mathbb{Z}^{n+1}$ and $T^\gamma = T_1^{\gamma_1} \cdot \dots \cdot T_n^{\gamma_n} \cdot T_{n+1}^{\gamma_{n+1}}$ then define the action

$$T^\gamma \circ (u_{x^\alpha})^\delta = (u_{x^\alpha})^{\delta+\gamma}$$

Note that negative shifts are indeed possible. This allows us to pick one representative generic point $\delta \in \mathbb{Z}^{n+1}$ and get all points just by shifting

it via these operators. By definition, the operators are multiplicative, that is:

$$T^\gamma \circ \left((u_{x^\alpha})^{\delta_1} \cdot (u_{x^\beta})^{\delta_2} \right) = T^\gamma \circ \left((u_{x^\alpha})^{\delta_1} \right) \cdot T^\gamma \circ \left((u_{x^\beta})^{\delta_2} \right)$$

Figure 3 shows an example of how the shift operators work in the (x, t) -plane.

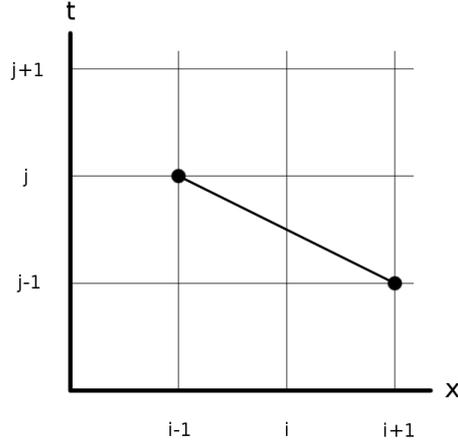


FIGURE 3. Action of the shift operator $(T_t T_x^{-2}) \circ (u_{i+1}^{j-1}) = u_{i-1}^j$

For convenience we will drop \circ when dealing with the T_i 's henceforth.

From this point it is necessary to incorporate the approximations into the framework for the discrete setting. Assume, that to a set

$$S = \left\{ \sum_{\gamma \in \Gamma_\alpha} \left(c_{\alpha\gamma} \cdot \prod_{\beta \in B_\gamma} u_{x^\beta} \right) \mid \alpha \in \Psi \right\} \subset D_0$$

of partial differential equations with

$$\Lambda = \{u_{x^{\alpha_1}}, \dots, u_{x^{\alpha_l}}\}$$

there are certain approximations

$$A^\delta = \left\{ (u_{x^\lambda})^\delta - \sum_{\omega \in \Omega_\lambda} \left(c_\omega \cdot \prod_{\nu \in N_\omega} T^{\gamma_\nu} (u_{x^\nu})^\delta \right) \mid \lambda \in \Phi \right\}$$

Note here, that nonlinearity in the trailing terms of the sum is possible. With these approximations in mind we define the set

$$M^\delta = \left\{ (u_{x^{\beta_1}})^\delta, \dots, (u_{x^{\beta_m}})^\delta \right\} = \bigcup_{\lambda \in \Phi} \bigcup_{\omega \in \Omega_\alpha} \bigcup_{\nu \in N_\omega} \left\{ (u_{x^\nu})^\delta \right\} \cup \left\{ (u_{x^\lambda})^\delta \right\}$$

of all terms of the type $(u_{x^\nu})^\delta$ that occur in A^δ .

Besides we want to denote the set of all terms that are being approximated by other terms, i.e. all the terms on the left hand side in A^δ :

$$L^\delta = \bigcup_{\lambda \in \Phi} \left\{ (u_{x^\lambda})^\delta \right\}$$

Before giving the final definition of the ring in which we will work while being in the discrete world, we shall take a look at the map φ that takes objects to their discrete analogs.

Recall the ring we defined before

$$D_0 = \mathbb{F} \otimes_{\mathbb{F}} C_1[\Lambda]$$

where C_1 describes the coefficients in S . These can be split up into coefficients $c' \in C_1^c$ that are constant and those $c'' \in C_1^d$ that depend on x_1, \dots, x_n, t . These coefficients are neglected with respect to the action of differentiation. The constants form a subring $C_1^c \subseteq C_1$ with the property

$$\partial^\alpha \circ c = 0 \quad \forall c \in C_1^c \quad \forall \alpha \in \mathbb{N} \setminus \{0\}$$

and accordingly the dependent coefficients C_1^d form a \mathbb{F} -algebra.

Example 2.2. *Let us consider the term $2 \cdot \sin + 3 \cdot \cos$. Then for C_1^d and for C_1^c we define for the dependent functions*

$$C_1^d = \mathbb{F}(\cos, \sin)$$

and for the constants

$$C_1^c = \mathbb{F}(a) \frac{[b]}{\langle b^2 + 1 \rangle}$$

and thus

$$2 \otimes \sin + 3 \otimes \cos \in C_1^c \otimes_{\mathbb{F}} C_1^d$$

Since different behavior of approximation and, hence, of shift operators on both, constants and non-constants, occurs when discretization takes place, we need to distinguish between them. A discussion about this

will proceed later in this chapter (confer 2.9). This gives rise to the map

$$\begin{aligned} \varphi : C_1 = C_1^c \otimes_{\mathbb{F}} C_1^d &\longrightarrow \{ \phi \mid \phi : \mathbb{Z}^{n+1} \rightarrow \mathbb{R} \} \\ (c', c'') &\longmapsto (c', \delta'(c'')) \end{aligned}$$

with $\delta'(c'') = c''(\delta)$ being the value of c'' at the generic point $\delta \in \mathbb{Z}^{n+1}$. Note that this map is well-defined since the coefficients are well-known and remark that the domain of the image function has changed. Let $\Lambda^\delta = \varphi(\Lambda)$ denote the image of φ at a symbolic point δ .

With the above setting and the convention that C_2 labels the discrete coefficients in the approximations the ring D_2 can be defined as

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(T_1, \dots, T_n, T_{n+1}) [\Lambda^\delta \cup M^\delta]$$

or, in a short notation

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta]$$

The philosophy here is to enlarge the ring by means of the shift operators \underline{T} in both directions, hence it suffices to focus on one generic symbolic point $\delta \in \mathbb{Z}^{n+1}$ because modulo the action of these operators all points can be identified.

Remark 2.3. Note here that according to this definition for any element in the ring D_2 the T_i can occur in fractions but one can avoid this situation by cancelling out all denominators during computations via multiplication with the least common multiple of the denominators. Thus, we regard only elements of the D_2 with no T_i occurring in the denominator of them.

But the formal allowance of fractions gives us the desirable case of

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta] = \mathbb{K} [\Lambda^\delta \cup M^\delta]$$

with \mathbb{K} being a *field*. This fact will be exploited later.

Orderings for schemes. We now formulate an important condition for the existence and uniqueness of numerical schemes and therefore we use the concept of monomial orderings.

Definition 2.4. A *monomial ordering* $<$ in a polynomial ring A is a *total* ordering on the set Mon_A of all monomials in A with the property

$$m_1 < m_2 \quad \Rightarrow \quad m_1 \cdot m_3 < m_2 \cdot m_3 \quad \forall m_1, m_2, m_3 \in Mon_A$$

We will restrict ourselves in the following to *global* orderings, that is we assume

$$m > 1 \quad \forall m \in \text{Mon}_A$$

Confer [1] for details.

Finding some ordering with a special property is crucial for our approach. Hereafter the ring to be considered shall be D_2 and as monomials we look upon the set

$$\text{Mon}_{D_2} = \Lambda^\delta \cup M^\delta$$

The shift operators are ignored with respect to an ordering.

Definition 2.5. The set A^δ is called *sufficient for scheme generation* if there exists a (global) ordering $>$ on Mon_{D_2} such that

$$(u_{x^\lambda})^\delta > \prod_{\nu \in N_\omega} (u_{x^\nu})^\delta \quad \forall \lambda \in \Phi \quad \forall \omega \in \Omega_\lambda$$

Likewise we call such an ordering $<$ *sufficient for scheme generation* with respect to a set A^δ .

An immediate consequence of 2.5 is:

Corollary 2.6. *If the ordering $<$ is sufficient for scheme generation, then*

$$|L^\delta| < |M^\delta|$$

Thus, there is the necessary condition $|M^\delta \setminus L^\delta| \geq 1$.

Proof. Since $L^\delta \subseteq M^\delta$ we have to prove the strictness of this relation. If $L^\delta = M^\delta$ was true this would imply a contradiction to the transitivity property of the monomial ordering $<$. \square

An easy example shows the reasoning of 2.6.

Example 2.7. *For a partial differential equation*

$$S^\delta = \{u_{tt} + a \cdot u_{xx}\}$$

and some approximations

$$A^\delta = \{u_{tt} - (u_x + u_t), u_t - (u + u^2), u_{xx} - (u_x + u), u_x - (u + u^3), u - (u_t + u_x)\}$$

we see that

$$L^\delta = \{u_{tt}, u_t, u_{xx}, u_x, u\} = M^\delta$$

However, the second and the last element in A^δ must hold the order

$$u_t > u > u_x$$

to fulfill the condition in 2.5. This is a contradiction to the transitivity of $<$.

Because of the same arguments as above the converse implication in 2.6 is not generally true, as the following example illustrates:

Example 2.8. Let

$$S^\delta = \{u_t + a \cdot u_x\}$$

and the formal approximations

$$A^\delta = \{u_t - (u_x + u_x \cdot u), u_x - (u_t + u^2)\}$$

Then we clearly have

$$L^\delta = \{u_t, u_x\} \subsetneq \{u_t, u_x, u\} = M^\delta.$$

For 2.5 we need the existence of a monomial ordering $<$ with

$$u_t > u_x \quad \text{and} \quad u_x > u_t$$

which, of course, is an obvious contradiction.

Remark 2.9. Note that in the case of non-constant coefficients that depend on the variables x_1, \dots, x_n, t in the \mathbb{F} -algebra $C_1^c \otimes_{\mathbb{F}} C_1^d$ the approximation of those $c \in C_1^d$ has to be conducted though these functions are well-known. Recall, that the shift operators are defined to be multiplicative, that is

$$T \circ (u_1 \cdot u_2) = T \circ u_1 \cdot T \circ u_2$$

for any two elements u_1, u_2 in the ring D_2 .

Consider the case of $u_1 = x_k$ being the identity for the k -th spatial variable, $u_2 = u_{x_k}$ and $T = T_k$. Then there is a natural discretization for the non-constant function x_k in any point $a = (i_1, \dots, i_{n+1})$ of the grid Ω with $x_k(a) = i_k$ for the k -th argument and hence omitting the operator notation \circ by limiting to multiplication \cdot in the ring D_2 we have in the continuous case generally

$$T \cdot (x \cdot u_x) = (T \cdot x) \cdot (T \cdot u_x) = (x + \Delta x) \cdot T \cdot u_x$$

and likewise in the discrete case the operator T_k is *not commutative* with the approximation of x_k

$$T_k \cdot (i_k \cdot u_{x_k}) = (T_k \cdot i_k) \cdot (T_k \cdot u_{x_k}) = (i_k + 1) \cdot T_k \cdot u_{x_k}$$

and thus

$$T_k \cdot i_k = (i_k + 1) \cdot T_k$$

for all $k \in \{1, \dots, n + 1\}$. This reasoning takes place when dealing with arbitrary non-constant functions.

Concerning the above remark and, consequently, the lacking property of commutativity in the case of occurring non-constant functions we assume for future discussions from now on that coefficients are constant and therefore $C_1 = C_1^c$.

Next we describe the procedure to generate and define a finite difference scheme:

Definition 2.10. Let S^δ , A^δ and the sets M^δ , L^δ be as above and let $<$ be a monomial ordering on the difference ring

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta]$$

Moreover, assume that the sufficiency for scheme generation is provided. Then D , defined via

$$D := (\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle_{D_2}) \cap \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [(\Lambda^\delta \cup M^\delta) \setminus L^\delta]$$

is called a *finite difference scheme ideal*.

Remark 2.11. Note, that we do not require the ideals $\langle S^\delta \rangle_{D_2}$ and $\langle A^\delta \rangle_{D_2}$ to be *difference ideals* in the definition above, so we can make several observations due to 2.10:

Clearly D is an *ideal* in the ring D_2 . That is

$$a_1 + a_2 \in D \quad \wedge \quad m \cdot a_1 \in D_2 \quad \forall a_1, a_2 \in D \quad \forall m \in D_2$$

But $D \trianglelefteq D_2$ is not necessarily a *difference ideal*, i.e. an ideal with the property

$$\Delta_i \circ f \in D \quad \forall f \in D \quad \forall \Delta_i$$

where the Δ_i are the occurring difference operators.

The ideal in 2.10 gives rise to work with Gröbner bases and the underlying theory, since all the objects defined so far are computable by means of computer algebra and its corresponding algorithms.

Since $\mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) = \mathbb{K}$ is a field, we can answer the question why the ideal

$$D \trianglelefteq \mathbb{K} [(\Lambda^\delta \cup M^\delta) \setminus L^\delta]$$

is called a *finite difference scheme* by stating the following lemma:

Lemma 2.12. *In the case of*

$$|(\Lambda^\delta \cup M^\delta) \setminus L^\delta| = 1$$

the ideal D is a principal ideal, that is

$$D = \langle d \rangle_{D_2}$$

and d is unique up to multiplication with constants.

Proof. As the ground ring is a field, the above statement is elementary commutative algebra (confer [1]). \square

In this case one can speak of *the* finite scheme like in the classical case and one can identify the ideal D with its unique generator d .

If

$$|(\Lambda^\delta \cup M^\delta) \setminus L^\delta| \geq 2$$

then D is not an ideal in a principal ideal domain and in general cannot be generated by exactly one element. This case would lead to a situation in which we deal with a system of equations in the corresponding ring.

Remark 2.13. Philosophy of 2.10: In a scheme we want all variables that are being approximated by others to be eliminated. Only those variables that do not have a given approximation remain in the final scheme.

We give an example of 2.10 and how to use Singular [6] in this context:

Example 2.14. *Take a look at the well known Cauchy problem*

$$u_t + a \cdot u_x = 0$$

Here we can choose $C_1 = \mathbb{F}(a) = C_1^c$ and want to approximate the derivatives u_t, u_x by simple difference quotients and with $k = \Delta t, h = \Delta x$:

$$u_t = \frac{u(x, t+k) - u(x, t)}{k} = \frac{T_t \circ u - u}{k}$$

respectively

$$u_x = \frac{u(x+2h, t) - u(x, t)}{2h} = \frac{T_x^2 \circ u - u}{2h}$$

In our terminology we can express this as follows:

$$S^\delta = \{u_t + au_x\}$$

and

$$A^\delta = \{k \cdot u_t - (T_t - 1)u, 2h \cdot u_x - (T_x^2 - 1)u\}$$

Note, that we do not distinguish between \cdot and \circ here and allow invertible coefficients h, k for u_x and u_t . So we have

$$L^\delta = \{u_t, u_x\} \subsetneq \{u_t, u_x, u\} = M^\delta$$

To compute the scheme according to 2.10 in Singular we need the suitable ring $A = \mathbb{Q}(a, h, k)[u_t, u_x, u]$ and an ordering $<$ due to 2.5. In Singular we proceed by introducing additional variables T_t and T_x (shift operators) coming together with a block-ordering that makes them subordinate to u_t, u_x, u :

```
> ring A=(0,a,h,k),(Ut,Ux,U,Tt,Tx),(lp(3),lp);
```

then initialize the ideals:

```
> ideal S=Ut+a*Ux;
> ideal L=Ut-(Tt-1)/k*U,Ux-(Tx^2-1)/(2*h)*U;
> ideal I=S+L; //this is the union of S and L
```

Next we compute the scheme

$$(\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle_{D_2}) \cap \mathbb{F} \otimes C_1^\delta \otimes C_2(\underline{T}) [(\Lambda^\delta \cup M^\delta) \setminus L^\delta]$$

i.e. we eliminate the first two variables u_t and u_x from the ideal:

```
> eliminate(I,intvec(1,2));
_[1]=(2*h)*U*Tt+(a*k)*U*Tx^2+(-a*k-2*h)*U
```

Depending on the taste of the user one could have computed the reduction of the generator of S^δ by the generators of A^δ to receive the same polynomial modulo multiplication with $2hk$:

```
> reduce(S,std(L));
_[1]=1/(k)*U*Tt+(a)/(2*h)*U*Tx^2+(-a*k-2*h)/(2*h*k)*U
```

The equality test

```
> reduce(S,L)[1]*2hk==eliminate(I,intvec(1,2))[1];
1
```

confirms our statement above. Finally we get the scheme

$$\left(T_t - 1 + \frac{ak}{2h} (T_x^2 - 1) \right) \circ u$$

or equivalently

$$T_t \circ u = u - \frac{ak}{2h} \cdot (T_x^2 \circ u - u)$$

respectively

$$u_i^{j+1} = u_i^j - \frac{ak}{2h} \cdot (u_{i+2}^j - u_i^j)$$

in the nodal form. The stencil of this scheme is shown in figure 4. For details of computation, see example 4.1.

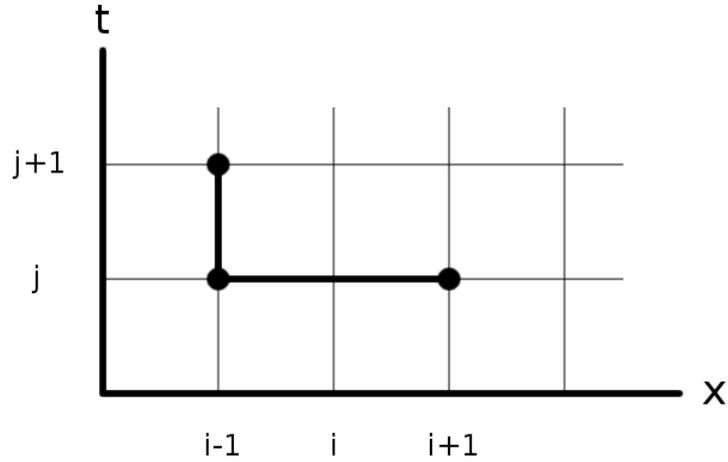


FIGURE 4. Stencil of the scheme in example 2.14

Below we shall illustrate the computation of the Lax-Wendroff-scheme within a Singular session:

Example 2.15. Consider the Cauchy problem

$$S^\delta = \{u_t + a \cdot u_x\}$$

as above with the forward approximation for the time

$$(u_t)_i^j = \frac{u_i^{j+1} - u_i^j}{k}$$

and a weighted mixture of upwind and downwind approximations for the space direction

$$(u_x)_i^j = \theta \frac{u_i^j - u_{i-1}^j}{h} + (1 - \theta) \frac{u_{i+1}^j - u_i^j}{h}$$

along with the weights

$$\theta = \frac{1 + \frac{ak}{h}}{2} \quad (1 - \theta) = \frac{1 - \frac{ak}{h}}{2}$$

So we have

$$A^\delta = \left\{ u_t - \frac{(T_t - 1)}{k} u, u_x - \frac{(1 + \frac{ak}{h})(1 - T_x^{-1})}{2h} u - \frac{(1 - \frac{ak}{h})(T_x - 1)}{2h} u \right\}$$

Note that we use shift operators both in positive and negative direction, since they occur in the approximations. Accordingly we define the ring

> ring A=(0,a,h,k),(Ut,Ux,U,Ttp,Ttm,Txp,Txm),(lp(3),lp);

and assure that the interaction of shift operators works correctly with the ideal

> ideal C=Ttp*Ttm-1,Txp*Txm-1;

Then declare S^δ and A^δ :

> ideal S=Ut+a*Ux;

> ideal L=Ut-(Ttp-1)*1/k*U,Ux-1/2*(1+k/h*a)*(1-Txm)/h*U
-1/2*(1-k/h*a)*(Txp-1)/h*U;

and eliminate the first two variables u_t and u_x from the ideal

$$\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle_{D_2}$$

in the basering:

> ideal I=reduce(S+L,std(C));

> intvec v=1,2;

> reduce(eliminate(I,v),std(C));

_ [1]=(-2*h^2)*U*Ttp+(a^2*k^2-a*h*k)*U*Txp+(a^2*k^2+a*h*k)*U*Txm
+(-2*a^2*k^2+2*h^2)*U

As mentioned above one can calculate the same result with the aid of reducing S^δ by A^δ

> reduce(reduce(S,std(L)),std(C));

_ [1]=1/(k)*U*Ttp+(-a^2*k+a*h)/(2*h^2)*U*Txp
+(-a^2*k-a*h)/(2*h^2)*U*Txm+(a^2*k^2-h^2)/(h^2*k)*U

Both results differ from each other only up to the constant $(-2h^2k)$:

> reduce(reduce(S,std(L)),std(C))[1]*-2*h^2*k

==reduce(eliminate(I,v),std(C))[1];

1

So finally we obtain with $c = \frac{ak}{h}$ the scheme

$$T_t u_t = T_x u \frac{(c^2 - c)}{2} + u(1 - c^2) + T_x^{-1} u \frac{(c^2 + c)}{2}$$

or in traditional form:

$$u_i^{j+1} = u_{i+1}^j \frac{(c^2 - c)}{2} + u_i^j (1 - c^2) + u_{i-1}^j \frac{(c^2 + c)}{2}$$

Figure 5 displays the relation of the grid points.
For details on computation, see 4.2.

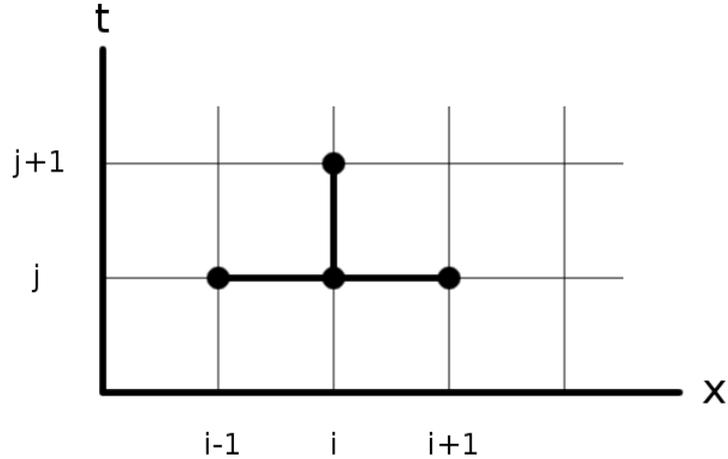


FIGURE 5. Stencil of the Lax-Wendroff-scheme in example 2.15

3. DISCUSSION

In this section we want to give some hints how to understand the proposed notations. Our reasoning will be based upon computer algebraic concepts.

For that reason we will give the relevant definitions in order to remind the reader of Gröbner bases. For more detailed explanations and examples confer [1].

Remark 3.1. Let $f \in K[x_1, \dots, x_n]$ be an arbitrary polynomial and $<$ a monomial ordering. Then f can uniquely be written as

$$f = a_\alpha \cdot x^\alpha + a_\beta \cdot x^\beta + \dots + a_\gamma \cdot x^\gamma$$

with $a_\alpha, a_\beta, a_\gamma \neq 0$ and

$$x^\alpha > x^\beta > \dots > x^\gamma$$

The (with respect to $<$) biggest term x^α is called the *leading term* of f or simply $lt(f)$.

An easy example for two different orderings shall be demonstrated with the polynomial $f = x^3 - 3x^2y^5 + xy^7 \in K[x, y]$. Note that $\text{Mon}_{K[x,y]} = \mathbb{N}^2$, $x = (1, 0)$ and $y = (0, 1)$ respectively.

(1) \leq_{l_p} with

$$(\alpha_1, \alpha_2) >_{l_p} (\beta_1, \beta_2) : \iff \exists 1 \leq i \leq 2 :$$

$$\alpha_1 = \beta_1, \dots, \alpha_{i-1} = \beta_{i-1}, \alpha_i > \beta_i$$

then

$$\text{lt}(f) = x^3 \text{ and } \text{tail}(f) = -3x^2y^5 + xy^7$$

(2) \leq_{D_p} with

$$(\alpha_1, \alpha_2) >_{D_p} (\beta_1, \beta_2) : \iff \sum_i \alpha_i > \sum_i \beta_i$$

$$\text{or } \left(\sum_i \alpha_i = \sum_i \beta_i \text{ and } \exists 1 \leq i \leq 2 : \right.$$

$$\left. \alpha_1 = \beta_1, \dots, \alpha_{i-1} = \beta_{i-1}, \alpha_i > \beta_i \right)$$

$$\text{lt}(f) = xy^7 \text{ and } \text{tail}(f) = -3x^2y^5 + x^3$$

Definition 3.2. Let $M \subseteq K[x_1, \dots, x_n]$ be any subset. The ideal

$$L(G) := \langle \text{lm}(g) \mid g \in G \setminus \{0\} \rangle_{K[x_1, \dots, x_n]}$$

is called the *leading ideal* of G .

Example 3.3. Let $G = \{x^2 - y, xy - y^2\}$ be a finite set and an ordering \leq_{l_p} with $y < x$. Then we have

$$L(G) = \langle x^2, xy \rangle_{K[x,y]} = \{f \cdot x^2 + g \cdot xy \mid f, g \in K[x, y]\}$$

Definition 3.4. Let $I \trianglelefteq A = K[x_1, \dots, x_n]$ be an ideal, $G \subseteq A$ a finite subset. Then G is called a *Gröbner basis* of I for a *global* ordering \preceq (i.e. well-ordering) if

$$G \subset I \quad \wedge \quad L(I) = L(G)$$

the last condition means that

$$\forall f \in I \quad \exists g \in G \quad lm(g) \mid lm(f)$$

We want to stress the fact that a Gröbner basis exists and is a finite set in the ring A .

Definition 3.5. A monomial ordering $<$ on a polynomial ring $A = \mathbb{K}[x_1, \dots, x_k, x_{k+1}, \dots, x_n]$ is called an *elimination ordering* for x_1, \dots, x_k , if it has the *elimination property* for the first k variables, that is

$$lm(g) \in \mathbb{K}[x_{k+1}, \dots, x_n] \quad \implies \quad g \in \mathbb{K}[x_{k+1}, \dots, x_n]$$

for any polynomial $g \in A$.

Elimination property assures that the non-occurrence of a suitable subset of variables in the leading monomial of a polynomial is sufficient for the membership of this polynomial in a subring not involving these variables anymore. A very prominent representant of these elimination orderings is $<_{lp}$ as defined above.

We next give a lemma that describes the interplay of elimination orderings and Gröbner bases and omit the proof (confer [1]):

Lemma 3.6.

Let $<$ be an elimination ordering in the ring $\mathbb{K}[x_1, \dots, x_k, x_{k+1}, \dots, x_n]$ for the variables x_1, \dots, x_k . Consider the Gröbner basis G of the ideal $I \leq \mathbb{K}[x_1, \dots, x_n]$. Then the set

$$\tilde{G} := \{g \in G \mid lm(g) \in \mathbb{K}[x_{k+1}, \dots, x_n]\} \subset \mathbb{K}[x_{k+1}, \dots, x_n]$$

is a Gröbner basis of

$$\tilde{I} := I \cap \mathbb{K}[x_{k+1}, \dots, x_n]$$

□

The concept of a *normal form* is essential for our further discussion:

Definition 3.7. Let $\mathcal{G} = \{G \mid G = \{g_1, \dots, g_s\} \subset A \text{ is finite}\}$. A *normal form* NF is a map

$$NF: A \times \mathcal{G} \longrightarrow A \quad (f, G) \longmapsto NF(f|G)$$

with the following characteristics: $\forall f \in A$ and $\forall G \in \mathcal{G}$

1. $NF(0|G) = 0$

2. $NF(f|G) \neq 0 \Rightarrow lm(NF(f|G)) \notin L(G)$
3. $f - NF(f|G)$ has *standard representation* with respect to $NF(\dots|G)$ i.e.

$$f - NF(f|G) = \sum_{k=1}^s a_k g_k$$

with $a_k \in A$ and $s \geq 0$, such that

$$lm\left(\sum_{k=1}^s a_k g_k\right) \geq lm(a_k g_k) \quad \forall k \text{ with } a_k g_k \neq 0$$

NF is called a *reduced*, if $NF(f|G)$ is reduced with respect to G for any polynomial $f \in A$. That means, no monomial of the power series expansion of $NF(f|G)$ is an element of $L(G)$. Confer [1] for further details.

Again without proof (see [1]) we state conditions for an extremely useful property of a normal form:

Theorem 3.8. *Let $NF(\dots|G)$ a reduced normal form and $G \subseteq A$ a standard basis of $\langle G \rangle_A$. Then NF is unique. \square*

Definition 3.9. Let $a, b \in K[x_1, \dots, x_n]$ be polynomials with

$$lt(a) = lc(a) lm(a) = lc(a) x^\alpha \quad lt(b) = lc(b) lm(b) = lc(b) x^\beta$$

and let

$$\gamma := lcm(lm(\alpha), lm(\beta)) := (\max(\alpha_1, \beta_1), \dots, \max(\alpha_n, \beta_n))$$

be the least common multiple of the leading monomials, then define the *spoly* via

$$spoly(a, b) := x^{\gamma-\alpha} a - \frac{lt(a)}{lt(b)} \cdot x^{\gamma-\beta} b$$

Remember the set A^δ , the set of formal approximations for the equation in S^δ . If the monomial ordering $<$ is sufficient for scheme generation, we can state some interesting property of A^δ :

Lemma 3.10. A^δ is a Gröbner basis with respect to the ordering $<$

Proof. Since all leading monomials u_{x^β} are pairwise distinct variables in the ring

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta]$$

we see on account of the product criterion (3.11) that A^δ is a Gröbner basis with respect to the ordering $<$. \square

The reasoning of 3.10 can be seen via the following lemma:

Lemma 3.11. *Let a and b be two polynomials with the property*

$$lm(a) \cdot lm(b) = lcm(lm(a), lm(b))$$

then

$$NF(spoly(a, b) | \{a, b\}) = 0$$

where $NF(\dots | \{a, b\})$ denotes a normal form.

Proof. This is a simple consequence and follows by looking at the reduction process and the construction of the *spoly* (see [1]). \square

We can state an obvious consequence of the above lemma as follows:

Corollary 3.12. *In particular, 3.11 means that $\{a, b\}$ is a Gröbner basis of the ideal $\langle a, b \rangle$.*

3.10 and 3.8 give rise to a very crucial observation:

Theorem 3.13. *Let $S^\delta = \{h\}$ any partial differential equation in an unknown function u and let A^δ be a set of approximations that is sufficient for scheme generation with a suitable ordering $<$ on the monomials of the ring*

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta] = \mathbb{K}(\underline{T}) [\Lambda^\delta \cup M^\delta]$$

as defined in 2.5 and the ordering $<$ with the elimination property (3.5) for the set L^δ . Let as before L^δ be the set of the occurring derivatives on the left hand side in A^δ , M^δ denote the set of all derivatives in A^δ and finally Λ^δ consist in all derivatives of h . And these sets shall have the property

$$|(\Lambda^\delta \cup M^\delta) \setminus L^\delta| = 1$$

Then there are two equivalent ways to compute the finite difference scheme from the given set:

- (1) $h \xrightarrow{\text{reduce}} NF(h|A^\delta) = a_1 \in D_2$
- (2) $(\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle_{D_2}) \cap \mathbb{K}(\underline{T}) [(\Lambda^\delta \cup M^\delta) \setminus L^\delta] = \langle a_2 \rangle_{D_2}$

With equivalent we mean the identity of a_1 and a_2 up to multiplication with constants:

$$a_1 = c \cdot a_2$$

Proof. Let without loss of generality $\Lambda^\delta \cup M^\delta = \{u_m, \dots, u_1, u\}$ and $(\Lambda^\delta \cup M^\delta) \setminus L^\delta = \{u\}$ holding the order $u_m > \dots > u_1 > u$. As a reduced normal form the reduced Buchberger Algorithm with tail reduction shall be chosen as a reduced normal form ([1] for details). The main iterative reduction step is performed by computing the appropriate *spoly*

$$\text{spoly}(h, m) = h - \frac{\text{lc}(h)}{\text{lc}(m)} \cdot \underline{u}^{\alpha-\beta} m$$

for an element $m \in A^\delta$, with $\text{lm}(m) = \underline{u}^\alpha | \underline{u}^\beta = \text{lm}(h)$ being provided by the set of approximations A^δ . Then clearly

$$\text{lm}(\text{spoly}(h, m)) < \text{lm}(h)$$

and during the reduction process one receives a sequence of leading monomials that becomes stationary:

$$\text{lm}(h) > \text{lm}(h_1) > \dots > \text{lm}(h_s)$$

Claim: $h_s = u$. This is obvious, since the approximations in A^δ give adequate substitutions for each occurring derivative and these are the ring variables. The assumption in the theorem statement assures that the claim holds true and consequently

$$h \in \mathbb{K}(\underline{T})[u]$$

Besides, a normal form has standard representation and hence

$$h \in (\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle_{D_2})$$

Here it is important that the normal form is *reduced* so the property of uniqueness is guaranteed (by 3.8), since furthermore the fact that A^δ is a Gröbner basis on account of 3.10 can be exploited in this context. After reduction the set $A^\delta \cup \{h\}$ is a Gröbner basis of $\langle A^\delta \cup \{h\} \rangle_{D_2}$ due to the Buchberger criterion (confer [1]) and with the reasoning above we see, that

$$(A^\delta \cup \{h\}) \cap \mathbb{K}(\underline{T})[u] = \{h\}$$

and is moreover a Gröbner basis for $(\langle S^\delta \rangle_{D_2} + \langle A^\delta \rangle) \cap \mathbb{K}(\underline{T})[u]$. Since the ring D_2 is a principal ideal domain we observe that every ideal has one unique generator up to multiplication with constants and hence the proof is done. \square

Suitable examples that show the computation in these two proposed ways of 3.13 are given in 4.1 and 4.2. The equality can be seen there easily.

Remark 3.14. Note, that we do not assume additional properties to our definition of schemes except the existence of an ordering that suffices for scheme generation. We do not exclude non-linear partial differential equations from our treatment, quite the contrary they are allowed explicitly. This is a fundamental difference between our attempt and, for instance, the Janet bases approach of V. Gerdt in [5] or the module approach of V. Levandovskyy in [3].

But for one linear partial differential equation with the characteristic of constant coefficients these three strategies are indeed equivalent according to a theorem in [3].

Remark 3.15. The generation of a scheme with an underlying partial differential equation of two or more unknown functions u, v, w etc. instead of the case with one single unknown function u is possible. Warning: the condition 2.5 is imposed to be valid for each function separately. I.e. we have to work in a ring

$$A = R[M_u, M_v, \dots, M_w]$$

with a suitable *block ordering*.

Remark 3.16. If $|S^\delta| > 1$, i.e. the case of several partial differential equations in the same unknown function, the problem of scheme generation can be reduced to the case of one equation by treating these separately i.e.

$$S^\delta = \{s_1^\delta, \dots, s_m^\delta\} = \{s_1^\delta\} \cup \dots \cup \{s_m^\delta\} = S_1^\delta \cup \dots \cup S_m^\delta$$

and receiving distinct schemes for each S_j^δ . For the several S_j^δ certain approximations A_j^δ have to be used that must be compatible to each other. Confer [5] for more material.

The following theorem describes two ways of computing difference schemes for a system of partial differential equations in several unknown functions if one single set of approximations is valid for the

occurring derivatives in all equations.

Theorem 3.17. *Let $S^\delta = \{s_1^\delta, \dots, s_N^\delta\}$ be the set of N distinct partial differential equations of M unknown functions $\underline{U} = \{u_1, \dots, u_M\}$ with the common approximations $A^\delta = \{a_1, \dots, a_k\}$ and let, moreover, the sufficiency of scheme generation be imposed on A^δ for each equation s_j^δ . Let as before Λ^δ be the set of derivatives in S^δ , M^δ denote all derivatives in A^δ and finally L^δ be all derivatives on the left hand side in the approximations such that*

$$(\Lambda^\delta \cup M^\delta) \setminus L^\delta = \underline{U}$$

and recall the ring D_2 as in 3.13

$$D_2 = \mathbb{F} \otimes_{\mathbb{F}} C_1^\delta \otimes_{\mathbb{F}} C_2(\underline{T}) [\Lambda^\delta \cup M^\delta] = \mathbb{K}(\underline{T}) [\Lambda^\delta \cup M^\delta]$$

Consider the following definitions for the ideals I_1 and I_2 :

(1)

$$I_1 = (\langle G \rangle_{D_2}) \cap \mathbb{K}(\underline{T}) [\underline{U}]$$

where G is a Gröbner basis of $S^\delta \cup A^\delta$ with respect to an elimination ordering

(2)

$$I_2 = (\langle h_1, \dots, h_N \rangle_{D_2} + \langle A^\delta \rangle_{D_2}) \cap \mathbb{K}(\underline{T}) [\underline{U}]$$

where $h_j = NF(s_j^\delta | A^\delta)$ for all j

Claim:

$$I_1 = I_2$$

Proof. The proof is obvious and follows simple reasoning in ideal theory. \square

Remark 3.18. Note that in $\mathbb{K}(\underline{T}) [\underline{U}]$ there do not occur any derivatives, since they are cancelled out by the approximations with the property of scheme sufficiency and on account of $(\Lambda^\delta \cup M^\delta) \setminus L^\delta = \underline{U}$.

It is clear that $h_j \in \mathbb{K}(\underline{T}) [\underline{U}]$ for these reasons and hence $h_j \in I_2 \forall j$. Moreover, $\{h_j\} \cup A^\delta$ is a Gröbner basis, but the set $\{h_1, \dots, h_N\} \cup A^\delta$ is in general not necessarily a Gröbner basis of $\langle h_1, \dots, h_N \rangle_{D_2} + \langle A^\delta \rangle_{D_2}$.

These two methods differ from a principal and from a practical point of view: the first ideal I_1 is computed by Gröbner basis computation of the whole union $S^\delta \cup A^\delta$ with all equations being involved, whereas the ideal I_2 is computed by calculating the several Gröbner bases $\{h_j\} \cup A^\delta$ independently from each other. The complexity of the first approach may be significantly higher than of the second one. The advantage

may be that certain hidden constraints between the objects are detected which may become lost in the second case that is known to be the classical one.

Remark 3.19. Note, that this paper does not focus on the convergence theory of numerical schemes. Algebraically this aspect is subordinate (though of high relevance in practice) and our intention is to give a general way of numerical scheme generation. For more details see [4] and [2].

4. EXAMPLES WITH SINGULAR

In this section we calculate the concrete examples with SINGULAR ([6]).

Example 4.1. *This example computes 2.14 in SINGULAR.*

```
> ring A=(0,a,h,k),(Ut,Ux,U,Tt,Tx),(lp(3),lp);
> ideal S=Ut+a*Ux;
> ideal L=Ut-(Tt-1)/k*U,Ux-(Tx^2-1)/(2*h)*U;
> ideal I=S+L;
> eliminate(I,intvec(1,2));
_[1]=(2*h)*U*Tt+(a*k)*U*Tx^2+(-a*k-2*h)*U
> reduce(S,std(L));
_[1]=1/(k)*U*Tt+(a)/(2*h)*U*Tx^2+(-a*k-2*h)/(2*h*k)*U
> reduce(S,L)[1]*2hk==eliminate(I,intvec(1,2))[1];
1
```

Example 4.2. *This example computes 2.15 in SINGULAR.*

```
> ring A=(0,a,h,k),(Ut,Ux,U,Ttp,Ttm,Txp,Txm),(lp(3),lp);
> ideal C=Ttp*Ttm-1,Txp*Txm-1;
> ideal S=Ut+a*Ux;
> ideal L=Ut-(Ttp-1)*1/k*U,Ux-1/2*(1+k/h*a)*(1-Txm)/h*U
-1/2*(1-k/h*a)*(Txp-1)/h*U;
> ideal I=reduce(S+L,std(C));
> intvec v=1,2;
> reduce(eliminate(I,v),std(C));
_[1]=(-2*h^2)*U*Ttp+(a^2*k^2-a*h*k)*U*Txp+(a^2*k^2+a*h*k)*U*Txm
```

```

+(-2*a^2*k^2+2*h^2)*U
> reduce(reduce(S,std(L)),std(C));
_[1]=1/(k)*U*Ttp+(-a^2*k+a*h)/(2*h^2)*U*Txp
+(-a^2*k-a*h)/(2*h^2)*U*Txm+(a^2*k^2-h^2)/(h^2*k)*U
> reduce(reduce(S,std(L)),std(C))[1]*-2*h^2*k
==reduce(eliminate(I,v),std(C))[1];
1

```

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TECHNISCHE UNIVERSITÄT KAISERSLAUTERN, KAISERSLAUTERN, GERMANY
E-mail address: dingler@mathematik.uni-kl.de

RWTH AACHEN, AACHEN, GERMANY
E-mail address: Viktor.Levandovskyy@math.rwth-aachen.de