

# On computer algebra-aided stability analysis of difference schemes generated by means of Gröbner bases

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# Outline

## Introduction

- Finite Difference Approach
- Stability of Difference Schemes

## Difference schemes for hyperbolic equations

- Difference Cauchy problem
- Notion of approximation for the initial problem

## First differential approximation of difference scheme

- Example: Lax Scheme

## Algorithmic Approach to Generation of Difference Schemes

## Algorithm for Construction of Differential Approximation

- Algorithm for Hyperbolic Form
- Algorithm for Hyperbolic Form
- Implementation in Maple
- Two-Step Lax-Wendroff Schemes

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# Finite Difference Approach

- ▶ The finite difference approach is the most popular discretization technique for numerical solving of ordinary or PDEs. In this approach derivatives are approximated by finite differences and the resulting algebraic system – difference scheme – is solved numerically.
- ▶ Recently (G.,B.,Mozzhilkin'06) we developed an algorithmic method to generation of finite difference schemes for linear PDEs with two independent variables. The method is based on difference elimination provided by construction of Gröbner bases for an appropriate elimination ranking.
- ▶ Sometimes Gröbner bases can be computed even for nonlinear difference systems obtained by discretization of PDEs and related integral equations. In this case nonlinear difference schemes can also be generated by our method.

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# Stability of Difference Schemes

- ▶ A difference scheme, to be of practical interest, must be stable. The stability study of difference schemes exploits symbolic mathematical operations. Thus it can be analyzed with help of **computer algebra methods and software** (Ganzha, Vorozhtsov'96).
- ▶ To analyze stability one can use **differential approximation** that is often called the **modified equation(s)** of the difference scheme. There are whole classes of different schemes for which their stability properties can be obtained with the aid of the differential approximation (Strikwerda'04). For all that, in many cases, the computation can be done by means of modern computer algebra software.
- ▶ In this talk **we shall demonstrate how Maple can be used** for this purpose and present a Maple program **for computation of differential approximations for difference schemes**.
- ▶ In the aggregate with the Maple package for construction of Gröbner bases for linear difference systems (G., Robertz'06) the program allows one to generate schemes possessing stability properties.

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# Difference Cauchy problem

Consider the following Cauchy problem

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{A} \mathbf{u}, \quad -\infty < 0 < \infty, \quad t > 0 \quad (1)$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad -\infty < 0 < \infty, \quad (2)$$

where  $\mathbf{x}$  is the spatial variable,  $t$  is the temporal variable,  $\mathbf{A}$  is a linear differential operator,  $\mathbf{u}_0(\mathbf{x})$  is a given function.

We approximate the Cauchy problem (1), (2) by the following difference Cauchy problem:

$$\frac{u_j^{n+1} - u_j^n}{\tau} = \Lambda_1 u_j^{n+1} + \Lambda_2 u_j^n, \quad j = 0, \pm 1, \pm 2, \dots; n = 0, 1, 2, \dots \quad (3)$$

$$u_j^0 = u_0(x_j) \quad (4)$$



# Difference Cauchy problem

Consider the following Cauchy problem

$$\frac{\partial u}{\partial t} = Au, \quad -\infty < x < \infty, \quad t > 0 \quad (1)$$

$$u(x, 0) = u_0(x), \quad -\infty < x < \infty, \quad (2)$$

where  $x$  is the spatial variable,  $t$  is the temporal variable,  $A$  is a linear differential operator,  $u_0(x)$  is a given function.

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$$u_j^0 = u_0(x_j) \quad (4)$$

## Notion of approximation

Let  $L$  be the operator of the initial equation (1), i.e.

$$Lu = \frac{\partial u}{\partial t} - Au, \quad (5)$$

and let  $L_h$  be a difference operator defined in accordance to (5) as

$$L_h u = \frac{u(x, t + \tau) - u(x, t)}{\tau} - \Lambda_1 u(x, t + \tau) - \Lambda_2 u(x, t), \quad (6)$$

Let  $u(x, t)$  be a solution of the Cauchy problem (1), (2) smooth enough. If

$$\|Lu - L_h u\| \leq C_1 h^{k_1} + C_2 \tau^{k_2}, \quad (7)$$

where  $k_1 > 0$ ,  $k_2 > 0$  and constants  $C_1$  и  $C_2$  do not depend on  $\tau$  and  $h$ , then (by definition) difference scheme (3) approximates equation (1) and has order of approximation  $k_1$  w.r.t.  $h$  and order  $k_2$  w.r.t.  $\tau$ .

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# First differential approximation of difference scheme

The **first differential approximation** (FDA) of difference schemes (3) is the partial differential equation which is obtained from (3) by substitution for the grid function their Taylor expansions and by keeping the main term (Shokin, Yanenko'85)

One distinguishes **hyperbolic** and **parabolic** forms of FDA (Ganzha, Vorozhtsov'96). To obtain parabolic form of FDA one uses differential consequences of the initial PDE(s)  $\frac{\partial u}{\partial t} = Au$ . as a result of differentiation of the both sides of PDE(s) w.r.t. the independent variables.

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# Error of Difference Scheme

Discretization of a PDE implies that a difference solution does not satisfy PDE. The deviation of difference solution from the exact one is called an **error of difference scheme**. Study and classification of errors is based on representation of the solution by a trigonometric Fourier series and detecting the variation in amplitude and phase of each harmonic in one step in time and, respectively, the variation of the exact solution (of PDE) on the same time interval.

If the harmonic amplitude decreases faster than that for the exact solution, then this effect is called the **amplitude error** of the scheme caused by an extra diffusion inherent to the scheme – **numerical viscosity**. The phase variation of the difference solution distinct from that for the exact solution is called the **phase error** caused by distinction in the phase velocities of the harmonic propagation – **numerical dispersion**.

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## Lax-type Scheme for Burgers' equation

$$u_t + f_x = \nu u_{xx}, \quad \nu = \text{const} \quad (8)$$

$$\frac{2u_{j+2}^{n+1} - (u_{j+3}^n + u_{j+1}^n)}{2\tau} + \frac{f_{j+3}^n - f_{j+1}^n}{2h} = \nu \frac{u_{j+4}^n - 2u_{j+2}^n + u_j^n}{4h^2} \quad (9)$$

Differential approximation in point  $(n, j+2)$

$$\begin{aligned} & \overbrace{u_t + f_x - \nu u_{xx}} - \frac{1}{2} u_{xx} \frac{h^2}{\tau} + \\ & + \frac{1}{2} u_{tt} \tau + \left( \frac{1}{6} f_{xxx} - \frac{1}{3} \nu u_{xxxx} \right) h^2 - \frac{1}{24} u_{xxxx} \frac{h^4}{\tau} + \\ & + \frac{1}{6} u_{ttt} \tau^2 + \left( \frac{1}{120} f_{xxxxx} - \frac{2}{45} \nu u_{xxxxx} \right) h^4 - \frac{1}{720} u_{xxxxx} \frac{h^6}{\tau} + \\ & + \dots = 0 \end{aligned} \quad (10)$$

From (10) it follows that scheme (9) does not approximate equation (8) at  $O(h^2/\tau) \sim 1$ . It is an example of **conditionally convergent scheme**.



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## Parabolic Form for FDA

For more detailed analysis of scheme (9) one can construct a **parabolic form** of FDA for  $f = u^2/2$ :

$$u_t + uu_x - \overbrace{\left( \nu + \frac{h^2}{2\tau} + (2\nu\tau + \frac{h^2}{2})u_x - \frac{\tau}{2}u^2 \right)} u_{xx} + (u\tau)u_x - (\nu u\tau + \frac{h^2}{3}u)u_{xxx} + \left( \frac{\nu^2\tau}{2} + \frac{\nu h^2}{6} + \frac{h^4}{12\tau} \right) u_{xxxx} = 0. \quad (11)$$

To be an approximation of the initial PDE it is necessary that expression marked by  $\overbrace{\dots}$  to be  $\sim \nu$  whereas the remaining terms which do not occur in PDE to be vanish.

For equation (8) and zero viscosity ( $\nu = 0$ ) the expression marked by  $\overbrace{\dots}$  must be  $> 0$ . Otherwise the diffusion coefficient becomes negative. Thereby the boundary-value problem becomes incorrect.

For some classes of PDE one can relate (equivalence theorem) the scheme stability with its differential approximation.

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# Algorithmic Generation of Difference Schemes

In (G.,B.,Mozzhilkin'06) we suggested an algorithmic approach to generation of difference schemes. By example consider equation (8).

$$\begin{aligned} \int u_t dt = u, & & u_t \tau = u_j^{n+1} - \frac{u_{j+2}^n + u_j^n}{2}, \\ \int f_x dx = f, & \implies & 2 h(f_x)_{j+1}^n = f_{j+2}^n - f_j^n, \\ \int u_x dx = u, & & 2 h(u_x)_{j+1}^n = u_{j+2}^n - u_j^n, \\ \int u_{xx} dx = u_x, & & 2 h(u_{xx})_{j+1}^n = (u_x)_{j+2}^n - (u_x)_j^n. \end{aligned} \quad (12)$$

Gröbner basis for  $u_{xx} \succ u_t \succ u_x \succ f_x \succ u \succ f \implies$  scheme (9).

If call such method of integration in time as Lax-type scheme, then one can use different numerical quadrature formulae for integration over  $x$ . For the midpoint or the trapezoidal rule for these integrals 8 different schemes are generated.

**Question:** how close are properties of these 8 schemes? A partial answer can be obtained by using the differential approximation technique.

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## Algorithm for Hyperbolic Form

Since in advance the order of ratio  $\frac{h}{\tau}$  is not known, one cannot specify a linear order for PDE in construction of the differential approximation. Equation (10) multiplied by  $\tau$  it can be partitioned into three groups:

$$\begin{aligned} & \left[ (u_t + f_x - \nu u_{xx})\tau - \frac{1}{2}u_{xx}h^2, \right. \\ & \left. \frac{1}{2}u_{tt}\tau^2 + \left(\frac{1}{6}f_{xxx} - \frac{1}{3}\nu u_{xxxx}\right)\tau h^2 - \frac{1}{24}u_{xxxx}h^4, \right. \\ & \left. \frac{1}{6}u_{ttt}\tau^3 + \left(\frac{1}{120}f_{xxxxx} - \frac{2}{45}\nu u_{xxxxx}\right)\tau h^4 - \frac{1}{720}u_{xxxxx}h^6 \right] \end{aligned}$$

- ▶ The first group does not divide.
- ▶ The second group has divisors in the first group.
- ▶ The third group has divisors from the first and the second groups.

The truncation order for the Taylor expansion is specified in such a way in order to provide a correct partition into groups.

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# Algorithm for Hyperbolic Form

To construct FDA for the parabolic form (it is sufficient to compare scheme properties), the derivatives in  $t$  in the second group are replaced by their values from the first group. It can be achieved by the sequential substitution derivatives  $u_{tt} \succ u_{tx} \succ u_t$  in accordance with the lexicographic order:

$$\begin{aligned} & \left[ (u_t + uu_x - \nu u_{xx})\tau - u_{xx} \frac{h^2}{2}, \right. \\ & \quad \left. + (-\nu uu_{xxx} - 2\nu u_x u_{xx} + \frac{1}{2}\nu^2 u_{xxxx} + \frac{1}{2}u^2 u_{xx} + uu_x^2)\tau^2 \right. \\ & \quad \left. + (\frac{1}{6}u_{xxxx}\nu - \frac{1}{3}u_{xxx}u - \frac{1}{2}u_{xx}u_x)\tau h^2 + \frac{1}{6}u_{xxxx}h^4 \right] \end{aligned}$$

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# Implementation in Maple

We implemented the above described method in Maple as a package FDA.

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>restart;  
>libname:=libname, "/usr/local/lib/lfdm", "/usr/local/lib/Janet", "/usr/local/lib/fda",  
"/opt/maple10/lib", "/usr/local/lib/lfdm", "/usr/local/lib/Janet", "/usr/local/lib/fda"  
>with(LFDM);
```

```
[AffEqn, AppShiftOp, AssertJanetBasis, CartesianCharacter, CompCond, CompCondBasis,  
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```
>with(FDA);  
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```

# Example: Burgers' Equation

```
>L:= [ut(n,j)+Fx(n,j)-nu*uxx(n,j),  
>   ut(n,j+1)*tau-(u(n+1,j+1)-(u(n,j+2)+u(n,j))/2),  
>   2*Fx(n,j+1)*h-(F(n,j+2)-F(n,j)),  
>   2*ux(n,j+1)*h-(u(n,j+2)-u(n,j)),  
>   2*uxx(n,j+1)*h-(ux(n,j+2)-ux(n,j))];
```

$$\begin{aligned} & [ut(n,j) + Fx(n,j) - \nu u_{xx}(n,j), ut(n,j+1)\tau - u(n+1,j+1) + \frac{1}{2}u(n,j+2) + \frac{1}{2}u(n,j), \\ & 2Fx(n,j+1)h - F(n,j+2) + F(n,j), \\ & 2ux(n,j+1)h - u(n,j+2) + u(n,j), \\ & 2uxx(n,j+1)h - ux(n,j+2) + ux(n,j)] \end{aligned}$$

```
>JanetBasis(L, [n,j], [uxx,ux,ut,Fx,u,F],2);
```

$$\begin{aligned} & [ [-2\nu\tau u(n,j+2) + \nu\tau u(n,j) + \nu\tau u(n,j+4) - 4h^2u(n+1,j+2) + 2h^2u(n,j+3) \\ & + 2h^2u(n,j+1) - 2\tau hF(n,j+3) + 2\tau hF(n,j+1), 2Fx(n,j+1)h - F(n,j+2) + F(n,j), \\ & 2ut(n,j+1)\tau - 2u(n+1,j+1) + u(n,j+2) + u(n,j), \\ & 2\tau h\nu ux(n,j) - \nu\tau u(n,j+3) + \nu\tau u(n,j+1) + 4h^2u(n+1,j+1) - 2h^2u(n,j+2) \\ & - 2h^2u(n,j) + 2\tau hF(n,j+2) - 2\tau hF(n,j), \\ & ut(n,j) + Fx(n,j) - \nu u_{xx}(n,j)], \\ & [n,j], [uxx, ux, ut, Fx, u, F] \end{aligned}$$

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$$\begin{aligned} & [ut(n,j) + Fx(n,j) - \nu uxx(n,j), ut(n,j+1)\tau - u(n+1,j+1) + \frac{1}{2}u(n,j+2) + \frac{1}{2}u(n,j), \\ & 2Fx(n,j+1)h - F(n,j+2) + F(n,j), \\ & 2ux(n,j+1)h - u(n,j+2) + u(n,j), \\ & 2uxx(n,j+1)h - ux(n,j+2) + ux(n,j)] \end{aligned}$$

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$$\begin{aligned} & [ut(n,j) + Fx(n,j) - \nu uxx(n,j), ut(n,j+1)\tau - u(n+1,j+1) + \frac{1}{2}u(n,j+2) + \frac{1}{2}u(n,j), \\ & 2Fx(n,j+1)h - F(n,j+2) + F(n,j), \\ & 2ux(n,j+1)h - u(n,j+2) + u(n,j), \\ & 2uxx(n,j+1)h - ux(n,j+2) + ux(n,j)] \end{aligned}$$

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>collect(%[1,1]/(4\*tau\*h^2),[tau,h,nu]);

$$\frac{-1/2 F(n,j+3) + 1/2 F(n,j+1)}{h} + \frac{(1/4 u(n,j+4) - 1/2 u(n,j+2) + 1/4 u(n,j)) \nu}{h^2}$$

$$+ \frac{1/2 u(n,j+3) + 1/2 u(n,j+1) - u(n+1,j+2)}{\tau}$$

>a:=-DForm(%,[u,F],[[n,tau,t],[j,h,x]],[0,2],2);

$$[D_2(F)(t,x) - D_{2,2}(u)(t,x) \nu + D_1(u)(t,x) - 1/2 \frac{D_{2,2}(u)(t,x) h^2}{\tau},$$

$$1/2 D_{1,1}(u)(t,x) \tau - (-1/6 D_{2,2,2}(F)(t,x) + 1/3 D_{2,2,2,2}(u)(t,x)) \nu h^2$$

$$- 1/24 \frac{D_{2,2,2,2}(u)(t,x) h^4}{\tau},$$

$$1/6 D_{1,1,1}(u)(t,x) \tau^2 - \left( -\frac{1}{120} D_{2,2,2,2,2}(F)(t,x) + \frac{2}{45} D_{2,2,2,2,2,2}(u)(t,x) \right) \nu h^4$$

$$- \frac{1}{720} \frac{D_{2,2,2,2,2,2}(u)(t,x) h^6}{\tau}]$$

>collect(%[1,1]/(4\*tau\*h^2),[tau,h,nu]);

$$\frac{-1/2 F(n,j+3) + 1/2 F(n,j+1)}{h} + \frac{(1/4 u(n,j+4) - 1/2 u(n,j+2) + 1/4 u(n,j)) \nu}{h^2}$$

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>F:=u^2/2;  
 >PForm(a);

$$\begin{aligned}
 & [D_2(u)(t, x) u(t, x) - D_{2,2}(u)(t, x) \nu + D_1(u)(t, x) - 1/2 \frac{D_{2,2}(u)(t, x) h^2}{\tau}, \\
 & (-\nu D_{2,2,2}(u)(t, x) u(t, x) - 2 \nu D_{2,2}(u)(t, x) D_2(u)(t, x) \\
 & + 1/2 \nu^2 D_{2,2,2,2}(u)(t, x) + 1/2 (u(t, x))^2 D_{2,2}(u)(t, x) + u(t, x) (D_2(u)(t, x))^2) \tau \\
 & + (-1/3 D_{2,2,2}(u)(t, x) u(t, x) - 1/2 D_{2,2}(u)(t, x) D_2(u)(t, x) + 1/6 D_{2,2,2,2}(u)(t, x) \nu) h^2 \\
 & + 1/12 \frac{D_{2,2,2,2}(u)(t, x) h^4}{\tau} ]
 \end{aligned}$$

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 & (-\nu D_{2,2,2}(u)(t, x) u(t, x) - 2 \nu D_{2,2}(u)(t, x) D_2(u)(t, x) \\
 & + 1/2 \nu^2 D_{2,2,2,2}(u)(t, x) + 1/2 (u(t, x))^2 D_{2,2}(u)(t, x) + u(t, x) (D_2(u)(t, x))^2) \tau \\
 & + (-1/3 D_{2,2,2}(u)(t, x) u(t, x) - 1/2 D_{2,2}(u)(t, x) D_2(u)(t, x) + 1/6 D_{2,2,2,2}(u)(t, x) \nu) h^2 \\
 & + 1/12 \frac{D_{2,2,2,2}(u)(t, x) h^4}{\tau} ]
 \end{aligned}$$

One can also use the trapezoidal rule for spatial integration. This derives other schemes. By selecting either the midpoint or the trapezoidal rule for the spatial integrals, we obtain 8 possible schemes. Among them there are 7 different schemes:

$$\begin{aligned}
 & \frac{2(u_{j+2}^{n+1} + u_{j+1}^{n+1}) - (u_{j+3}^n + u_{j+2}^n + u_{j+1}^n + u_j^n)}{4\tau} + \frac{(f_{j+3}^n + f_{j+2}^n) - (f_{j+1}^n + f_j^n)}{4h} = \nu \frac{(u_{j+3}^n - u_{j+2}^n) - (u_{j+1}^n - u_j^n)}{2h^2}, \\
 & \frac{2u_{j+1}^{n+1} - (u_{j+2}^n + u_j^n)}{2\tau} + \frac{f_{j+2}^n - f_j^n}{2h} = \nu \frac{u_{j+2}^n - 2u_{j+1}^n + u_j^n}{h^2}, \\
 & \frac{2(u_{j+3}^{n+1} + 2u_{j+2}^{n+1} + u_{j+1}^{n+1}) - (u_{j+4}^n + 2u_{j+3}^n + 2u_{j+2}^n + 2u_{j+1}^n + u_j^n)}{8\tau} \\
 & \quad + \frac{(f_{j+4}^n + 2f_{j+1}^n) - (2f_{j+1}^n + f_j^n)}{8h} = \nu \frac{u_{j+3}^n - 2u_{j+2}^n + u_{j+1}^n}{h^2}, \\
 & \frac{2(u_{j+3}^{n+1} + u_{j+2}^{n+1}) - (u_{j+4}^n + u_{j+3}^n + u_{j+2}^n + u_{j+1}^n)}{4\tau} + \frac{f_{j+3}^n - f_{j+2}^n}{h} \\
 & \quad = \nu \frac{((u_{j+5}^n + u_{j+4}^n) - 2u_{j+3}^n) - (2u_{j+2}^n - (u_{j+1}^n + u_j^n))}{8h^2}, \\
 & \frac{2(u_{j+2}^{n+1} + u_{j+1}^{n+1}) - (u_{j+3}^n + u_{j+2}^n + u_{j+1}^n + u_j^n)}{4\tau} + \frac{f_{j+2}^n - f_{j+1}^n}{h} = \nu \frac{(u_{j+3}^n - u_{j+2}^n) - (u_{j+1}^n - u_j^n)}{2h^2}, \\
 & \frac{2(u_{j+3}^{n+1} + 2u_{j+2}^{n+1} + u_{j+1}^{n+1}) - (u_{j+4}^n + 2u_{j+3}^n + 2u_{j+2}^n + 2u_{j+1}^n + u_j^n)}{8\tau} + \frac{f_{j+3}^n - f_{j+1}^n}{2h} \\
 & \quad = \nu \frac{u_{j+3}^n - 2u_{j+2}^n + u_{j+1}^n}{h^2}.
 \end{aligned}$$

Computation of differential approximations for them gives:

$$\begin{aligned}
 (9) \quad & [\dots, (\dots)\tau \quad +(\frac{1}{6}\mathbf{u}_{xxxx}\nu - \frac{1}{3}\mathbf{u}_{xxx}\mathbf{u} - \frac{1}{2}\mathbf{u}_{xx}\mathbf{u}_x)h^2 \quad +\frac{1}{12}\mathbf{u}_{xxxx}\frac{h^4}{\tau}] \\
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 \end{aligned} \tag{13}$$

These schemes have similar properties, and three of them have identical differential approximations. By inspection of the schemes we see that these schemes have

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Denoting the values of functions on the intermediate time level by  $\bar{u}$ ,  $\bar{F}$  we obtain the following difference system:

$$\left\{ \begin{array}{l} u_t^n + F_x^n = \nu u_{xx}^n \\ u_t^n \tau = \bar{u}_j^{n+1} - \frac{u_{j+2}^n + u_j^n}{2} \\ 2F_{x,j+1}^n h = F_{j+2}^n - F_j^n \\ 2u_{x,j+1}^n h = u_{j+2}^n - u_j^n \\ 2u_{xx,j+1}^n h = u_{x,j+2}^n - u_{x,j}^n \\ \bar{u}_t^n + \bar{F}_x^n = \nu \bar{u}_{xx}^n \\ \bar{u}_t^n \tau = \bar{u}_j^{n+1} - \bar{u}_j^n \\ 2\bar{F}_{x,j+1}^n h = \bar{F}_{j+2}^n - \bar{F}_j^n \\ 2\bar{u}_{x,j+1}^n h = \bar{u}_{j+2}^n - \bar{u}_j^n \\ 2\bar{u}_{xx,j+1}^n h = \bar{u}_{x,j+2}^n - \bar{u}_{x,j}^n. \end{array} \right. \quad (14)$$

The trapezoidal or midpoint rule for the integral relation between  $u_x$  and  $u$  yields 36 different schemes whose are similar the Lax-Wendroff scheme.

# Conclusions

- ▶ Gröbner bases provide algorithmic construction of finite difference schemes for linear PDEs in two independent variables.
- ▶ Having a difference scheme constructed the method of differential approximation (modified equation) allows to study stability of schemes for a wide class of PDEs. In particular, the first differential approximation (FDA) plays an important role in the stability analysis.
- ▶ For linear and some quasilinear PDEs differential approximations can be constructed algorithmically, and the underlying algorithms have been implemented in Maple.
- ▶ Algorithms for computing parabolic and hyperbolic forms of FDA are available together with their implementation in Maple.
- ▶ The methods and software designed were applied to many different PDEs, for example, to Burgers' equation. A number of difference schemes for them was generated and their stability properties were studied by the method of differential approximation.

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