Gröbner Bases Applied to Generation of Difference Schemes for PDEs

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Introduction

Though partial differential equations (PDEs) may admit some explicit closed-form solutions, in practice one has to solve them numerically.

Example: the Laplace equation $\triangle u(x,y) := u_{xx} + u_{yy} = 0$ has exact solutions

$$u = (x+a)^2-(y+b)^2,\ u = e^{x+a}cos(y+b),\ u = \log[(x+a)^2+(y+b)^2],\ldots$$

The Dirichlet problem

$$\forall (x,y) \in \Omega\ :\ \triangle u(x,y) = 0, \quad \forall (x,y) \in \partial\Omega\ :\ u(x,y) = f(x,y),$$

where $\partial\Omega$ is the boundary of domain Ω and $f(x,y)$ is a given function, can be solved only numerically.

Introduction (cont.)

Finite differences along with finite elements and finite volumes are most important discretization schemes for numerical solving of PDEs.

Mathematical operations used in the construction of difference schemes are substantially symbolic.

Thereby, it is a challenge to computer algebra to provide an algorithmic tool for automatization of the difference schemes constructing as well as for investigating properties of the difference schemes. In (Gerdt, Blinkov, Mozzhilkin'06) we suggest difference elimination to generate the schemes.

Introduction (cont.)

One of the most fundamental requirements for a difference scheme is its stability which can be analyzed with the use of computer algebra methods and software (Ganzha, Vorozhtsov'96; Gerdt, Blinkov, Mozzhilkin'06).

Furthermore, if PDEs admit a conservation law form or/and have some symmetries, it is worthwhile to preserve these features at the level of difference schemes too.

In particular, a tool for automatic construction of difference schemes should produce conservative schemes whenever the original PDEs can be written in the integral conservation law form.

Basic Idea: Conservation Law Form

A wide class of PDEs can be written in the conservation law form

$$\frac{\partial \mathbf{v}}{\partial x} + \frac{\partial}{\partial y}\mathbf{F}(\mathbf{v}) = 0$$

Here $\mathbf{v}$ is a $m-$vector function in unknown $n-$vector function $\mathbf{u}$ and its partial derivatives $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_{xx} \ldots$; $\mathbf{F}$ is a function that maps R^m into R^m.

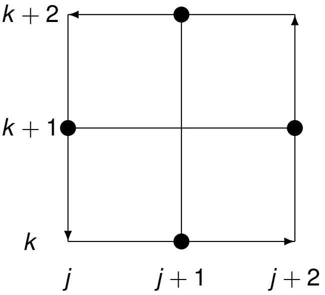
By Green's theorem (curl theorem in the plane), the above equation is equivalent to

$$\oint_{\Gamma} -\mathbf{F}(\mathbf{v})dx + \mathbf{v}dy = 0\,.$$

where Γ is arbitrary closed contour.

Basic Idea: Discretization

We set $\mathbf{u}(x,y) = \mathbf{u}(x_j, y_k) \equiv \mathbf{u}_{j\,k},\ \mathbf{u}_x(x,y) = \mathbf{u}_x(x_j, y_k) \equiv (\mathbf{u}_x)_{j\,k}, \ldots$,
choose the integration contour, e.g.,



and add the relations

$$\int_{x_j}^{x_{j+2}} \mathbf{u}_x dx = \mathbf{u}(x_{j+2}, y) - \mathbf{u}(x_j, y),\quad \int_{y_k}^{y_{k+2}} \mathbf{u}_y dy = \mathbf{u}(x, y_{k+2}) - \mathbf{u}(x, y_k), \ldots .$$

Basic Idea: Difference Elimination

Using a numerical integration method, e.g. the midpoint one, with

$$x_{j+1} - x_j = y_{k+1} - y_k = \triangle h$$

we rewrite the equations and the relations as

$$\begin{array}{c} -(\mathbf{F}(\mathbf{v})_{j+1\,k} - \mathbf{F}(\mathbf{v})_{j+1\,k+2}) + (\mathbf{v}_{j+2\,k+1} - \mathbf{v}_{j\,k+1}) = 0, \\ (\mathbf{u}_x)_{j+1\,k} \cdot 2\triangle h = \mathbf{u}_{j+2\,k} - \mathbf{u}_{j\,k}, \\ (\mathbf{u}_y)_{j\,k+1} \cdot 2\triangle h = \mathbf{u}_{j\,k+2} - \mathbf{u}_{j\,k}, \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \end{array}$$

A fully conservative difference scheme for $\mathbf{u}$ is obtained by elimination of all partial derivatives $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_{xx}, \ldots$. The elimination can be achieved by constructing a Gröbner basis (GB), if they exist (finite), e.g., for linear PDEs.

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Rings of Difference Polynomials

Let $\{y^1, \ldots, y^m\}$ be the set of *difference indeterminates*, e.g. functions of $n-$variables $\{x_1, \ldots, x_n\}$, and $\theta_1, \ldots, \theta_n$ be the set of mutually commuting *difference operators (differences)*, e.g.,

$$\theta_i \circ y^j = y^j(x_1, \ldots, x_i + 1, \ldots, x_n).$$

A *difference ring R with differences $\theta_1, \ldots, \theta_n$* is a commutative ring R with a unity such that $\forall f, g \in R,\ 1 \leq i, j \leq n\ \theta_i \circ f \in R$ and

$$\theta_i\theta_j = \theta_j\theta_i,\ \theta_i \circ (f + g) = \theta_i \circ f + \theta_i \circ g,\ \theta_i \circ (f\,g) = (\theta_i \circ f)(\theta_i \circ g)$$

Similarly one defines a *difference field*.

Rings of Difference Polynomials (cont.)

Let $\mathbb{K}$ be a difference field. Denote by $\mathbb{R} := \mathbb{K}\{y^1, \ldots, y^m\}$ the difference ring of polynomials over $\mathbb{K}$ in variables

$$\{\ \theta^\mu \circ y^k \ \mid \mu \in \mathbb{Z}^n_{\geq 0},\ k = 1, \ldots, m\ \}\,.$$

Denote by $\mathbb{R}_L$ the set of linear polynomials in $\mathbb{R}$ and use the notations

$$\Theta = \{\ \theta^\mu \ \mid\ \mu \in \mathbb{Z}^n_{\geq 0}\ \},.$$

A *difference ideal* I in $\mathbb{R}$ is an ideal $I \in \mathbb{R}$ close under the action of any operator from Θ. If $F := \{f_1, \ldots, f_k\} \subset \mathbb{R}$ is a finite set, then the smallest difference ideal containing F denoted by $\mathrm{Id}(F)$. If $F \subset \mathbb{R}_L$, then $\mathrm{Id}(F)$ is *linear difference ideal*.

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Ranking

A total ordering $\prec$ over the set of $\theta_\mu y^j$ is a *ranking* if it satisfies

1. $\theta_i \theta^\mu \circ y^j \succ \theta^\mu \circ y^j$
2. $\theta^\mu y^j \succ \theta^\nu \circ y^k \quad \Longleftrightarrow \quad \theta_i \theta^\mu \circ y^j \succ \theta_i \theta^\nu \circ y^k \quad \forall\, i, j, k, \mu, \nu.$

If $\mu \succ \nu \Longrightarrow \theta_\mu \circ y^j \succ \theta_\nu \circ y^k$ the ranking is *orderly*.
If $i \succ j \Longrightarrow \theta_\mu \circ y^j \succ \theta_\nu \circ y^k$ the ranking is *elimination*.

Given a ranking $\succ$,

- every linear polynomial $f \in \mathbb{R}_L \setminus \{0\}$ has the *leading term* $a\,\theta \circ y^j$, $\theta \in \Theta$;
- $\mathrm{lc}(f) := a \in \mathbb{K} \setminus \{0\}$ is the *leading coefficient*;
- $\mathrm{lm}(f) := \theta \circ y^j$ is the *leading monomial*.

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Gröbner Bases

Given nonzero linear difference ideal $I = \mathrm{Id}(G)$ and term order $\succ$, its generating set $G = \{g_1, \dots, g_s\} \subset \mathbb{R}_L$ is a *Gröbner basis* (GB) (Buchberger,Winkler'98; Kondratieva,Levin,Mikhalev,Pankratiev'99) of I if

$$\forall f \in I \cap \mathbb{R}_L \setminus \{0\}\ \exists g \in G, \theta \in \Theta \ :\ \mathrm{lm}(f) = \theta \circ \mathrm{lm}(g)\,.$$

It follows that $f \in I$ *is reducible modulo G*

$$f \underset{g}{\longrightarrow} f' := f - \mathrm{lc}(f)\,\theta \circ (g/lc(g)), \quad f' \in I, \dots, \quad f \underset{G}{\longrightarrow} 0\,.$$

In our algorithmic construction of GB we shall use a restricted set of reductions called *Janet-like* (Gerdt, Blinkov'05)

Based on these reductions an involutive algorithm that computes **Janet-like Gröbner bases** has been implemented in Maple (Gerdt, Robertz'06) extends the polynomial algorithm (Gerdt, Blinkov'05) to linear difference ideals.

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Laplace Equation

Consider the Laplace equation $u_{xx} + u_{yy} = 0$ and rewrite it as the conservation law

$$\oint_{\Gamma} -u_y dx + u_x dy = 0\,.$$

Add the integral relations

$$\int_{x_j}^{x_{j+2}} u_x dx = u(x_{j+2}, y) - u(x_j, y), \;\; \int_{y_k}^{y_{k+2}} u_y dy = u(x, y_{k+2}) - u(x, y_k)\,.$$

Thus, we obtain 3 integral relations for 3 unknown functions

$$u(x, y),\;\; u_x(x, y),\;\; u_y(x, y)\,.$$

Laplace Equation (cont.)

Choose the midpoint integration method for above rectangular contour.

This yields the discrete system

$$\left\{\begin{array}{c} -((u_y)_{j+1\,k} - (u_y)_{j+1\,k+2}) + ((u_x)_{j+2\,k+1} - (u_y)_{j\,k+1}) = 0, \\ (u_x)_{j+1\,k} \cdot 2\triangle h = u_{j+2\,k} - u_{j\,k}, \\ (u_y)_{j\,k+1} \cdot 2\triangle h = u_{j\,k+2} - u_{j\,k}. \end{array}\right.$$

Its difference form is

$$\left\{\begin{array}{l} (\theta_x\theta_y^2 - \theta_x) \circ u_y + (\theta_x^2\theta_y - \theta_y) \circ u_x = 0\,, \\ 2\triangle h\,\theta_x \circ u_x - (\theta_x^2 - 1) \circ u = 0\,, \\ 2\triangle h\,\theta_y \circ u_y - (\theta_y^2 - 1) \circ u = 0\,. \end{array}\right.$$

Laplace Equation (cont.)

Computation of GB for elimination order with $u_x \succ u_y \succ u$ and $\theta_x \succ \theta_y$ gives

$$\begin{cases} \theta_x \circ u_x - \frac{1}{2\triangle h}\,(\theta_x^2 - 1) \circ u = 0\,, \\ \theta_y \circ u_x + \theta_x \circ u_y - \frac{1}{2\triangle h}\,(\theta_x\theta_y((\theta_x^2 - 1) + (\theta_y^2 - 1))) \circ u = 0\,, \\ \theta_x^2 \circ u_y - \frac{1}{2\triangle h}\,(\theta_x^2\theta_y((\theta_x^2 - 1) + (\theta_y^2 - 1)) - \theta_y(\theta_x^2 - 1)) \circ u = 0\,, \\ \theta_y \circ u_y - \frac{1}{2\triangle h}\,(\theta_y^2 - 1) \circ u = 0\,, \\ \frac{1}{2\triangle h}\,(\theta_x^4\theta_y^2 + \theta_x^2\theta_y^4 - 4\theta_x^2\theta_y^2 + \theta_x^2 + \theta_y^2) \circ u = 0\,. \end{cases}$$

Laplace Equation (cont.)

The last equation gives the difference scheme written in double nodes

$$\frac{u_{j+2\,k} - 2u_{j\,k} + u_{j-2\,k}}{4\triangle h^2} + \frac{u_{j\,k+2} - 2u_{j\,k} + u_{j\,k-2}}{4\triangle h^2} = 0.$$

Similarly, the trapezoidal rule for the relation integrals generates the same difference scheme but written in ordinary nodes

$$\frac{u_{j+1\,k} - 2u_{j\,k} + u_{j-1\,k}}{\triangle h^2} + \frac{u_{j\,k+1} - 2u_{j\,k} + u_{j\,k-1}}{\triangle h^2} = 0.$$

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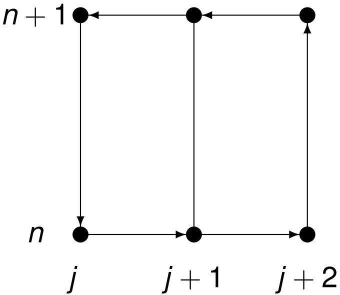
Heat Equation

Consider now the Heat equation $u_t + \alpha u_{xx} = 0$ in its conservation law form

$$\oint_{\Gamma} -\alpha u_x dt + u dx = 0$$

Again let $u(x,t) = u(x_j, t_k)$ and choose the contour



Heat Equation (cont.)

Add the integral relation

$$\int_{x_j}^{x_{j+1}} u_x dx = u(x_{j+1}, t) - u(x_j, t),$$

and use the midpoint rule for the contour integral and the trapezoidal method for the relation integral we find two difference equations for two indeterminates u, u_x in the form

$$\begin{cases} \alpha \frac{\triangle t}{2} (1 + \theta_t - \theta_x^2 - \theta_t \theta_x^2) \circ u_x - 2\triangle h (\theta_x \theta_t - \theta_x) \circ u = 0\,, \\ \frac{\triangle h}{2} (\theta_x + 1) \circ u_x - (\theta_x - 1) \circ u = 0\,. \end{cases}$$

Heat Equation (cont.)

Eliminating u_x by means of GB we obtain the famous Crank-Nicholson scheme

$$\frac{u_j^{n+1} - u_j^n}{\triangle t} + \alpha \frac{(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (u_{j+1}^n - 2u_j^n + u_{j-1}^n)}{2\triangle h^2} = 0.$$

The same scheme is obtained for the midpoint integration method applied to the relation integral.

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Wave Equation

The Wave equation $u_{tt} - u_{xx} = 0$ in the conservation law form is

$$\oint_{\Gamma} u_x dt + u_t dx = 0$$

For the same cell contour as for Laplace equation and the same additional integral relations by applying the midpoint rule for the contour integral and the trapezoidal rule for the integral relations we obtain the operator equations

$$\begin{cases} (\theta_x - \theta_x\theta_t^2) \circ u_t + (\theta_x^2\theta_t - \theta_t) \circ u_x = 0\,, \\ \frac{\triangle h}{2}\,(\theta_x + 1) \circ u_x - (\theta_x - 1) \circ u = 0\,, \\ \frac{\triangle t}{2}\,(\theta_t + 1) \circ u_t - (\theta_t - 1) \circ u = 0\,. \end{cases}$$

They yield the well-known finite difference scheme

$$u_j^{n+1} + u_j^{n-1} - u_{j+1}^n - u_{j-1}^n = 0\,.$$

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Burgers' Equation

Consider Burgers' equation in the form

$$u_t + f_x = \nu\, u_{xx}, \quad \nu = \mathrm{const}\,,$$

where we denoted u^2 by f. Convert the this equation into the conservation law form

$$\oint_{\Gamma} (\nu u_x - f)dt + udx = 0\,,$$

choose the same rectangular contour as earlier and add the integral relation

$$\int_{x_j}^{x_{j+2}} u_x dx = u(x_{j+2}, t) - u(x_j, t)\,.$$

Burgers' Equation (cont.)

For temporal and spartial discretization steps $\triangle t$ and $\triangle h$ we obtain

$$\left\{ \begin{array}{l} \triangle h\,(\theta_x\theta_t^2 - \theta_x)\circ u - \triangle t\,(\theta_x^2\theta_t - \theta_t)\circ(\nu u_x + f) = 0\,, \\ 2\triangle h\,\theta_x \circ u_x - (\theta_x^2 - 1)\circ u = 0\,. \end{array} \right.$$

GB for the elimination order with $u_x \succ u \succ f$ and $\theta_t \succ \theta_x$ is

$$\left\{ \begin{array}{l} 2\nu\triangle t\triangle h\,\theta_t \circ u_x + 2\triangle h^2\theta_t^2(\theta_x - 1)\circ u + 2\triangle t\triangle h\theta_t(\theta_x^2 - 1)\circ f - \\ \qquad \nu\triangle t\,\theta_t\theta_x(\theta^2 - 1)\circ u = 0, \\ 2\triangle h\,\theta_x \circ u_x - (\theta_x^2 - 1)\circ u = 0, \\ 2\triangle h^2\theta_x^2(\theta_t^2 - 1)\circ u - \nu\triangle t\,\theta_t(\theta_x^4 - 2\theta_x^2 + 1)\circ u + \\ \qquad 2\triangle t\triangle h\,\theta_t\theta_x(\theta_x^2 - 1)\circ f = 0. \end{array} \right.$$

The obtained difference scheme (FTFS) is

$$\frac{u_{j+2}^{n+2} - u_{j+2}^{n}}{\triangle t} - \nu\frac{u_{j+4}^{n+1} - 2u_{j+2}^{n+1} + u_j^{n+1}}{2\triangle h^2} + \frac{f_{j+3}^{n+1} - f_{j+1}^{n+1}}{\triangle h} = 0.$$

Burgers' Equation (cont.)

Derivation of (generally nonconservative) difference schemes without recourse to conservation law needs usually more computation.
Example: Burgers' equation along with with integral relations

$$\begin{cases} u_t + f_x = \nu u_{xx} \\ \int u_t dt = u \\ \int f_x dx = f \\ \int u_x dx = u \\ \int u_{xx} dx = u_x \end{cases} \Longrightarrow \begin{cases} (u_t)_j^n + (f_x)_j^n = \nu (u_{xx})_j^n \\ (u_t)_{j+1}^n \triangle t = u_{j+1}^{n+1} - \frac{u_{j+2}^n + u_j^n}{2} \\ 2\triangle h\,(f_x)_{j+1}^n = f_{j+2}^n - f_j^n \\ 2\triangle h\,(u_x)_{j+1}^n = u_{j+2}^n - u_j^n \\ 2\triangle h\,(u_{xx})_{j+1}^n = (u_x)_{j+2}^n - (u_x)_j^n \end{cases}$$

Elimination with $u_{xx} \succ u_x \succ f_x \succ u \succ f$ yields the Lax scheme

$$\frac{2u_{j+2}^{n+1} - (u_{j+3}^n + u_{j+1}^n)}{2\triangle t} + \frac{f_{j+3}^n - f_{j+1}^n}{2\triangle h} - \nu \frac{u_{j+4}^n - 2u_{j+2}^n + u_j^n}{4\triangle h^2} = 0\,.$$

Burgers' Equation (cont.)

One can also generate other schemes, for example, the two-step Lax-Wendroff scheme.

Let $\overline{u}$ and $\overline{f}$ denote the values of u and f on the intermediate time levels. Then the midpoint rule for the spatial integrals, gives:

$$\begin{cases} (u_t)_j^n + (f_x)_j^n &= \nu\,(u_{xx})_j^n\,, \\ (u_t)_{j+1}^n\,\tau &= \overline{u}_{j+1}^{\,n+1} - \frac{u_{j+2}^n + u_j^n}{2}\,, \\ 2(f_x)_{j+1}^n\,h &= f_{j+2}^n - f_j^n\,, \\ 2(u_x)_{j+1}^n\,h &= u_{j+2}^n - u_j^n\,, \\ 2(u_{xx})_{j+1}^n\,h &= (u_x)_{j+2}^n - (u_x)_j^n\,, \\ (\overline{u}_t)_j^n + (\overline{f}_x)_j^n &= \nu\,(\overline{u}_{xx})_j^n\,, \\ 2(\overline{u}_t)_j^n\,\tau &= u_j^{n+1} - u_j^n\,, \\ 2(\overline{f}_x)_{j+1}^n\,h &= \overline{f}_{j+2}^n - \overline{f}_j^n\,, \\ 2(\overline{u}_x)_{j+1}^n\,h &= \overline{u}_{j+2}^n - \overline{u}_j^n\,, \\ 2(\overline{u}_x x)_{j+1}^n\,h &= (\overline{u}_x)_{j+2}^n - (\overline{u}_x)_j^n\,. \end{cases}$$

Burgers' Equation (cont.)

For the elimination ranking with

$$u_{xx} \succ \bar{u}_{xx} \succ u_x \succ \bar{u}_x \succ u_t \succ \bar{u}_t \succ f_x \succ \bar{f}_x \succ f \succ u \succ \bar{f} \succ \bar{u}$$

the Gröbner basis contains the Lax-Wendroff scheme

$$\begin{cases} \frac{\bar{u}^{n+1}_{j+2} - (u^n_{j+3} + u^n_{j+1})}{2\,\triangle t} + \frac{f^n_{j+3} - f^n_{j+1}}{2\,\triangle h} = \nu \frac{u^n_{j+4} - 2u^n_{j+2} + u^n_j}{4\,\triangle h^2}\,, \\ \frac{u^{n+1}_{j+3} - \bar{u}^n_{j+2}}{2\,\triangle t} + \frac{\bar{f}^n_{j+3} - \bar{f}^n_{j+1}}{2\,\triangle h} = \nu \frac{\bar{u}^n_{j+4} - \bar{u}^n_{j+2} + \bar{u}^n_j}{4\,\triangle h^2}\,. \end{cases}$$

With all possible combinations of the trapezoidal and midpoint rules one obtains 49 different Lax-Wendroff schemes.

Burgers' Equation (cont.)

It is especially difficult to simulate numerically nonsmooth and discontinuous solutions which are among most interesting problems in computational fluid and gas dynamics. Most of the known difference schemes fail to handle these singularities. The most appropriate are Godunov's schemes based on solving a local Riemann problem.

We apply the Gröbner bases technique to generate the Godunov-type scheme for inviscid Burgers' equation when $\nu = 0$. For this purpose we discretize the corresponding system in in the following way

$$\begin{cases} (u_t)_j^n + (f_x)_j^n = 0\,, \\ (u_t)_j^n \triangle t = u_j^{n+1} - u_j^n\,, \\ ((f_x)_j^n \triangle h - (f_{j+1}^n - f_j^n))((f_x)_{j+1}^n \triangle h - (f_{j+1}^n - f_j^n)) = 0\,, \\ 2\,(u_x)_{j+1}^n \triangle h = u_{j+2}^n - u_j^n\,, \\ 2\,(u_{xx})_{j+1}^n \triangle h = (u_x)_{j+2}^n - (u_x)_j^n\,. \end{cases}$$

Burgers' Equation (cont.)

To do the elimination from the nonlinear system we apply the Gröbner factoring approach: if a Gröbner basis contains a polynomial which factors, then the computation is split into the computation of two or more Gröbner bases corresponding to the factors.

We choose the elimination ranking

$$u_{xx} \succ u_x \succ u_t \succ f_x \succ f \succ u$$

and compute two Gröbner bases, for every of two factors. Then we compose the product of two obtained difference polynomials in u and f that gives us the Godunov-type difference scheme

$$\left(\frac{u_{j+2}^{n+1} - u_{j+2}^{n}}{\triangle t} + \frac{f_{j+2}^{n} - f_{j+1}^{n}}{\triangle h} \right) \cdot \left(\frac{u_{j+2}^{n+1} - u_{j+2}^{n}}{\triangle t} + \frac{f_{j+3}^{n} - f_{j+2}^{n}}{\triangle h} \right) = 0.$$

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Falkowich-Karman Equation

Consider now one more nonlinear equation, namely, the Falkowich-Karman equation describing transonic flow in gas dynamics

$$\varphi_{xx}(K - (\gamma + 1)\varphi_x) + \varphi_{yy} - 2\varphi_{xt} - \varphi_{tt} = 0$$

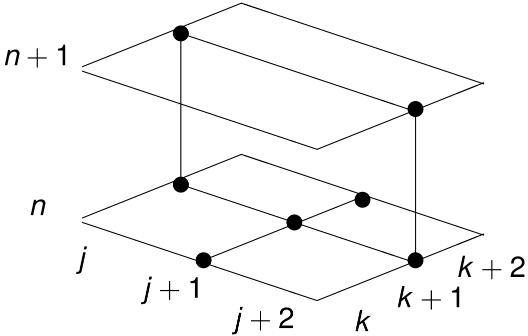
in its non-stationary form. One can use this form to find a stationary solution by the steady-state method. Rewrite the equation in the (partially discrete) conservation law form

$$\int_{t_n}^{t_{n+1}} \left(\oint_{\Gamma} -\varphi_y dx + \varphi_x (K - \frac{(\gamma+1)}{2}\varphi_x) dy \right) dt -$$

$$- \int_{x_j}^{x_{j+2}} \int_{y_k}^{y_{k+2}} (2\varphi_x + \varphi_t) \Big|_{t_n}^{t_{n+1}} dxdy = 0.$$

Falkowich-Karman Equation (cont.)

We use a grid decomposition of the three-dimensional domain in (x, y, t) into the elementary volumes of the form



Falkowich-Karman Equation (cont.)

Again we add the integral relations similar to those used for the Laplace Equation and use the trapezoidal integration rule for φ_x, φ_y and the midpoint rule for φ_t.

Then it gives the nonlinear difference equations

$$\left\{ \begin{array}{l} (-(\theta_x - \theta_x\theta_y^2) \circ \varphi_y + (\theta_x^2\theta_y - \theta_y) \circ (\varphi_x(K - \frac{(\gamma+1)}{2}\varphi_x))) \cdot 2\triangle h \triangle t - \\ \quad -(\theta_t - 1)(\theta_x^2\theta_y - \theta_y) \circ 2\varphi \cdot 2\triangle h - \theta_x\theta_y \circ \varphi_t \cdot 4\triangle h^2 = 0 \\ (\theta_x + 1) \circ \varphi_x \cdot \frac{\triangle h}{2} = (\theta_x - 1) \circ \varphi \\ (\theta_y + 1) \circ \varphi_y \cdot \frac{\triangle h}{2} = (\theta_y - 1) \circ \varphi \\ \theta_t \circ \varphi_t \cdot 2\triangle t = (\theta_t^2 - 1) \circ \varphi \end{array} \right. .$$

To construct GB, we use the lexicographical term order such that $\varphi_x \succ \varphi_y \succ \varphi_t \succ \varphi$ and then $\theta_x \succ \theta_y \succ \theta_t$.

Falkowich-Karman Equation (cont.)

$$
\begin{cases}
(\theta_x - 1)^2\theta_y \circ \varphi \cdot (\gamma+1)\varphi_x \frac{\triangle t}{\triangle h} + \theta_x\theta_y \circ \varphi_t \cdot \triangle h = \\
\quad = ((\theta_x - 1)^2\theta_y \circ \varphi \cdot (K - (\theta_x - 1)^2\theta_y \circ (\gamma+1)\varphi) + \\
\quad +\theta_x(\theta_y - 1)^2 \circ \varphi)\frac{\triangle t}{\triangle h} - (\theta_x^2\theta_y - \theta_y)(\theta_t - 1) \circ \varphi\,, \\
(\theta_y + 1) \circ \varphi_y = (\theta_y - 1) \circ \varphi \cdot \frac{2}{\triangle h}\,, \\
\theta_t \circ \varphi_t = (\theta_t^2 - 1) \circ \varphi \cdot \frac{1}{2\triangle t}\,, \\
0 = \theta_x(\theta_x - 1)^2\theta_y\theta_t \circ \varphi \cdot [((\theta_x - 1)^2\theta_y\theta_t \circ \varphi \cdot (K - \\
\quad -(\theta_x^3 - \theta_x^2 + \theta_x - 1)\theta_y\theta_t \circ \frac{(\gamma+1)}{2}\varphi) + \\
\quad +\theta_x(\theta_y - 1)^2\theta_t \circ \varphi)\frac{\triangle t}{\triangle h} - (\theta_x^2 - 1)\theta_y(\theta_t^2 - \theta_t) \circ \varphi - \\
\quad -\theta_x\theta_y(\theta_t - 1)^2 \circ \varphi \cdot \frac{\triangle h}{2\triangle t}] + \\
\quad +(\theta_x - 1)^2\theta_y\theta_t \circ \varphi \cdot [(\theta_x(\theta_x - 1)^2\theta_y\theta_t \circ \varphi \cdot (K - \\
\quad -(\theta_x^3 - \theta_x^2 + \theta_x - 1)\theta_y\theta_t \circ \frac{(\gamma+1)}{2}\varphi) + \\
\quad +\theta_x^2(\theta_y - 1)^2\theta_t \circ \varphi)\frac{\triangle t}{\triangle h} - (\theta_x^3 - \theta_x)\theta_y(\theta_t^2 - \theta_t) \circ \varphi - \\
\quad -\theta_x^2\theta_y(\theta_t - 1)^2 \circ \varphi \cdot \frac{\triangle h}{2\triangle t}].
\end{cases}
$$

Falkowich-Karman Equation (cont.)

The last element is the finite-difference scheme

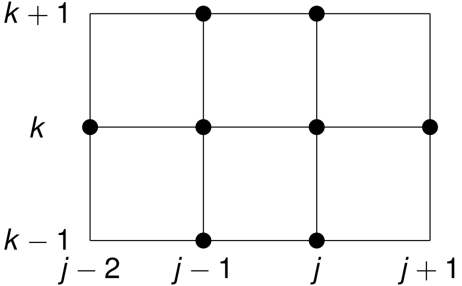
$$(\varphi^n_{j+1\,k} - 2\varphi^n_{j\,k} + \varphi^n_{j-1\,k}) \cdot [((\varphi^n_{j\,k} - 2\varphi^n_{j-1\,k} + \varphi^n_{j-2\,k})(K - \frac{(\gamma+1)}{2\triangle h}(\varphi^n_{j+1\,k}$$
$$-\varphi^n_{j\,k} + \varphi^n_{j-1\,k} - \varphi^n_{j-2\,k}) + (\varphi^n_{j-1\,k+1} - 2\varphi^n_{j-1\,k} + \varphi^n_{j-1\,k-1}))\frac{\triangle t}{\triangle h} -$$
$$(\varphi^{n+1}_{j\,k} - \varphi^{n+1}_{j-2\,k} - \varphi^n_{j\,k} + \varphi^n_{j-2\,k}) - (\varphi^{n+1}_{j-1\,k} - 2\varphi^n_{j-1\,k} + \varphi^{n-1}_{j-1\,k})\frac{\triangle h}{2\triangle t}] +$$
$$(\varphi^n_{j\,k} - 2\varphi^n_{j-1\,k} + \varphi^n_{j-2\,k}) \cdot [((\varphi^n_{j+1\,k} - 2\varphi^n_{j\,k} + \varphi^n_{j-1\,k})(K - \frac{(\gamma+1)}{2\triangle h}(\varphi^n_{j+1\,k}$$
$$-\varphi^n_{j\,k} + \varphi^n_{j-1\,k} - \varphi^n_{j-2\,k}) + (\varphi^n_{j\,k+1} - 2\varphi^n_{j\,k} + \varphi^n_{j\,k-1}))\frac{\triangle t}{\triangle h} -$$
$$(\varphi^{n+1}_{j+1\,k} - \varphi^{n+1}_{j-1\,k} - \varphi^n_{j+1\,k} + \varphi^n_{j-1\,k}) - (\varphi^{n+1}_{j\,k} - 2\varphi^n_{j\,k} + \varphi^{n-1}_{j\,k})\frac{\triangle h}{2\triangle t}] = 0.$$

In its stationary form this scheme is given by

$$D_{xx}(\varphi^n_{j\,k}) \cdot [D_{xx}(\varphi^n_{j-1\,k})(K - \frac{(\gamma+1)}{2}(D_x(\varphi^n_{j+1\,k}) + D_x(\varphi^n_{j-1\,k}))) + D_{yy}(\varphi^n_{j-1\,k})] +$$
$$D_{xx}(\varphi^n_{j-1\,k}) \cdot [D_{xx}(\varphi^n_{j\,k})(K - \frac{(\gamma+1)}{2}(D_x(\varphi^n_{j+1\,k}) + D_x(\varphi^n_{j-1\,k}))) + D_{yy}(\varphi^n_{j\,k})] = 0$$

Falkowich-Karman Equation (cont.)

Note that the scheme obtained is fully conservative and does not contain switches that are typically used in calculation of transonic flows. The stencil used for the stationary case is



We applied this scheme to the one-dimensional flow in a channel with a straight density jump.

Conclusions

- GB are the most universal algorithmic tool for linear difference systems.
- GB can be effectively applied to derivation of differences schemes for linear PDEs.
- By construction, the schemes derived from the conservation law form are fully conservative. Their form depends on the numerical integration rules used.
- There is an efficient algorithm for construction of GB for linear difference ideals. The algorithm is based on the concept of Janet-like reductions. Its first implementation in Maple is already available.
- For classical linear PDEs: Laplace Equation (elliptic), Heat Equation (parabolic), Wave Equation (hyperbolic) and Advection Equation (hyperbolic) our algorithmic technique leads to the well-known finite difference schemes.

Conclusions (cont.)

- For Burgers' equation by applying Gröbner bases for the difference elimination of partial derivatives we generated such well-known schemes as FTFS, Lax and Lax-Wendroff and also Godunov-type scheme.
- The new finite-difference scheme generated for the Falkowich-Karman Equation possesses a stable convergence in time to the exact solution with a one-dimensional shock wave. As a consequence of the full conservatism of the scheme, it does not reveal non-uniqueness in solution of difference equations that is a typical feature of the traditional difference schemes.
- An area of the shock transition has a size of one grid step what can be explained by preserving, at the discrete level, all algebraic properties of the initial continuous equations.

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