Computer algebra aided generation and analysis of difference approximations to quasilinear evolution equations

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Plan

1. Introduction
2. Evolution equations
3. KdV equation
4. Discretization
5. Numerical experiments
6. Conclusion

Research problem

Solving PDE(s) in practice:

PDE(s) (+ IC or/and BC)

$\Downarrow$

Discretization (FDM, FEM, FVM)

$\Downarrow$

Algebraic equations

$\Downarrow$

Numerical solving

$\Downarrow$

Approximate solution

The main research problem here is to construct a **compatible (mimetic) discretization** which **inherits within the required accuracy** such fundamental properties of the PDE(s) as **conservation laws**, symmetries, maximum principle, etc.

Discretization (Gerdt,Blinkov,Mozzhilkin'2006)

Construction of finite difference approximation (FDA):

1. For an input PDE system complete it to involution.
2. If possible convert PDE into integral conservation law form with a polynomial integrand and choose a control volume (integration contour/surface).
3. Add to the output of the previous step the exact integral relations between derivatives of dependent variables that occur in the output of Step 2.
4. Discretize the obtained equations (on a Cathesian solution grid) by using methods of numerical integration.
5. Eliminate partial derivatives of dependent variables from the obtained difference equations by applying the Gröbner bases technique. This yields FDA to PDE(s) (difference scheme) as the subset of the Gröbner basis that does not contain partial derivatives.

Evolution equations

Let ∂_x be the derivation operator and $\mathcal{R} := \mathbb{Q}(\alpha, \beta, \ldots)\{u\}$ be the ordinary differential polynomial ring over the field $\mathbb{Q}(\alpha, \beta, \ldots)$ of constants (parameters).

Here we consider quasilinear evolution equations (QLEE) of the form

$$u_t = a\, u_m + F(u_{m-1}, \ldots, u_1, u)\,, \quad 0 \neq a \in \mathbb{Q}\,, \quad m \in \mathbb{N}_{>0}$$

where $u_k := \partial_x^k u$ $(0 \leq k \leq m)$, $u_0 := u$ and $F \in \mathcal{R}$ is a differential polynomial of order $m-1$ in ∂_x (denotation: $\mathrm{ord}(F) = m-1$).

If there is a differential polynomial $P \in \mathcal{R}$ such that $F = \partial_x P$ then the equation admits the differential conservation law form

$$u_t = \partial_x\,(a\, u_{m-1} + P)\,, \quad P \in \mathcal{R}\,, \quad \mathrm{ord}(P) = m-2$$

Examples

The set of QLEEs contains most of classical equations (Kudryashov'10):

- Korteveg-de Vries (KdV) hierarchy

$$u_t + u_{xxx} + 6uu_x = 0 \quad \text{(KdV)}$$

$$u_t + u_{xxxxx} + 10u_{xx} + 30u^2u_x + 20u_xu_{xx} = 0$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

- Burgers hierarchy (Burgers equation for $n = 1$)

$$u_t + a\,\partial_x\,(\partial_x + u)^n\,u = 0\,, \quad a \neq 0\,, \quad n \in \mathbb{N}_{\geq 0}$$

- Kuramoto-Sivashinsky equation

$$u_t + uu_x + a\,u_{xx} + b\,u_{xxx} + c\,u_{xxxx} = 0$$

- Burgers-Huxley equation

$$u_t + a\,u_{xx} + b\,uu_x + c\,u + \delta u^2 + d\,u^3 = 0$$

and their various generalizations.

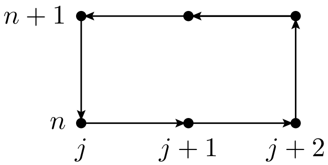
Discretization of QLEE I

If a QLEE admits the differential polynomial conservation law form we convert it into the equivalent integral conservation law form

$$\oint_{\Gamma} (P + a u_{m-1})\, dt + u\, dx = 0$$

where Γ is an arbitrary singly connected integration contour.

We choose the Cartesian grid with $t_{n+1} - t_n = \tau$, $x_{j+1} - x_j = h$ and choose simple rectangular integration contour as a "control volume"



Discretization of QLEE II

To discretize the contour integral we apply a numerical method of its evaluation in term of the grid function

$$u_j^n := u(t_n, x_j)$$

Then we add the (exact) integral relations

$$\int_{x_j}^{x_{j+1}} u_{k+1}\, dx = u_k(t, x_{j+1}) - u_k(t, x_j)\,, \quad k = 1, \ldots, m-2$$

and approximate the integrals numerically on the grid.

As a result, we obtain a system of difference equations containing

$$u_j^n, {u_1}_j^n, \ldots, {u_{m-1}}_j^n$$

Finally, difference elimination of partial derivatives yields FDA.

KdV equation

To be specific, we consider the nonlinear evolution Korteveg-de Vries equation (KdV) in the following form

$$f = 0, \quad f := u_t + \alpha u u_x + \beta u_{xxx}\,, \quad u = u(t,x)\,, \quad \alpha, \beta \in \mathcal{R}\,.$$

It has **infinitely many** local conservation laws

$$\{\,\underbrace{\partial_t T_i + \partial_x X_i}_{\mathfrak{C}_i} = 0|_{f=0} \implies \frac{d}{dt}\int_{-\infty}^{\infty} T_i dx + [X_i]_{-\infty}^{\infty} = 0 \mid i \in \mathbb{N}_{\geq 1}\,\}$$

where $T_i = T_i(u)$ are densities and $X_i = X_i(u)$ are fluxes.

Conserved densities and fluxes

For $\alpha = 3$, $\beta = 1$ the low order conservation laws are given by

i	T_i and X_i
1	$T_1 = u \qquad X_1 = 3u^2 + u_{xx}$
2	$T_2 = u_x \qquad X_2 = 6uu_x + u_{xxx}$
3	$T_3 = u^2 + u_{xx} \quad X_3 = 5u_x^2 + 8uu_{xx} + 4u^3 + u_{xxxx}$
4	$T_4 = 4uu_x + u_{xxx}$
	$X_4 = 18u_x u_{xx} + 24u^2 u_x + 10uu_{xxx} + u_{xxxxx}$
5	$T_5 = 2u^3 + 6uu_{xx} + 10u_x^2 + u_{xxxx}$
	$X_5 = 42u^2 u_{xx} + 19u_{xx}^2 + 60uu_x^2 + 28u_x u_{xxx} + 12uu_{xxxx} + 9u^4 + u_{xxxxxx}$
...	....

These conservation laws were computed by using Maple package PDEBellII (Miao,Wang,Chen,Yang'14).

Conservation laws expressed via f

Conservation laws $\mathfrak{C}_i$ belong to the radical differential ideal $[\![f]\!] \subset \mathcal{R} = \mathbb{Q}(\alpha,\beta)\{u\}$ generated by f. In particular,

i	$\mathfrak{C}_i$	$\mathrm{ord}_x(\mathfrak{C}_i)$
1	f	3
2	f_x	4
3	$f_{xx} + 2uf$	5
4	$f_{xxx} + uf_x^4 + u_x^4 f$	6
5	$f_{xxxx} + 6uf_{xx} + 5u_x f_x + 6u_{xx} f + 6u^2 f$	7
...	....	......

$\mathfrak{C}_i$ were computed by using Maple package DifferentialThomas (Bächler,Gerdt,Lange-Hegermann,Robertz'12).

Discretization of KdV I

Integral conservation law form

$$u_t + (P + \beta u_{xx})_x = 0 \iff \oint_\Gamma -(P + \beta u_{xx})\, dt + u\, dx = 0$$

and chose the integration contour with $t_{n+1} - t_n = \tau$, $x_{j+1} - x_j = h$
Integral relations

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

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

Discretization of KdV II

To approximate numerically the contour integral, we apply the trapezoidal rule to integration over t and the midpoint rule to integration over x.

For numerical approximations of the integral relations we apply the trapezoidal rule for the integration of u_x and the midpoint rule for the integration of u_{xx}. This leads to the difference approximation to KdV which is outputted by the following MAPLE code (Gerdt, Blinkov, Marinov'17)

Maple code

```
> restart:
> with(LDA):
> L:=[(-(P(n,j)+P(n+1,j)-P(n,j+2)-P(n+1,j+2))-(beta*uxx(n,j)+beta*uxx(n+1,j)
  -beta*uxx(n,j+2)-beta*uxx(n+1,j+2)))*tau/2+(u(n+1,j+1)-u(n,j+1))*2*h,
   (ux(n,j+1)+ux(n,j))*h/2-(u(n,j+1)-u(n,j)),
    2*uxx(n,j+1)*h-(ux(n,j+2)-ux(n,j))]:
> JanetBasis(L,[n,j],[uxx,ux,u,F],2):
> collect(%[1,1]/(4*tau*h**3),[tau,h]);
```

$$\frac{\frac{1}{4}P(n+1,j+3)+\frac{1}{4}P(n,j+3)-\frac{1}{4}P(n+1,j+1)-\frac{1}{4}P(n,j+1)}{h}+\frac{1}{h^3}\Big(\frac{1}{4}\beta\,u(n+1,j+4)-\frac{1}{2}\beta\,u(n+1,j+3)+\frac{1}{4}\beta\,u(n,j+4)-\frac{1}{2}\beta\,u(n,j+3)+\frac{1}{2}\beta\,u(n+1,j+1)-\frac{1}{4}\beta\,u(n+1,j)+\frac{1}{2}\beta\,u(n,j+1)-\frac{1}{4}\beta\,u(n,j)\Big)+\frac{u(n+1,j+2)-u(n,j+2)}{\tau}$$

Computer algebra software used

To perform algebraically the difference elimination of the grid functions, that correspond to partial derivatives of u, from the obtained discrete system we use the Maple package LDA (Linear Difference Algebra).

LDA created by D.Robertz (RWTH, Aachen) is freely available (http://wwwb.math.rwth-aachen.de/Janet/). It implements the involutive algorithm (Gerdt,Blinkov'98) based on Janet division and specialized to difference ideals generated by linear difference polynomials.

Note that to apply LDA we "hide" the nonlinearity (caused by the presence of u^2 in the input difference equations) into the extra grid function $P_j^n := \alpha(u_j^n)^2/2$.

Numerical solving of KdV

In the conventional notations the obtained discretization (difference scheme) reads

$$\tilde{f} = 0\,, \quad \text{where} \quad \tilde{f} := \frac{u_j^{n+1} - u_j^n}{\tau} + \frac{(P_{j+1}^{n+1} - P_{j-1}^{n+1}) + (P_{j+1}^n - P_{j-1}^n)}{4h}$$
$$+ \frac{\beta(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + 2u_{j-1}^{n+1} - u_{j-2}^{n+1}) + \beta(u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n)}{4h^3}\,.$$

To construct a numerical solution to KdV we apply the method of simple iteration and exploit the following approximation

$$v_{k+1}^2 = v_{k+1}^2 - v_k^2 + v_k^2 = (v_{k+1} - v_k)(v_{k+1} + v_k) + v_k^2 \approx v_{k+1} \cdot 2v_k - v_k^2\,.$$

Properties of the FDA (scheme) derived I

Using the library SymPy (http://www.sympy.org/en/) written in Python we computed the modified equation for KdV with $\alpha = 3, \beta = 1$.

$$
\begin{gathered}
u_t + 6u_1 u + u_3 + \\
\tau^2 (108 u_1^3 u + 81 u_1^2 u_3 + 99 u_1 u_2^2 + 162 u_1 u_2 u^2 + \\
63 u_1 u_4 u + 6 u_1 u_6 + 99 u_2 u_3 u + \frac{27}{2} u_2 u_5 + 21 u_3 u_4 + \\
18 u_3 u^3 + 9 u_5 u^2 + \frac{3}{2} u_7 u + \frac{1}{12} u_9) + \\
h^2 (3 u_1 u_2 + u_3 u + \frac{1}{4} u_5) + O(h^4) + O(\tau^4) + O(\tau^2 h^2) = 0\,,
\end{gathered}
$$

where

$$u_k := u_{\underbrace{xx\cdots x}_{k \text{ times}}}.$$

Properties of the FDA (scheme) derived II

1. The modified equation shows that the scheme has the 2-nd order in τ and in h.
2. This also implies that the scheme is (strongly) consistent.
3. The scheme is implicit, and hence it is unconditionally stable.
4. Because of universally adopted condition for convergency of difference schemes (rigorously proved for linear Cauchy problem - the Lax-Richtmyer equivalence theorem):

$$\text{convergence} = \text{consistency} + \text{stability}$$

the obtained scheme is convergent.

FDA to conservation laws I

The difference polynomial $\tilde{f}$ generates the perfect difference ideal $[\![\tilde{f}]\!]$ in the inversive difference polynomial ring with differences σ_t, $\sigma_x, \sigma_t^{-1}, \sigma_x^{-1}$ where

$$\sigma_t \circ \tilde{f}_j^n = \tilde{f}_j^{n+1},\ \sigma_x \circ \tilde{f}_j^n = \tilde{f}_{j+1}^n,\ \sigma_t^{-1} \circ \tilde{f}_j^n = \tilde{f}_j^{n-1},\ \sigma_x^{-1} \circ \tilde{f}_j^n = \tilde{f}_{j-1}^n .$$

The consistency of $\tilde{f} = 0$ with $f = 0$ implies that every element in $[\![f]\!]$ is approximated by an element in $[\![\tilde{f}]\!]$ (strong consistency).

We illustrate this fact by the 3rd and 4th KdV conservation laws

$$\begin{aligned} \mathfrak{C}_3 &= f_{xx} + 2uf\ , \\ \mathfrak{C}_4 &= f_{xxx} + uf_x^4 + u_x^4 f\ . \end{aligned}$$

FDA to conservation laws II

With regard to forward and backward differences

$$\Delta_p := \frac{1}{h}\left(\sigma_x - 1\right), \qquad \Delta_m := \frac{1}{h}\left(1 - \sigma_x^{-1}\right).$$

we obtain

$$\frac{1}{2}\left(\Delta_p + \Delta_m\right) \circ u \xrightarrow[h\longrightarrow 0]{} u_x + \mathcal{O}(h^2),$$

$$\frac{1}{2}\left(\Delta_p + \Delta_m\right) \circ f \xrightarrow[h\longrightarrow 0]{} f_x + \mathcal{O}(h^2),$$

$$\Delta_m\,\Delta_p \circ f \xrightarrow[h\longrightarrow 0]{} f_{xx} + \mathcal{O}(h^2),$$

$$\Delta_p\,\Delta_m\,\Delta_p \circ f - \frac{h}{2}\,\Delta_m\,\Delta_p\,\Delta_m\,\Delta_p \circ f \xrightarrow[h\longrightarrow 0]{} f_{xxx} + \mathcal{O}(h^2).$$

Other schemes with $\mathcal{O}(\tau^2, h^2)$ approximation

Scheme I

$$u_i^{n+1} = u_i^{n-1} - \frac{\alpha\tau}{h} u_i^n \left(u_{i+1}^n - u_{i-1}^n\right) - \frac{\beta\tau}{h^3}\left(u_{i+2}^n - 2u_{i+1}^n + 2u_{i-1}^n - u_{i-2}^n\right)$$

This explicit scheme (Belashov,Vladimirov'05, Eq.1.80) is stable for

$$\tau \leq \frac{2h^3}{3\sqrt{3}\beta} \cong 0.384\frac{h^3}{\beta}\,.$$

Scheme II

The implicit scheme (Belashov,Vladimirov'05, Eq.1.96)

$$\frac{u_j^{n+1} - u_j^n}{\tau} + \frac{\alpha}{4h}\left[u_j^n\left(u_{j+1}^{n+1} - u_{j-1}^{n+1}\right) + u_j^{n+1}\left(u_{j+1}^n - u_{j-1}^n\right)\right] +$$
$$+ \frac{\beta}{4h^3}\left(\left(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + 2u_{j-1}^{n+1} - u_{j-2}^{n+1}\right) + \right.$$
$$\left. + \left(u_{j+2}^n - 2u_j^{n+1} + 2u_{j-1}^n - u_{j-2}^n\right)\right) = 0\,.$$

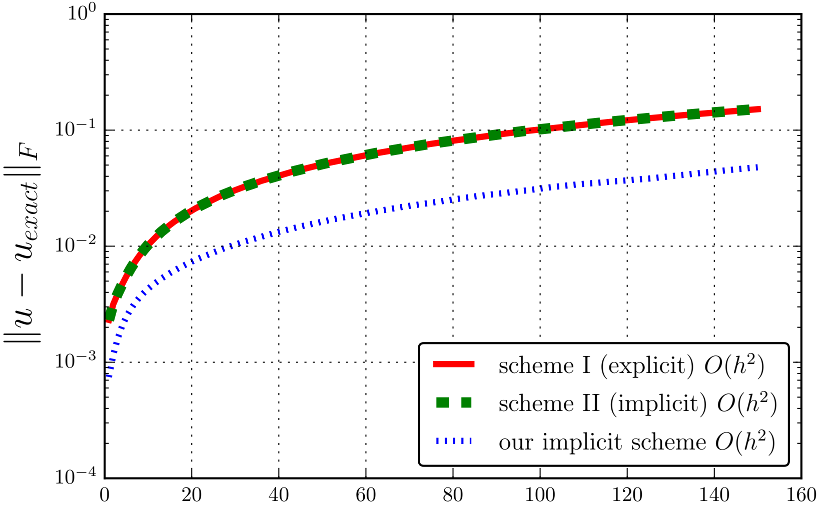
Computational experiment I

Our numerical analysis of the above difference schemes was done with the Python package SciPy (http:\scipy.org). As a benchmark, we used the exact one-soliton solution

$$u_{\text{exact}}(x,y) = \frac{2k_1^2}{\cosh(k_1(x - 4k_1^2 t))^2}$$

to the KdV with $\alpha = 6$, $\beta = 1$ and $k_1 = 0.4$. In so doing, we fixed $h = 0.25$ and considered the solution in interval $-50 \le x \le 50$ with periodic boundary conditions (cf. Belashov,Vladimirov'05, p.49). The numerical inaccuracy was estimated by the Frobenius norm.

Computational experiment II



Conclusions

- We considered a class of nonlinear evolution PDEs containing the classical KdV equation which has exact multi-soliton solutions and infinitely many conservation laws.
- We generated a FDA (implicit difference scheme) to KdV with $\mathcal{O}(\tau^2, h^2)$ approximation. The scheme is consistent and stable.
- The conservation laws of KdV are approximated with accuracy $\mathcal{O}(\tau^2, h^2)$ by difference consequences of the scheme.
- Experimental comparison, on the exact one-soliton solution, of the constructed scheme with some other schemes of the same accuracy reveals its numerical superiority.

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