A Symbolic Approach to Finite Difference Schemes and their von Neumann Stability

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Introduction

Joint work with M. Fröhner, B. Martin (Cottbus).

Given

- a system S of linear PDE's in unknown functions u_i in variables $\{t, x, y, z, \ldots\}$ with constant coefficients
- a set of approximations for differential operators involved

Tasks

- Compute the finite difference scheme for a given data
- Analyze the scheme for consistency, stability, dispersion etc.

Symbolic approach

Via the operator formulation the process of generation does not depend on initial resp. boundary conditions.

Difference Approximations

Notation: difference operators $T_x : f(t,x,y,z) \to f(t,x+\triangle x,y,z)$.

Taylor Expansion

$$u(x \pm \triangle x) = u(x) \pm \triangle x u_x(x) + \frac{\triangle x^2}{2} u_{xx}(x) + \mathcal{O}(\triangle x^3).$$

$$u_x(x) = \frac{u(x+\triangle x) - u(x)}{\triangle x} + \mathcal{O}(\triangle x) \text{ (forward difference)}$$

$$u_x(x) = \frac{u(x) - u(x-\triangle x)}{\triangle x} + \mathcal{O}(\triangle x) \text{ (backward difference)}$$

$$u_x(x) = \frac{u(x+\triangle x) - u(x-\triangle x)}{2\triangle x} + \mathcal{O}(\triangle x^2) \text{ (central } 1^{st} \text{ order diff.)}$$

$$\frac{u(x+\triangle x) - 2u(x) + u(x-\triangle x)}{\triangle x^2} = u_{xx}(x) + \mathcal{O}(\triangle x^2)$$

Forward difference

$$(T_x - 1) \bullet u = \triangle x \bullet u_x \quad \Leftrightarrow \quad (\triangle x,\ 1 - T_x) \cdot (u_x, u)^T = 0.$$

Difference Approximations: Rules

Approximation Rules

- **Forward difference** $(\triangle x,\ 1 - T_x) \cdot (u_x, u)^T = 0$
- **Backward difference** $(\triangle x \cdot T_x,\ 1 - T_x) \cdot (u_x, u)^T = 0$
- A 1^{st} **order central appr.** $(2\triangle x \cdot T_x,\ 1 - T_x^2) \cdot (u_x, u)^T = 0$
- A 2^{nd} **order central appr.** $(-\triangle x^2 \cdot T_x,\ (1 - T_x)^2) \cdot (u_{xx}, u)^T = 0$
- **Trapezoid rule** $(\frac{1}{2}\triangle x \cdot (T_x + 1), 1 - T_x) \cdot (u_x, u)^T = 0$
- **Midpoint rule** $(2\triangle x \cdot T_x, 1 - T_x^2) \cdot (u_x, u)^T = 0.$
- **Pyramid rule** $(\frac{1}{3}\triangle x \cdot (T_x^2 + T_x + 1), T_x(1 - T_x^2)) \cdot (u_x, u)^T = 0$

Computing Finite Difference Schemes I

The equation $u_{tt} - \lambda^2 u_{xx} = 0$

We approximate x via trapezoid rule and t via backward difference. We obtain the matrix formulation

$$\begin{pmatrix} -\lambda^2 & 0 & 1 & 0 & 0 \\ \triangle x/2 \cdot (T_x + 1) & 1 - T_x & 0 & 0 & 0 \\ 0 & \triangle x/2 \cdot (T_x + 1) & 0 & 0 & 1 - T_x \\ 0 & 0 & \triangle t \cdot T_t & 1 - T_t & 0 \\ 0 & 0 & 0 & \triangle t \cdot T_t & 1 - T_t \end{pmatrix} \bullet \begin{pmatrix} u_{xx} \\ u_x \\ u_{tt} \\ u_t \\ u \end{pmatrix}$$

Computational Task

Let M be a submodule of a free module, generated by the rows of the matrix above. We look for a submodule $N \subset M$, involving only u.

Elimination of module components

Suppose there is a monomial well–ordering $\prec_A$ on a ring A.
The ordering $\prec_m$ on a free left module $A^r = \bigoplus_{i=1}^{r} Ae_i$ is the **position–over–term** ordering with $e_1 \succ e_2 \succ \ldots$, defined as follows:

$$x^{\alpha} e_i \prec_m x^{\beta} e_j \;\Leftrightarrow\; j < i \text{ or } j = i \text{ and } x^{\alpha} \prec_A x^{\beta}.$$

Lemma

Let $M \subseteq A^r$ be a submodule. Let $G = \{g_1, \ldots, g_m\}$ be a Gröbner basis of M with respect to $\prec_m$ as before.
Then $\forall\ 1 \leq s \leq r \quad G \cap \bigoplus_{i=s}^{r} Ae_i$ is a Gröbner basis of $M \cap \bigoplus_{i=s}^{r} Ae_i$.

Computing Finite Difference Schemes II

Continue with the example before. Gröbner basis computation gives us the submodule, generated by the difference polynomial

$$\frac{4\lambda^2 \triangle t^2}{\triangle h^2}(T_x^2 T_t^2 - 2T_x T_t^2 + T_t^2) =$$

$$= T_x^2 T_t^2 - 2T_x^2 T_t + 2T_x T_t^2 + T_x^2 - 4T_x T_t + T_t^2 + 2T_x - 2T_t + 1$$

Written in the nodes of the mesh, it looks as follows

$$\frac{4\lambda^2 \triangle t^2}{\triangle h^2} \cdot (u_{j+2}^{n+2} - 2u_{j+1}^{n+2} + u_j^{n+2}) =$$

$$= (u_{j+2}^{n+2} - 2u_{j+2}^{n+1} + u_{j+2}^{n}) + 2(u_{j+1}^{n+2} - 2u_{j+1}^{n+1} + u_{j+1}^{n}) +$$
$$+ (u_j^{n+2} - 2u_j^{n+1} + u_j^{n})$$

One can easily see that this scheme is consistent.

The Importance of Stability

Consistency and Convergence

A scheme is **consistent** if it converges towards the original PDE equation for $\triangle t, \triangle x \to 0$. We say that **convergence** takes place, if the (numerical) solution of the scheme converges towards the real solution of the PDE for $\triangle t, \triangle x \to 0$.

Lax's Equivalence Theorem

Given a properly posed initial value problem and a finite-difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.

Using nice approximations, we often get consistent schemes.
The stability analysis is more involved.

von Neumann Stability Analysis I

The idea is to let the error terms grow with the time.
Due to linearity of equations, error terms satisfy the same difference equations as the scheme does.

Substitutions

Let $J^2 = -1$. For spatial variables x, y, z and for the time t, we substitute $\quad \chi' : E^m_{ijk} \mapsto \Gamma^i_n \Lambda^j_\ell \Upsilon^k_s \xi^m_{n\ell s}, \quad$ where
$\Gamma_n := e^{J\beta_n h_x}$, $\Lambda_\ell := e^{J\gamma_\ell h_y}$ and $\Upsilon_s := e^{J\delta_s h_z}$, $\xi_{n\ell s} = e^{\alpha_{n\ell s} \triangle t}$.

Let us denote by $E := E^0_{000}$ the error in the initial point.

Interpretation

Indeed, $\chi'(E) = 1$, $\chi'(E^m_{000}) = \xi^m_{n\ell s} = \chi'(T^m_t \bullet E)$,
$\chi'(E^0_{i00}) = \Gamma^i_n = \chi'(T^i_x \bullet E)$ and so on.

von Neumann Stability Analysis II

Let R be a ring of linear difference operators on E over a field C with $C \supseteq \mathbb{C}(\triangle t, \triangle x, \triangle y, \triangle z)$.
A map χ' induces a morphism of rings

$$\chi : R = C[T_x, T_y, T_z, T_t] \;\rightarrow\; C(\Gamma_n, \Lambda_\ell, \Upsilon_s)[\xi_{n\ell}],$$

defined by $\chi(T_x^i T_y^j T_z^k T_t^m) = \Gamma_n^i \Delta_\ell^j \Upsilon_s^k \xi_{n\ell s}^m$.

Constructive Approach

1. use the morphism $\chi_t : C[T_x, T_y, T_z, T_t] \;\rightarrow\; C(\Gamma_n, \Lambda_\ell, \Upsilon_s)[T_t]$
2. map a difference equation of a given scheme to $C(\Gamma_n, \Lambda_\ell, \Upsilon_s)[T_t]$ using χ_t, obtain a polynomial in one variable
3. solve the equation in T_t, get the roots $\{t_s\}$
4. the scheme is stable, if $|t_s| \leq 1$ for all the roots
5. obtain the conditions for stability

von Neumann Stability Analysis: Machinery

Yet easier formulation

In order to reduce computations to the polynomial case, we switch to the ring $\mathbb{C}(\triangle t, \triangle x, \triangle y, \triangle z)[g, sin_x, cos_x, \ldots]/\langle sin_x^2 + cos_x^2 - 1, \ldots \rangle$, where $g := T_t = \xi_{n\ell s}$ and $cos_x = \cos(\beta_n \triangle x)$, $sin_x = \sin(\beta_n \triangle x)$ represent $\Gamma_n := e^{J\beta_n \triangle x} = \cos(\beta_n \triangle x) + i \sin(\beta_n \triangle x)$ (analogous for Λ_ℓ, Υ_s).

Constructive Approach

- One needs a routine to solve parametric polynomial equations symbolically and represent the roots in different ways (trigonometric or polynomial).
- For solving the inequalities for the roots symbolically, we use Cylindrical Algebraic Decomposition (CAD). However, one needs to exclude extra components manually.

von Neumann Stability of λ–wave equation I

Let us continue with the example before. Denote $d^2 := \dfrac{4\lambda^2 \triangle t^2}{\triangle h^2}$. Then

$$T_x^2 T_t^2 - 2T_x^2 T_t + 2T_x T_t^2 + T_x^2 - 4T_x T_t + T_t^2 + 2T_x - 2T_t + 1 -$$
$$-d^2(T_x^2 T_t^2 - 2T_x T_t^2 + T_t^2) = 0$$

After performing substitutions $T_t^a T_x^b \mapsto g^a(\cos(\alpha) + isin(\alpha))^b$, we obtain that $g^2 - 2bg + b = 0$ must be true $\forall\ \alpha$, where

$$b = \frac{cos^2(\alpha)}{d^2(1 - cos^2(\alpha)) + cos^2(\alpha)} = \frac{1}{1 + d^2 \tan^2(\alpha)}.$$

The solutions are staightforward: $g = b \pm \sqrt{b^2 - b}$.

Note that $0 \le b \le 1$, then $b^2 - b \le 0$ and the absolute value of each root is $b^2 + b - b^2 = b \le 1$.

Hence, this scheme is **unconditionally stable**.

von Neumann Stability of λ–wave equation II

If we use 2^{nd} order central approximations for both x and t and denote $d := \lambda \frac{\triangle t}{\triangle h}$, we obtain the scheme

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

Denote $b := -1 + 2d^2 \sin^2(\alpha/2)$, then, in terms of operators, $d^2 T_x^2 T_t - T_x T_t^2 + (-2d^2 + 2) T_x T_t - Tx + d^2 T_t = 0$.
The stability polynomial is $g^2 + 2bg + 1 = 0$ and the roots are $b \pm \sqrt{b^2 - 1}$. If $b^2 > 1$, then absolute value of one of the roots is bigger, than one. If $b^2 \leq 1$, the absolute value of both roots equals $b^2 + 1 - b^2 = 1$. And $b^2 \leq 1 \Leftrightarrow d \leq 1$.
This scheme is **conditionally stable** with the condition for the Courant number $d := \lambda \frac{\triangle t}{\triangle h} \leq 1$.

Dispersion Analysis

Continuous dispersion

We call $e^{i(kx-wt)}$ a **Fourier node.** One gets continuous dispersion from the PDE by substituting Fourier nodes into the equation and deriving a relation $w = w(k)$. For the equation above,

$$0 = (\frac{\partial}{\partial t^2} - \lambda^2 \frac{\partial}{\partial x^2}) e^{i(kx-wt)} = -e^{i(kx-wt)} \cdot (w^2 - \lambda^2 k^2)$$

Hence, $w = \pm\lambda k$ is the continuous dispersion relation.

Discrete dispersion

We substitute **discrete Fourier nodes** $F_j^n := e^{i(kx_j - wt_n)}$ into the difference scheme (for u_j^n) and derive a relation $w = w(k)$.
We can see, that $(T_t^a T_x^b) \bullet F_j^n = (e^{-iw\triangle t})^a (e^{ik\triangle x})^b \cdot F_j^n$.

Dispersion Analysis: Symbolic Approach

Discrete dispersion

Presenting discrete Fourier nodes via trigonometrical functions, we are able to compute discrete dispersion relations symbolically.

For simplicity, assume we are dealing with the one–dimensional situation.

Ring and Action

We work in the ring $\mathbb{C}(\triangle t, \triangle x)[sin_t, cos_t, sin_x, cos_x]$ modulo the ideal $\langle sin_x^2 + cos_x^2 - 1, sin_t^2 + cos_t^2 - 1\rangle$, where
$cos_x := \cos(k\triangle x)$, $cos_t := \cos(w\triangle t)$ and so on.
We utilize the action $(T_t^a T_x^b) \bullet F_j^n = (\cos_t - i\sin_t)^a(\cos_x + i\sin_x)^b \cdot F_j^n$.

Dispersion for λ–wave equation

In the scheme, obtained with the 2^{nd} order central approximations for x and t, we denote $d := \lambda \frac{\triangle t}{\triangle h}$.
The correspondent difference polynomial is
$d^2 T_x^2 T_t - T_x T_t^2 + (-2d^2 + 2) T_x T_t - Tx + d^2 T_t = 0$.

Performing computations, we obtain $d^2 \cos_x - cos_t + 1 - d^2 = 0$, that is $\cos(w \triangle t) = 1 - d^2(1 - \cos(k \triangle x))$.
In the so-called stability limit $d \rightarrow 1$, we have even
$\cos(w \triangle t) = \cos(k \triangle x) \Rightarrow w = \pm \frac{\triangle x}{\triangle t} k$.
Since $d \rightarrow 1 \Rightarrow \frac{\triangle x}{\triangle t} \rightarrow \lambda$, In the stability limit the discrete dispersion relation goes to $w = \pm \lambda k$, the continuous dispersion relation.

Main Instruments

Specialized Computer Algebra System SINGULAR

- one of the fastest systems in the area of polynomial computations
- distributed under GPL License (free for academic use)
- many different flavors of Gröbner bases thoroughly implemented
- a non–commutative subsystem PLURAL
- easy C–like programming language
- dynamical modules, namespaces, OPENMATH etc.

General Purpose Computer Algebra System MATHEMATICA

- the system with overwhelmingly many abilities
- very widely used Computer Algebra System
- graphical, user–friendly interface
- a package for intercommunication with SINGULAR

Methodology

1. represent the module and compute the difference scheme by eliminating the module components. (SINGULAR)
2. compute factorized difference polynomials and their mesh presentations. (SINGULAR or MATHEMATICA)
3. apply the stability morphism and perform simplifications (SINGULAR or MATHEMATICA)
4. use Cylindrical Algebraic Decomposition (CAD) for solving the inequalities for the roots (MATHEMATICA)

Work in progress

- algorithmic check of consistency
- application to systems of PDE
- variable coefficients lead us to non–commutative algebras
- Godunov–type schemes, Two–step methods (Lax–Wendroff etc.)