Stability theory for finite-difference schemes using modified equations

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Introduction to modified equations

For instance, let us consider the scalar transport equation :

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

where $c > 0$, and let us consider the following numerical scheme, for example :

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 \qquad (1)$$

where Δt and Δx are respectively the discrete time step and the mesh size.
After we use Taylor expansions in the vicinity of (x_i, t^n)

$$u_i^{n+1} = u(x_i, t^{n+1}) = u(x_i, t^n + \Delta t) = u_i^n + \Delta t\frac{\partial u_i^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u_i^n}{\partial t^2} + O(\Delta t^3)$$

$$u_{i-1}^n = u(x_{i-1}, t^n) = u(x_i - \Delta x, t^n) = u_i^n - \Delta x\frac{\partial u_i^n}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 u_i^n}{\partial x^2} + O(\Delta x^3)$$

and replace in the scheme (1) in order to get the scheme truncation error :

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} - \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + c\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + O(\Delta t^2, \Delta x^2) \qquad (2)$$

Now, for physical interpretation, we would like to have only space derivatives in the right hand side.

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Replace $\frac{\partial^2 u_i^n}{\partial t^2}$ by $\frac{\partial}{\partial t}(2)$ in (2), then :

$$\begin{aligned}\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} &= -c^2\frac{\Delta t}{2}\frac{\partial^2 u}{\partial x^2} + c\frac{\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + O(\Delta t^2, \Delta x^2) \\ &= c\frac{\Delta x}{2}\left(1 - c\frac{\Delta t}{\Delta x}\right)\frac{\partial^2 u}{\partial x^2} + O(\Delta t^2, \Delta x^2)\end{aligned}$$

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After we use Taylor expansions in the vicinity of $(x_i; t^n)$ and replace in the scheme (1) in order to get the scheme truncation error :

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Then, the modified equation is :

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = c\frac{\Delta x}{2}\left(1 - c\frac{\Delta t}{\Delta x}\right)\frac{\partial^2 u}{\partial x^2} + O(\Delta t^2; \Delta x^2)$$

The scheme is stable only if

$$1 - c\frac{\Delta t}{\Delta x} \geq 0$$

Heuristic stability theory : heat equation

PDE

$$\frac{\partial u}{\partial t} \quad Q\frac{\partial^2 u}{\partial x^2} = 0; \quad Q > 0$$

Scheme

$$\frac{u_i^{n+1} \quad u_i^n}{\Delta t} \quad Q\frac{u_{i+1}^n \quad 2u_i^n + u_{i\ \ 1}^n}{\Delta x^2} = 0$$

This scheme is stable under the condition :

$$Q\frac{\Delta t}{\Delta x^2} \quad \frac{1}{2}$$

Modified equation

$$\frac{\partial u}{\partial t} = Q\frac{\partial^2 u}{\partial x^2} \quad \frac{Q}{12}\ \ 6Q\Delta t \quad \Delta x^2\ \ \frac{\partial^4 u}{\partial x^4} + \frac{Q}{360}(\Delta x^4 + 30Q\Delta t(\quad \Delta x^2 + 4Q\Delta t))\frac{\partial^6 u}{\partial x^6} + O(\Delta t^2; \Delta x^4)$$

Heuristic stability theory : heat equation

PDE

$$\frac{\partial u}{\partial t} - Q\frac{\partial^2 u}{\partial x^2} = 0; \quad Q > 0$$

Scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - Q\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = 0$$

This scheme is stable under the condition :

$$Q\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$$

Modified equation

$$\frac{\partial u}{\partial t} = Q\frac{\partial^2 u}{\partial x^2} - \frac{Q}{12}\left(6Q\Delta t - \Delta x^2\right)\frac{\partial^4 u}{\partial x^4} + \frac{Q}{360}\left(\Delta x^4 + 30Q\Delta t(-\Delta x^2 + 4Q\Delta t)\right)\frac{\partial^6 u}{\partial x^6} + O(\Delta t^2; \Delta x^4)$$

We look at the sign of the even order coefficients

$Q \geq 0$

$\frac{Q}{12}(6Q\Delta t - \Delta x^2) \geq 0 \;,\; Q\frac{\Delta t}{\Delta x^2} \geq \frac{1}{6}$

...

Heuristic stability theory : heat equation

PDE

$$\frac{\partial u}{\partial t} - Q\frac{\partial^2 u}{\partial x^2} = 0, \quad Q > 0$$

Scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - Q\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = 0$$

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- $Q \geq 0$
- $\frac{Q}{12}(6Q\Delta t - \Delta x^2) \leq 0 \ , \ Q\frac{\Delta t}{\Delta x^2} \leq \frac{1}{6}$
- ...

This shows the limitations of the heuristic approach.

Project goal and subject

Project goal

To establish a clear link between the stability condition of a numerical scheme for a given PDE system and an associated modified equation.

Next step : Once this is completed, retrieve the stability conditions presented in (P. Noble and J. P. Vila. "Stability theory for difference approximations of euler korteweg equations and application to thin film flows". In: (2014), pp. 1–22. arXiv: arXiv:1304.3805v2)

State of the art

Presented the heuristic stability theory and also tried for non linear pdes.
M. C. Hirt. \Heuristic Stability Theory for Finite-Di erence Equations". In:Journal of Computational Physics2 (1968), pp. 339{355

The connection between the modi ed equation and the von Neumann (Fourier) method is established.
R. F. Warming and B. J. Hyett. \The Modi ed Equation Approach to the Stability and Accuracy Analysis of Finite-Di erence Methods". In:Journal of Computational Physics179 (1974), pp. 159{179

An alternative approach on how to derive the modi ed equation for linear problems
Romuald Carpentier, Armel de la Bourdonnaye, and Larrouturou Bernard. \On the derivation of the modi ed equation for the analysis of linear numerical methods". In: 31.4 (1997), pp. 459{4

Von Neumann stability analysis

Given a linear PDE :

$$u_t + L_x(u) = 0$$

assume we have a consistent one-step linear scheme given in general as :

$$\sum_{q=-m_l}^{m_r} B_q u_{j+q}^{n+1} = \sum_{p=-n_l}^{n_r} A_p u_{j+p}^{n}$$

We replace every u_j^n by $v(k)^n \exp(ikj\Delta x)$ and define the amplification factor as:

$$g(k) = \frac{v(k)^{n+1}}{v(k)^n} = \frac{\sum_{p=-n_l}^{n_r} A_p \exp(ipk\Delta x)}{\sum_{q=-m_l}^{m_r} B_q \exp(iqk\Delta x)}$$

A necessary and sufficient stability condition is :

$$|g(k)| \leq 1$$

Von Neumann stability analysis

In order to get a more practical formulation of this condition, we can show that the square of the modulus can be given by :

$$|g(k)|^2 = 1 - 4z^r \frac{S(z)}{P(z)}$$

where :

- $z = \sin^2(k\Delta x/2)$.
- $r \geq 1$ is an integer. It is the maximum power of z that can be put as a common factor in the numerator.
- $S(z) = \sum_{i=0}^{s} \sigma_i z^i$ is a polynomial function of z such that $S(0) \neq 0$.
- $P(z) = \sum_{i=0}^{d} \pi_i z^i > 0$ is a polynomial function of z such that $P(0) = 1$

Therefore, the stability condition becomes :

$$|g(k)|^2 \leq 1 \quad \Leftrightarrow \quad S(z) \geq 0 \quad \forall z \in [0;1]$$

Modified equations - Elementary wave solution

Consider the modified equation obtained after replacing all the time derivatives by space derivatives

$$\frac{\partial u}{\partial t} = \sum_{p=1}^{\infty} \alpha(p) \frac{\partial^p u}{\partial x^p}$$

We split even and odd derivatives of this series as follows :

$$\frac{\partial u}{\partial t} = \sum_{p=0}^{\infty} \alpha(2p+1) \frac{\partial^{2p+1} u}{\partial x^{2p+1}} + \sum_{p=1}^{\infty} \alpha(2p) \frac{\partial^{2p} u}{\partial x^{2p}}$$

Assume an elementary solution of the modified equation (9) in the form $u = e^{\omega t} e^{ikx}$ then this solution must verify :

$$\omega = \sum_{p=0}^{\infty} i(-1)^p \alpha(2p+1) k^{2p+1} + \sum_{p=1}^{\infty} (-1)^p \alpha(2p) k^{2p}$$

If we further divide $\omega = a + ib$ where a and b are reals we get :

$$\boxed{a = \sum_{p=1}^{\infty} (-1)^p \alpha(2p) k^{2p}} \quad ; \quad b = \sum_{p=0}^{\infty} (-1)^p \alpha(2p+1) k^{2p+1}$$

Link to the Von Neumann stability analysis

The amplification factor $g_m(k)$ of the elementary solution $u = e^{\omega t}e^{ikx}$ is :

$$\frac{u(x;t+\Delta t)}{u(x;t)} = \frac{e^{\omega(t+\Delta t)}e^{ikx}}{e^{\omega t}e^{ikx}} = e^{\omega\Delta t} = e^{a\Delta t}e^{ib\Delta t} = |g_m(k)|\,e^{ib\Delta t}$$

Therefore :

$$|g_m(k)| = e^{a\Delta t} = \exp\left(\Delta t\sum_{p=1}^{\infty}(-1)^p\alpha(2p)k^{2p}\right)$$

Since the numerical solution verifies the modified equation (9) then its amplification factor is the same as the elementary solution :

$$|g(k)| = |g_m(k)| \Rightarrow |g(k)|^2 - |g_m(k)|^2 = 0$$

Which yields:

$$\boxed{1 - 4z^r\frac{S(z)}{P(z)} - \exp\left(2\Delta t\sum_{p=1}^{\infty}(-1)^p\alpha(2p)k^{2p}\right) = 0}$$

Which we can express as :

$$H(\xi) = 0; \qquad \xi = k\Delta x$$

Expanding the left hand side into power series of ξ permits to obtain coefficients of $S(z)$.

Determining the form of the ampli cation factor

If we note n_{ex} = The number of grid points around u_j^n. n_{im} = The number of grid points around u_j^{n+1} then :

- The least even order appearing in the modi ed equation is $2r$
- $s = \max(n_{ex}; n_{im}) - r$ (except very particular cases)
- $d = n_{im}$

This gives a precise form of the ampli cation factor :

$$|g(k)| = 1 - 4z^r \frac{\sum_{i=0}^{s} \alpha_i z^i}{1 + \sum_{i=1}^{d} \beta_i z^i}$$

$\Rightarrow$ The unknowns in the ampli cation factor are $(\alpha_0 \ldots \alpha_s; \beta_1 \ldots \beta_d) \Rightarrow s + d + 1$ unknowns.

Optimizing the procedure

Instead of developing $H(\ )$ as a function of , it is better to develop the following function :

$$\frac{H(\ )}{2r} = F(\ ^{2}) = F(\ )$$

It is sufficient to develop F in a power series to the order $s + d$:

$$F(\ ) = \sum_{k=0}^{s+d} c_k(\ (i);\ _0 \ldots\ _s;\ _1 \ldots\ _d)\ ^k + R(\ )$$

and set then set all the coefficients equal to zero :

$$c_k(\ (i);\ _0 \ldots\ _s;\ _1 \ldots\ _d) = 0 \qquad \forall k \in \{0, \ldots, s + d\}$$

Which permits to obtain $|g(k)|^2$.

Example : scheme for the heat equation

We consider the heat equation ($Q > 0$):

$$\frac{\partial u}{\partial t} = Q \frac{\partial^2 u}{\partial x^2}$$

$$\frac{u_i^{n+1} \quad u_i^n}{t} = \quad Q \frac{u_{i\ 1}^n \quad 2u_i^n + u_{i+1}^n}{x^2} + (1 \quad) Q \frac{u_{i\ 1}^{n+1} \quad 2u_i^{n+1} + u_{i+1}^{n+1}}{x^2}$$

The grid points used in the scheme besides u_i^n and u_i^{n+1} are $u_{i\ 1}^n$ and $u_{i\ 1}^{n+1}$ therefore :

$$n_{ex} = n_{im} = 2 \Rightarrow \boxed{d = 2}$$

The modified equation up to 4th order is given by :

$$\frac{\partial u}{\partial t} = Q \frac{\partial^2 u}{\partial x^2} \quad \frac{Q \quad x^2}{12} (\quad 1 + 6 \quad (2 \quad 1)) \frac{\partial^4 u}{\partial x^4}$$

least non-zero even order derivative : $2r = 2 \Rightarrow \boxed{r = 1}$ and $s = \max(n_{ex}; n_{im}) \quad r \Rightarrow \boxed{s = 1}$.

$$\Rightarrow |g(k)|^2 = 1 \quad 4z \frac{_0 + \ _1 z}{1 + \ _1 z + \ _2 z^2}$$

Possible extensions

Linear scalar equations

- nice code
- gives stability condition for a large class of schemes
- based on a combination of Von Neumann analysis and modified equations

Nonlinear scalar equations

Linear systems

Possible extensions: difficulties

Nonlinear scalar equations

Von Neumann analysis requires Fourier transformation which demands linearization.

If one finally decides to linearize, it will kill the nonlinear nature of the equation.

Burgers equation:

$$u_t + uu_x = 0 \qquad \Longrightarrow \qquad u_t + u_0 u_x = 0.$$

Linear systems

It is not obvious how to get the same S-form of the amplification factor of the scheme.

Operators do not commute $\Longrightarrow$ the same code can not be used to derive the modified equations.

What next?

Linear scalar equations

- nice code
- gives stability condition for a large class of schemes
- based on a combination of Von Neumann analysis and modified equations

Nonlinear scalar equations

Problems:

- Von Neumann analysis kills nonlinearity

Linear systems

Warming approach

Problems:

- Operators do not commute
- Amplification factor for Von Neumann analysis is more difficult to obtain

Entropy stability

+ modified equations

?

Entropy stability of linear systems

Linear hyperbolic system:

$$\mathbf{u}_t + A\mathbf{u}_x = 0;$$

Entropy conservation law:

$$(\mathbf{u})_t + H(\mathbf{u})_x = 0.$$

Entropy stability condition:

$$\frac{d}{dt}\int_\Omega (\mathbf{u})dx \quad 0.$$

The numerical analog:

$$\sum_{i=1}^{N} \frac{(\ {}_i^{n+1} \quad {}_i^{n})\Delta x}{\Delta t} \quad 0.$$

Entropy stability + modified equations

Question: how can we use modified equations for the entropy stability study?

- Write a numerical scheme for a hyperbolic system which admits an entropy conservation law,
- Multiply it by the vector of entropy variables $\frac{\partial}{\partial \mathbf{u}}$,
- Derive a numerical analog of the entropy equation,
- Apply Warming's approach for the obtained equation.

Example: linearized shallow water equations

Shallow water system linearized around the steady state $u = 0$, $h = h_0$:

$$
\begin{aligned}
{}_t + h_0 v_x &= 0; \\
v_t + g \ {}_x &= 0:
\end{aligned}
$$

The entropy equation:

$$
\left(\begin{aligned} g \quad {}_t + g h_0 \ v_x &= 0 \\ h_0 v v_t + g h_0 v \ {}_x &= 0 \end{aligned} \right. \quad =) \quad \boxed{ \left(\frac{g \ ^2 + h_0 v^2}{2} \right)_t + (g h_0 \ v)_x = 0: }
$$

The entropy couple of the system:

$$
(\mathbf{u}) = \frac{g \ ^2 + h_0 v^2}{2}; \qquad H(\mathbf{u}) = g h_0 \ v:
$$

Associated entropy variables:

$$
\frac{@}{@} = g \ ; \qquad \frac{@}{@v} = h_0 v:
$$

Example: linearized shallow water equations

Backward Euler scheme:

$$\frac{\mathbf{u}_i^{n+1} - \mathbf{u}_i^n}{\Delta t} + A\frac{\mathbf{u}_i^n - \mathbf{u}_{i-1}^n}{\Delta x} = 0, \qquad \mathbf{u}_i^n = (\eta_i^n, v_i^n)^T.$$

Multiplying it by $\left(\frac{\partial \mathcal{U}}{\partial \mathbf{u}}\right)_i^n = (g\eta_i^n, h_0 v_i^n)^T$, we get the numerical entropy equation:

$$\frac{\mathcal{U}_i^{n+1} - \mathcal{U}_i^n}{\Delta t} + \frac{H_i^n - H_{i-1}^n}{\Delta x} = -\frac{gh_0}{\Delta x}(\eta_i^n - \eta_{i-1}^n)(v_i^n - v_{i-1}^n) + \frac{g}{2\Delta t}(\eta_i^{n+1} - \eta_i^n)^2 + \frac{h_0}{2\Delta t}(v_i^{n+1} - v_i^n)^2.$$

It is possible to derive the modified equation, but a more complex algorithm is needed. However, the obtained modified equation will be non-linear.

Conclusions and perspectives

Done: Developed the code which

- Computes the modified equation for a given linear scalar PDE
- Automatically derives the stability condition, based on Warming's approach.

In progress:

- Study of the entropy stability coupled with modified equations (dealing with non-linearities)
- Development of the code to derive modified equations for linear PDE systems