Analysis of numerical dissipation and dispersion

Modified equation method: *the exact solution of the discretized equations satisfies a PDE which is generally different from the one to be solved*

Original PDE | Modified equation $Au^{n+1} = Bu^n$

$$\frac{\partial u}{\partial t} + \mathcal{L}u = 0 \qquad \approx \qquad \frac{\partial u}{\partial t} + \mathcal{L}u = \sum_{p=1}^{\infty} \alpha_{2p} \frac{\partial^{2p} u}{\partial x^{2p}} + \sum_{p=1}^{\infty} \alpha_{2p+1} \frac{\partial^{2p+1} u}{\partial x^{2p+1}}$$

Motivation: PDEs are difficult or impossible to solve analytically but their *qualitative behavior* is easier to predict than that of discretized equations

- Expand all nodal values in the difference scheme in a double Taylor series about a single point (x_i, t^n) of the space-time mesh to obtain a PDE
- Express high-order time derivatives as well as mixed derivatives in terms of space derivatives using **this** PDE to transform it into the desired form

Derivation of the modified equation

Example. Pure convection equation $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0, \quad v > 0$

BDS in space, FE in time: $\frac{u_i^{n+1} - u_i^n}{\Delta t} + v\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$ (upwind)

Taylor series expansions about the point (x_i, t^n)

$$u_i^{n+1} = u_i^n + \Delta t \left(\frac{\partial u}{\partial t}\right)_i^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n + \frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)_i^n + \dots$$

$$u_{i-1}^n = u_i^n - \Delta x \left(\frac{\partial u}{\partial x}\right)_i^n + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n - \frac{(\Delta x)^3}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i^n + \dots$$

Substitution into the difference scheme yields

$$\left(\frac{\partial u}{\partial t}\right)_i^n + v\left(\frac{\partial u}{\partial x}\right)_i^n = -\frac{\Delta t}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n - \frac{(\Delta t)^2}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)_i^n + \frac{v\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n - \frac{v(\Delta x)^2}{6}\left(\frac{\partial^3 u}{\partial x^3}\right)_i^n + \dots$$

original PDE $\mathcal{O}[\Delta t, \Delta x]$ *truncation error* $(*)$

Next step: replace both time derivatives in the RHS by space derivatives

Derivation of the modified equation

Differentiate $(*)$ with respect to t

$$\frac{\partial^2 u}{\partial t^2} + v\frac{\partial^2 u}{\partial x \partial t} = -\frac{\Delta t}{2}\frac{\partial^3 u}{\partial t^3} - \frac{(\Delta t)^2}{6}\frac{\partial^4 u}{\partial t^4} + \frac{v\Delta x}{2}\frac{\partial^3 u}{\partial x^2 \partial t} - \frac{v(\Delta x)^2}{6}\frac{\partial^4 u}{\partial x^3 \partial t} + \dots \quad (1)$$

Differentiate $(*)$ with respect to x and multiply by v

$$v\frac{\partial^2 u}{\partial t \partial x} + v^2\frac{\partial^2 u}{\partial x^2} = -\frac{v\Delta t}{2}\frac{\partial^3 u}{\partial t^2 \partial x} - \frac{v(\Delta t)^2}{6}\frac{\partial^4 u}{\partial t^3 \partial x} + \frac{v^2\Delta x}{2}\frac{\partial^3 u}{\partial x^3} - \frac{v^2(\Delta x)^2}{6}\frac{\partial^4 u}{\partial x^4} + \dots \quad (2)$$

Subtract (2) from (1) and drop high-order terms

$$\frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2} + \frac{\Delta t}{2}\left[-\frac{\partial^3 u}{\partial t^3} + v\frac{\partial^3 u}{\partial t^2 \partial x} + \mathcal{O}(\Delta t)\right] + \frac{\Delta x}{2}\left[v\frac{\partial^3 u}{\partial x^2 \partial t} - v^2\frac{\partial^3 u}{\partial x^3} + \mathcal{O}(\Delta x)\right] \quad (3)$$

Differentiate formula (3) with respect to t $$\frac{\partial^3 u}{\partial t^3} = v^2\frac{\partial^3 u}{\partial x^2 \partial t} + \mathcal{O}[\Delta t, \Delta x] \quad (4)$$

Differentiate formula (2) with respect to x $$\frac{\partial^3 u}{\partial x^2 \partial t} = -v\frac{\partial^3 u}{\partial x^3} + \mathcal{O}[\Delta t, \Delta x] \quad (5)$$

Differentiate formula (3) with respect to x $$\frac{\partial^3 u}{\partial t^2 \partial x} = v^2\frac{\partial^3 u}{\partial x^3} + \mathcal{O}[\Delta t, \Delta x] \quad (6)$$

Derivation of the modified equation

Equations (4) and (5) imply that $\frac{\partial^3 u}{\partial t^3} = -v^3 \frac{\partial^3 u}{\partial x^3} + \mathcal{O}[\Delta t, \Delta x]$ (7)

Plug (5)–(7) into (3) $\Rightarrow$ $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} + v^2 (v\Delta t - \Delta x) \frac{\partial^3 u}{\partial x^3} + \mathcal{O}[\Delta t, \Delta x]$ (8)

Substitute (7) and (8) into (∗) to obtain the modified equation

$$\frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} = -\frac{v^2 \Delta t}{2} \left[\frac{\partial^2 u}{\partial x^2} + (v\Delta t - \Delta x) \frac{\partial^3 u}{\partial x^3} \right] + \frac{v^3 (\Delta t)^2}{6} \frac{\partial^3 u}{\partial x^3} + \frac{v \Delta x}{2} \frac{\partial^2 u}{\partial x^2} - \frac{v (\Delta x)^2}{6} \frac{\partial^3 u}{\partial x^3} + \ldots$$

which can be rewritten in terms of the Courant number $\nu = v \frac{\Delta t}{\Delta x}$ as follows

$$\frac{\partial u}{\partial t} + v \frac{\partial u}{\partial x} = \underbrace{\frac{v \Delta x}{2} (1 - \nu) \frac{\partial^2 u}{\partial x^2}}_{numerical\ diffusion} + \underbrace{\frac{v (\Delta x)^2}{6} (3\nu - 2\nu^2 - 1) \frac{\partial^3 u}{\partial x^3}}_{numerical\ dispersion} + \ldots$$

Remark. The CFL stability condition $\nu \leq 1$ must be satisfied for the discrete problem to be well-posed. In the case $\nu > 1$, the numerical diffusion coefficient $\frac{v \Delta x}{2}(1 - \nu)$ is negative, which corresponds to a *backward heat equation*

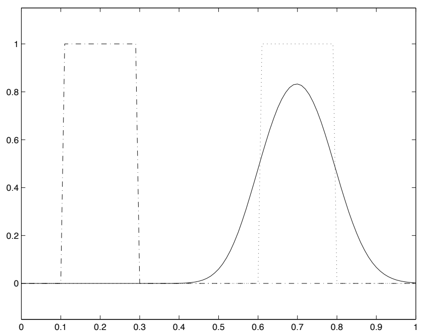
Significance of terms in the modified equation

Exact solution of the discretized equations

$$Au^{n+1} = Bu^n \quad \longleftrightarrow \quad \frac{\partial u}{\partial t} + \mathcal{L}u = \sum_{p=1}^{\infty} \alpha_{2p} \frac{\partial^{2p} u}{\partial x^{2p}} + \sum_{p=1}^{\infty} \alpha_{2p+1} \frac{\partial^{2p+1} u}{\partial x^{2p+1}}$$

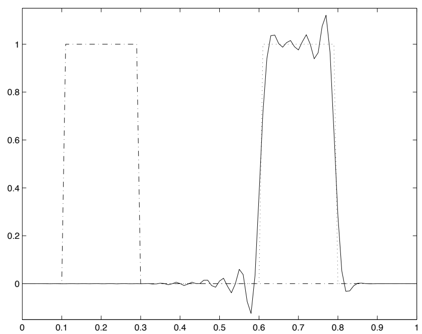
Even-order derivatives $\frac{\partial^{2p} u}{\partial x^{2p}}$ cause numerical dissipation

Odd-order derivatives $\frac{\partial^{2p+1} u}{\partial x^{2p+1}}$ cause numerical dispersion



smearing (amplitude errors)

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



wiggles (phase errors)

Qualitative analysis: the numerical behavior of the discretization scheme largely depends on the relative importance of dispersive and dissipative effects

Stabilization by means of artificial diffusion

Stability condition (necessary but not sufficient)

The coefficients of the even-order derivatives in the modified equation must have alternating signs, the one for the second-order term being positive

If this condition is violated, it can be enforced by adding artificial diffusion:

Stabilized methods	$+\delta(\mathbf{v}\cdot\nabla)^2 u$	*streamline diffusion*
Nonoscillatory methods	$+\delta(\mathbf{v}\cdot\nabla)^2 u + \epsilon(u)\Delta u$	*shock-capturing viscosity*

Remark. In the one-dimensional case both terms are proportional to $\frac{\partial^2 u}{\partial x^2}$

Free parameters $\delta = \frac{c_\delta h}{1+|\mathbf{v}|}, \quad \epsilon(u) = c_\epsilon h^2 R(u)$ where h is the mesh size and $R(u)$ is the residual

Problem: how to determine proper values of the constants c_δ and c_ϵ ???

Alternative: use a high-order time-stepping method or flux/slope limiters

Lax-Wendroff time-stepping

Consider a time-dependent PDE $\frac{\partial u}{\partial t} + \mathcal{L}u = 0 \quad \text{in} \quad \Omega \times (0,T)$

1. Discretize it in time by means of the Taylor series expansion

$$u^{n+1} = u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2} \left(\frac{\partial^2 u}{\partial t^2}\right)^n + \mathcal{O}(\Delta t)^3$$

2. Transform time derivatives into space derivatives using the PDE

$$\frac{\partial u}{\partial t} = -\mathcal{L}u, \qquad \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial t}(-\mathcal{L}u) = -\mathcal{L}\frac{\partial u}{\partial t} = \mathcal{L}^2 u$$

3. Substitute the resulting expressions into the Taylor series

$$u^{n+1} = u^n - \Delta t \mathcal{L} u^n + \frac{(\Delta t)^2}{2} \mathcal{L}^2 u^n + \mathcal{O}(\Delta t)^3$$

4. Perform space discretization using finite differences/volumes/elements

Lax-Wendroff scheme for pure convection

Example. Pure convection equation $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0$ (1D case)

Time derivatives $\mathcal{L} = v\frac{\partial}{\partial x} \quad \Rightarrow \quad \frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}, \qquad \frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2}$

Semi-discrete scheme $u^{n+1} = u^n - v\Delta t\left(\frac{\partial u}{\partial x}\right)^n + \frac{(v\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)^n + \mathcal{O}(\Delta t)^3$

Central difference approximation in space

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1}-u_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x)^2, \qquad \left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i+1}-2u_i+u_{i-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x)^2$$

Fully discrete scheme (second order in space and time)

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} + v\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \frac{v^2\Delta t}{2}\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + \mathcal{O}[(\Delta t)^2, (\Delta x)^2]$$

Remark. LW/CDS is equivalent to FE/CDS stabilized by numerical dissipation due to the second-order term in the Taylor series (no adjustable parameter)

Forward Euler vs. Lax-Wendroff (CDS)

Modified equation for the FE/CDS scheme

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v\Delta x}{2}\nu\frac{\partial^2 u}{\partial x^2} - \frac{v(\Delta x)^2}{6}(1+2\nu^2)\frac{\partial^3 u}{\partial x^3} + \dots \qquad \text{where} \quad \nu = v\frac{\Delta t}{\Delta x}$$

- unconditionally unstable since the coefficient $-\frac{v\Delta x}{2}\nu = -\frac{v^2\Delta t}{2}$ is negative

Modified equation for the LW/CDS scheme

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v(\Delta x)^2}{6}(1-\nu^2)\frac{\partial^3 u}{\partial x^3} - \frac{v(\Delta x)^3}{8}\nu(1-\nu^2)\frac{\partial^4 u}{\partial x^4} - \frac{v(\Delta x)^4}{120}(1+5\nu^2-6\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

- conditionally stable for $\nu^2 \leq 1$ in 1D, $\nu^2 \leq \frac{1}{8}$ in 2D, $\nu^2 \leq \frac{1}{27}$ in 3D
- the second-order derivative (leading dissipation error) has been eliminated
- the negative dispersion coefficient corresponds to a lagging phase error i. e.
- harmonics travel too slow, spurious oscillations occur *behind* steep fronts
- the leading truncation error vanishes for $\nu^2 = 1$ (unit CFL property)

Forward Euler vs. Lax-Wendroff (FEM)

Galerkin FEM $\quad \left(\frac{\partial u}{\partial t}\right)_i \approx \mathcal{M}\frac{u_i^{n+1}-u_i^n}{\Delta t}, \quad$ where $\quad \mathcal{M}u_i = \frac{u_{i+1}+4u_i+u_{i-1}}{6}$

Modified equation for the FE/FEM scheme

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v\Delta x}{2}\nu\frac{\partial^2 u}{\partial x^2} - \frac{v(\Delta x)^2}{3}\nu^2\frac{\partial^3 u}{\partial x^3} + \dots \qquad \text{where} \quad \nu = v\frac{\Delta t}{\Delta x}$$

- unconditionally unstable since the numerical diffusion coefficient is negative
- the leading dispersion error due to space discretization has been eliminated

Modified equation for the LW/FEM scheme

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \frac{v(\Delta x)^2}{6}\nu^2\frac{\partial^3 u}{\partial x^3} - \frac{v(\Delta x)^3}{24}\nu(1-3\nu^2)\frac{\partial^4 u}{\partial x^4} + \frac{v(\Delta x)^4}{180}(1-\frac{15}{2}\nu^2+9\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

- conditionally stable for $\nu^2 \le \frac{1}{3}$ in 1D, $\nu^2 \le \frac{1}{24}$ in 2D, $\nu^2 \le \frac{1}{81}$ in 3D
- the positive dispersion coefficient corresponds to a leading phase error i. e.
- harmonics travel too fast, spurious oscillations occur *ahead* of steep fronts
- the truncation error does not vanish for $\nu^2 = 1$ (no unit CFL property)

Lax-Wendroff FEM in multidimensions

Pure convection equation $\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = 0 \quad \text{in } \Omega \times (0, T) \qquad \mathbf{v} = \mathbf{v}(\mathbf{x})$

Boundary conditions $\quad u = g \quad \text{on } \Gamma_{\text{in}} = \{\mathbf{x} \in \Gamma : \mathbf{v} \cdot \mathbf{n} < 0\}$ inflow boundary

Time derivatives $\quad \mathcal{L} = \mathbf{v} \cdot \nabla \quad \Rightarrow \quad \frac{\partial u}{\partial t} = -\mathbf{v} \cdot \nabla u$ streamline derivative

$\frac{\partial^2 u}{\partial t^2} = (\mathbf{v} \cdot \nabla)^2 u$ streamline diffusion (second derivative in the flow direction)

Semi-discrete scheme $\quad u^{n+1} = u^n - \Delta t\, \mathbf{v} \cdot \nabla u^n + \frac{(\Delta t)^2}{2} (\mathbf{v} \cdot \nabla)^2 u^n + \mathcal{O}(\Delta t)^3$

Weak formulation for the Galerkin method

$$\int_\Omega w(u^{n+1} - u^n)\, d\mathbf{x} = -\Delta t \int_\Omega w\, \mathbf{v} \cdot \nabla u^n\, d\mathbf{x} + \frac{(\Delta t)^2}{2} \int_\Omega w(\mathbf{v} \cdot \nabla)^2 u^n\, d\mathbf{x}$$

Integration by parts using the identity $\nabla \cdot (a\mathbf{b}) = a\nabla \cdot \mathbf{b} + \mathbf{b} \cdot \nabla a$ yields

$$\int_\Omega w\mathbf{v} \cdot \nabla \mathbf{v} \cdot \nabla u\, d\mathbf{x} = -\int_\Omega \nabla \cdot (w\mathbf{v})\ \mathbf{v} \cdot \nabla u\, d\mathbf{x} + \int_{\Gamma_{\text{out}}} w\mathbf{v} \cdot \mathbf{n}\ \mathbf{v} \cdot \nabla u\, ds$$

$$= -\int_\Omega \mathbf{v} \cdot \nabla w\ \mathbf{v} \cdot \nabla u\, d\mathbf{x} - \int_\Omega w \nabla \cdot \mathbf{v}\ \mathbf{v} \cdot \nabla u\, d\mathbf{x} + \int_{\Gamma_{\text{out}}} w\mathbf{v} \cdot \mathbf{n}\ \mathbf{v} \cdot \nabla u\, ds$$

Taylor-Galerkin methods

Donea (1984) introduced a family of high-order time-stepping schemes which stabilize the convective terms by means of intrinsic streamline diffusion

Convection-dominated PDE $\quad \frac{\partial u}{\partial t} + \mathcal{L}u = 0 \quad$ in $\Omega \times (0, T)$

Taylor series expansion up to the third order

$$u^{n+1} = u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n + \frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \mathcal{O}(\Delta t)^4$$

Time derivatives $\quad \frac{\partial u}{\partial t} = -\mathcal{L}u, \quad \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial t}(-\mathcal{L}u) = -\mathcal{L}\frac{\partial u}{\partial t} = \mathcal{L}^2 u$

$\frac{\partial^3 u}{\partial t^3} = \mathcal{L}^2 \frac{\partial u}{\partial t} = \mathcal{L}^2 \frac{u^{n+1} - u^n}{\Delta t} + \mathcal{O}(\Delta t) \quad$ to avoid third-order space derivatives

Substitution $\quad u^{n+1} = u^n - \Delta t \mathcal{L}u^n + \frac{(\Delta t)^2}{2}\mathcal{L}^2 u^n + \frac{(\Delta t)^2}{6}\mathcal{L}^2(u^{n+1} - u^n) + \mathcal{O}(\Delta t)^4$

Remark. The Lax-Wendroff scheme is recovered for $u^{n+1} = u^n$ (steady state)

Euler Taylor-Galerkin scheme

Semi-discrete FE/TG scheme $$\left[\mathcal{I} - \frac{(\Delta t)^2}{6}\mathcal{L}^2\right]\frac{u^{n+1}-u^n}{\Delta t} = -\mathcal{L}u^n + \frac{\Delta t}{2}\mathcal{L}^2 u^n$$

Space discretization: Galerkin FEM (finite differences/volumes also feasible)

The third-order term results in a modification of the consistent mass matrix

Example. Pure convection in 1D $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0, \qquad \mathcal{L} = v\frac{\partial}{\partial x}$

Modified equation for the FE/TG scheme (Galerkin FEM, linear elements)

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v(\Delta x)^3}{24}\nu(1-\nu^2)\frac{\partial^4 u}{\partial x^4} + \frac{v(\Delta x)^4}{180}(1-5\nu^2+4\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

- conditionally stable for $\nu^2 \leq 1$ in 1D, $\nu^2 \leq \frac{1}{8}$ in 2D, $\nu^2 \leq \frac{1}{27}$ in 3D
- the leading dispersion error is of higher order than that for LW/FEM
- the leading truncation error vanishes for $\nu^2 = 1$ (unit CFL property)

Leapfrog Taylor-Galerkin scheme

Taylor series $$u^{n\pm1} = u^n \pm \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n \pm \frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \mathcal{O}(\Delta t)^4$$

It follows that $$u^{n+1} - u^{n-1} = 2\Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^3}{3}\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \mathcal{O}(\Delta t)^4$$

Time derivatives $$\frac{\partial u}{\partial t} = -\mathcal{L}u, \quad \frac{\partial^3 u}{\partial t^3} = \mathcal{L}^2 \frac{\partial u}{\partial t} = \mathcal{L}^2 \frac{u^{n+1}-u^n}{\Delta t} + \mathcal{O}(\Delta t)$$

Semi-discrete LF/TG scheme $$\left[\mathcal{I} - \frac{(\Delta t)^2}{6}\mathcal{L}^2\right] \frac{u^{n+1}-u^{n-1}}{2\Delta t} = -\mathcal{L}u^n$$

Modified equations for leapfrog schemes with $\mathcal{L} = v\frac{\partial}{\partial x}$

LF/CDS $$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v(\Delta x)^2}{6}(1-\nu^2)\frac{\partial^3 u}{\partial x^3} + \frac{v(\Delta x)^4}{120}(1-10\nu^2+9\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

LF/FEM $$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \frac{v(\Delta x)^2}{6}\nu^2\frac{\partial^3 u}{\partial x^3} + \frac{v(\Delta x)^4}{360}(2-27\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

LF/TG $$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \frac{v(\Delta x)^4}{360}(2+5\nu^2-7\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$$

- fourth-order accurate, non-dissipative and conditionally stable for $\nu^2 \leq 1$
- the truncation error shrinks as compared to that for 2nd-order LF schemes
- the unit CFL property is satisfied for phase angles in the range $0 \leq \theta \leq \frac{\pi}{2}$

Crank-Nicolson Taylor-Galerkin scheme

Taylor series expansions up to the fourth order

$$u^{n+1} = u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n + \frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \mathcal{O}(\Delta t)^4$$

$$u^n = u^{n+1} - \Delta t \left(\frac{\partial u}{\partial t}\right)^{n+1} + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^{n+1} - \frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^{n+1} + \mathcal{O}(\Delta t)^4$$

It follows that $u^{n+1} = u^n + \frac{\Delta t}{2}\left[\left(\frac{\partial u}{\partial t}\right)^n + \left(\frac{\partial u}{\partial t}\right)^{n+1}\right]$

$$+\frac{(\Delta t)^2}{4}\left[\left(\frac{\partial^2 u}{\partial t^2}\right)^n - \left(\frac{\partial^2 u}{\partial t^2}\right)^{n+1}\right] + \frac{(\Delta t)^3}{12}\left[\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \left(\frac{\partial^3 u}{\partial t^3}\right)^{n+1}\right] + \mathcal{O}(\Delta t)^4$$

Time derivatives $\frac{\partial u}{\partial t} = -\mathcal{L}u, \quad \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial t}(-\mathcal{L}u) = -\mathcal{L}\frac{\partial u}{\partial t} = \mathcal{L}^2 u$

$$\left(\frac{\partial^3 u}{\partial t^3}\right)^n + \left(\frac{\partial^3 u}{\partial t^3}\right)^{n+1} = \mathcal{L}^2\left[\left(\frac{\partial u}{\partial t}\right)^n + \left(\frac{\partial u}{\partial t}\right)^{n+1}\right] = 2\mathcal{L}^2\frac{u^{n+1}-u^n}{\Delta t} + \mathcal{O}(\Delta t)$$

Fourth-order accurate Crank-Nicolson time-stepping

$$u^{n+1} = u^n - \frac{\Delta t}{2}\mathcal{L}(u^n + u^{n+1}) + \frac{(\Delta t)^2}{4}\mathcal{L}^2(u^n - u^{n+1}) + \frac{(\Delta t)^2}{6}\mathcal{L}^2(u^{n+1} - u^n)$$

Crank-Nicolson Taylor-Galerkin scheme

Semi-discrete CN/TG scheme $\left[\mathcal{I} + \frac{\Delta t}{2}\mathcal{L} + \frac{(\Delta t)^2}{12}\mathcal{L}^2\right]\frac{u^{n+1}-u^n}{\Delta t} = -\mathcal{L}u^n$

Modified equations for Crank-Nicolson schemes with $\mathcal{L} = v\frac{\partial}{\partial x}$

CN/CDS $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v(\Delta x)^2}{6}\left(1 + \frac{\nu^2}{2}\right)\frac{\partial^3 u}{\partial x^3} + \frac{v(\Delta x)^4}{120}(1 + 5\nu^2 + \frac{3}{2}\nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$

CN/FEM $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = -\frac{v(\Delta x)^2}{12}\nu^2\frac{\partial^3 u}{\partial x^3} + \dots$

CN/TG $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \frac{v(\Delta x)^4}{720}(4 - 5\nu^2 + \nu^4)\frac{\partial^5 u}{\partial x^5} + \dots$

- fourth-order accurate, non-dissipative and unconditionally stable
- cannot be operated at $\nu^2 > 1$ since the matrix becomes singular
- the phase response is far superior to that for 2nd-order CN schemes
- the leading truncation error vanishes for $\nu^2 = 1$ (unit CFL property)

Remark. Both LF/TG and CN/TG degenerate into the unstable Galerkin discretization if the solution reaches a steady state so that $u^{n+1} = u^n$

Multistep Taylor-Galerkin schemes

Fractional step algorithms of predictor-corrector type lend themselves to the treatment of (nonlinear) problems described by PDEs of complex structure

Purpose: to avoid a repeated application of spatial differential operators to the governing equation and/or enhance the accuracy of time discretization

Taylor series $$u^{n+1} = u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2} \left(\frac{\partial^2 u}{\partial t^2}\right)^n + \mathcal{O}(\Delta t)^3$$

Factorization $$\mathcal{I} + \Delta t \frac{\partial}{\partial t} + \frac{(\Delta t)^2}{2} \frac{\partial^2}{\partial t^2} = \mathcal{I} + \Delta t \frac{\partial}{\partial t} \left[\mathcal{I} + \frac{\Delta t}{2} \frac{\partial}{\partial t}\right]$$

Richtmyer scheme (two-step Lax-Wendroff method)

$$\begin{aligned} u^{n+1/2} &= u^n + \frac{\Delta t}{2} \left(\frac{\partial u}{\partial t}\right)^n \\ u^{n+1} &= u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^{n+1/2} \end{aligned} \quad \Rightarrow \quad \begin{aligned} u^{n+1/2} &= u^n - \frac{\Delta t}{2} \mathcal{L} u^n \\ u^{n+1} &= u^n - \Delta t \mathcal{L} u^{n+1/2} \end{aligned}$$

- second-order RK method (forward Euler predictor + midpoint rule corrector)
- stability and phase characteristics as for the single-step Lax-Wendroff scheme

Multistep Taylor-Galerkin schemes

Taylor series $$u^{n+1}=u^n+\Delta t\left(\frac{\partial u}{\partial t}\right)^n+\frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n+\frac{(\Delta t)^3}{6}\left(\frac{\partial^3 u}{\partial t^3}\right)^n+\mathcal{O}(\Delta t)^4$$

Factorization $$\mathcal{I}+\Delta t\frac{\partial}{\partial t}+\frac{(\Delta t)^2}{2}\frac{\partial^2}{\partial t^2}+\frac{(\Delta t)^3}{6}\frac{\partial^3}{\partial t^3}=\mathcal{I}+\Delta t\frac{\partial}{\partial t}\left[\mathcal{I}+\frac{\Delta t}{2}\frac{\partial}{\partial t}+\frac{(\Delta t)^2}{6}\frac{\partial^2}{\partial t^2}\right]$$

$$=\mathcal{I}+\Delta t\frac{\partial}{\partial t}\left[\mathcal{I}+\frac{\Delta t}{2}\frac{\partial}{\partial t}\left(\mathcal{I}+\frac{\Delta t}{3}\frac{\partial}{\partial t}\right)\right]$$ no high-order derivatives

Three-step Taylor-Galerkin method *(Jiang and Kawahara, 1993)*

$$\begin{aligned} u^{n+1/3}&=u^n+\frac{\Delta t}{3}\left(\frac{\partial u}{\partial t}\right)^n \\ u^{n+1/2}&=u^n+\frac{\Delta t}{2}\left(\frac{\partial u}{\partial t}\right)^{n+1/3} \\ u^{n+1}&=u^n+\Delta t\left(\frac{\partial u}{\partial t}\right)^{n+1/2}\end{aligned}\quad\Rightarrow\quad\begin{aligned} u^{n+1/3}&=u^n-\frac{\Delta t}{3}\mathcal{L}u^n \\ u^{n+1/2}&=u^n-\frac{\Delta t}{2}\mathcal{L}u^{n+1/3} \\ u^{n+1}&=u^n-\Delta t\mathcal{L}u^{n+1/2}\end{aligned}$$

- third-order time-stepping method, conditionally stable for $\nu^2\leq 1$ (optimal)
- no improvement in phase accuracy as compared to the two-step TG algorithm
- lagging phase error at intermediate and short wavelengths, unit CFL property

High-order Taylor-Galerkin schemes

Multistep TG methods involving second time derivatives offer high accuracy and an isotropic stability domain for nonlinear multidimensional problems

Two-step third-order TG scheme *(Selmin, 1987)*

$$u^{n+1/2} = u^n + \frac{\Delta t}{3}\left(\frac{\partial u}{\partial t}\right)^n + \alpha(\Delta t)^2\left(\frac{\partial^2 u}{\partial t^2}\right)^n \qquad \text{predictor}$$

$$u^{n+1} = u^n + \Delta t\left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^{n+1/2} \qquad \text{corrector}$$

- α is chosen so as to obtain the desired stability/accuracy characteristics
- excellent phase response of the FE/TG method is reproduced for $\alpha = \frac{1}{9}$
- stable for $\nu^2 \leq \frac{3}{4}$ in 1D/2D/3D (no loss of stability in multidimensions)

Underlying factorization vs. Taylor series expansion

$$\mathcal{I} + \Delta t\frac{\partial}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2}{\partial t^2}\left[\mathcal{I} + \frac{\Delta t}{3}\frac{\partial}{\partial t} + \alpha(\Delta t)^2\frac{\partial^2}{\partial t^2}\right] = \mathcal{I} + \Delta t\frac{\partial}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2}{\partial t^2} + \frac{(\Delta t)^3}{6}\frac{\partial^3}{\partial t^3} + \alpha\frac{(\Delta t)^4}{2}\frac{\partial^4}{\partial t^4}$$

Remark. A fourth-order accurate time-stepping method is recovered for $\alpha = \frac{1}{12}$

Two-step fourth-order TG schemes

TTG-4A scheme *(Selmin and Quartapelle, 1993)*

$$u^{n+1/2} = u^n - \frac{\Delta t}{3}\mathcal{L}u^n + \frac{(\Delta t)^2}{12}\mathcal{L}^2 u^n \qquad \text{predictor}$$

$$u^{n+1} = u^n - \Delta t \mathcal{L}u^n + \frac{(\Delta t)^2}{2}\mathcal{L}^2 u^{n+1/2} \qquad \text{corrector}$$

- fourth-order accurate in time, isotropic stability condition $\nu^2 \leq 1$
- poor phase response at intermediate and short wavelengths as $|\nu| \to 1$

TTG-4B scheme $\alpha \approx 0.1409714, \quad \beta \approx 0.1160538, \quad \gamma \approx 0.3590284$

$$u^{n+1/2} = u^n - \alpha \Delta t \mathcal{L}u^n + \beta(\Delta t)^2 \mathcal{L}^2 u^n \qquad \text{predictor}$$

$$u^{n+1} = u^n - \Delta t \mathcal{L}u^{n+1/2} + \gamma(\Delta t)^2 \mathcal{L}^2 u^{n+1/2} \qquad \text{corrector}$$

- fourth-order accurate in time, isotropic stability condition $\nu^2 \leq 0.718$
- excellent phase response in the whole range of Courant numbers

Semi-implicit Taylor-Galerkin schemes

Problem: fully explicit schemes are doomed to be conditionally stable

Semi-implicit Lax-Wendroff method *(Hassan et al., 1989)*

$$u^{n+1} = u^n - \Delta t \mathcal{L} u^n + \frac{(\Delta t)^2}{2} \mathcal{L}^2 u^{n+1} + \mathcal{O}(\Delta t)^3 \qquad \text{unconditionally stable}$$

High-order multistep TG schemes *(Safjan and Oden, 1993)*

$$[\mathcal{I} - \lambda (\Delta t)^2 \mathcal{L}^2] u^{n+\alpha_i} = u^n + \sum_{j=0}^{i-1} [-\mu_{ij} \Delta t \mathcal{L} + \nu_{ij} (\Delta t)^2 \mathcal{L}^2] u^{n+\alpha_j}, \quad i = 1, \dots, s$$

Here $0 = \alpha_0 \leq \ldots \leq \alpha_s = 1$, the free parameter λ is to be chosen from stability considerations and the coefficients $\alpha_i, \mu_{ij}, \nu_{ij}$ must satisfy the *order conditions*

$$\alpha_i^k - k \sum_{j=1}^{s} [\mu_{ij} \alpha_j^{k-1} + \nu_{ij} (k-1) \alpha_j^{k-2}] = \begin{cases} \mu_{i0}, & i = 1 \\ 2\nu_{i0}, & i = 2 \\ 0, & \text{otherwise} \end{cases} \qquad \begin{array}{l} i = 1, \dots, s \\ k = 1, \dots, p \end{array}$$

for an s-step scheme to be of $p-$th order ($p = 2s$ is the highest possible accuracy)

Padé approximations

Taylor series expansion *(Donea et al., 1998)*

$$u^{n+1} = \left[1 + \Delta t \frac{\partial}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2}{\partial t^2} + \frac{(\Delta t)^3}{6}\frac{\partial^3}{\partial t^3} + \dots\right] u^n = \exp\left(\Delta t \frac{\partial}{\partial t}\right) u^n$$

Padé approximations of order $p = m + n$ to the exponential of $x = \Delta t \frac{\partial}{\partial t}$

$$R_{n,m}(x) := \frac{P_n(x)}{Q_m(x)} \approx \exp(x)$$

multistage Taylor-Galerkin methods

Example. $R_{2,0} = 1 + x + \frac{x^2}{2}$ (second order)

$$u^{n+1} = \left(1 + x\left(1 + \tfrac{x}{2}\right)\right) u^n = u^n + \Delta t \left(\tfrac{\partial u}{\partial t}\right)^{n+1/2}$$

where $u^{n+1/2} = u^n + \frac{\Delta t}{2}\left(\frac{\partial u}{\partial t}\right)^n$

$R_{2,0}$ – Richtmyer scheme

$R_{3,0}$ – Jiang-Kawahara

$R_{1,1}$ – Crank-Nicolson

$R_{2,2}$ – CNTG scheme

Padé approximations

m, n	0	1	2	3
0	1	$1 + x$	$1 + x + \frac{1}{2}x^2$	$1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3$
1	$\frac{1}{1-x}$	$\frac{1+\frac{1}{2}x}{1-\frac{1}{2}x}$	$\frac{1+\frac{2}{3}x+\frac{1}{6}x^2}{1-\frac{1}{3}x}$	$\frac{1+\frac{3}{4}x+\frac{1}{4}x^2+\frac{1}{24}x^3}{1-\frac{1}{4}x}$
2	$\frac{1}{1-x+\frac{1}{2}x^2}$	$\frac{1+\frac{1}{3}x}{1-\frac{2}{3}x+\frac{1}{6}x^2}$	$\frac{1+\frac{1}{2}x+\frac{1}{12}x^2}{1-\frac{1}{2}x+\frac{1}{12}x^2}$	$\frac{1+\frac{3}{5}x+\frac{3}{20}x^2+\frac{1}{60}x^3}{1-\frac{2}{5}x+\frac{1}{20}x^2}$
3	$\frac{1}{1-x+\frac{1}{2}x^2-\frac{1}{6}x^3}$	$\frac{1+\frac{1}{4}x}{1-\frac{3}{4}x+\frac{1}{4}x^2-\frac{1}{24}x^3}$	$\frac{1+\frac{2}{5}x+\frac{1}{20}x^2}{1-\frac{3}{5}x+\frac{3}{20}x^2+\frac{1}{60}x^3}$	$\frac{1+\frac{1}{2}x+\frac{1}{10}x^2+\frac{1}{120}x^3}{1-\frac{1}{2}x+\frac{1}{10}x^2-\frac{1}{120}x^3}$

$m = 0$ explicit TG schemes, $m > 0$ implicit TG schemes