Lectures Références

Roger Peyret (NICE ESSI : 89),
Tim Warburton (Boston MIT : 03-05),
Pierre Charrier (Bordeaux Matmeca 96-08)

Numerical Methods for PDE: Finite Differences and Finites Volumes

B. Nkonga

JAD/INRIA

2009

1. Finite Difference(FD) and Finite volume(FV) : Overview
2. Modelization and Simplified models of PDE.
3. Scalar Advection-Diffusion Eqation.
4. Approximation of a Scalar 1D ODE.
5. FD for 1D scalar poisson equation (elliptic).
6. FD for 1D scalar difusion equation (parabolic).
7. FD for 1D scalar advection-diffusion equation.
8. Scalar Nonlinear Conservation law : 1D (hyperbolic).
9. FV for scalar nonlinear Conservation law : 1D
10. Multi-Dimensional extensions

Plan

Plan

Plan

Plan

Solution of a periodic Advection-Diffusion Equation.

Is defined by the Solution of the linear ODE :

$$\left\{ \begin{array}{l} \dfrac{dA_m}{dt} = \mu_m A_m \\ A_m(0) = A(\omega_m) \end{array} \right. \Longrightarrow A_m(t) = A(\omega_m)\exp\left(\mu_m t\right)$$

- When $\mathcal{R}e\left(\mu_m\right) < 0$ the solution decays exponentially fast in time. Rate is determined by the magnitude of $\mathcal{R}e\left(\mu_m\right)$.
- When $\mathcal{R}e\left(\mu_m\right) > 0$ the solution grows exponentially fast in time. Rate is determined by the magnitude of $\mathcal{R}e\left(\mu_m\right)$.
- When $\mathcal{I}m\left(\mu_m\right) \neq 0$ the solution oscillates in time. The larger $\mathcal{I}m\left(\mu_m\right)$ is, the faster the solution oscillates in time.

Numerical Approximation of an ODE

$$\frac{dA}{dt} = \mathcal{F}(A) \quad \text{with} \quad A(0) = A_0$$
$$\Longrightarrow A(t + \delta t) = \mathcal{L}(A(t))$$

Question : Can we solve this equation numerically such as to recover the different behavior, described in the previous slide, when $\mathcal{F}$ is linear ?
Answer : YES, by using a recurrence relation which approximates $A(t^n + \delta t)$ as a function of the previous discrete times $t^n, ..., t^{n-k}, ..., t^0 = 0$. Example of a one step scheme,

"Euler Forward " : $\quad \tilde{A}(t^n + \delta t) = \tilde{\mathcal{L}}(\tilde{A}) = \tilde{A}(t^n) + \delta t \mathcal{F}(\tilde{A}(t^n))$

But we have to take care of :
Consistency, Stability, Accuracy, Convergence.

Numerical Approximation of an ODE

- Consistency and Accuracy : what is the local discretization error (or local truncation error $\mathcal{E} = \mathcal{L}(A) - \tilde{\mathcal{L}}(A)$) for the discrete formula when we substitute the exact solution ?
  - For any smooth function ϑ is $\|\tilde{\mathcal{L}}(\vartheta) - \mathcal{L}(\vartheta)\| = O(\delta t^{1+\alpha})$ with $\alpha > 0$?
- Stability : Does the numerical solution behave in the same way as the exact solution ? Is $\tilde{A}$ bounded in a similar way to A ? Discrete operator does not amplify "noise" ?
- Accuracy : How close to the exact solution is the numerical solution ? Can we choose δt small enough for the error to be below some threshold ?
- Convergence : As we decrease the time step δt, does the end iterate converge to the solution at a given time $t = t_* > 0$. $\|\tilde{A} - A\| = \|e\| = O(\delta t^{\beta})$

Euler-Forward : Stability for $\mathcal{F}(A) = \mu A$

We consider the case of constant time step δt and denote $\tilde{A}^n = \tilde{A}(n\delta t)$:

"Euler Forward " : $\tilde{A}^{n+1} = \tilde{A}^n + \delta t \mathcal{F}(\tilde{A}^n) = (1 + \mu\delta t)\tilde{A}^n$

For a given $\tilde{A}^0 = A(0)$, Euler-Forward scheme gives :

$$\tilde{A}^{n+1} = (1 + \mu\delta t)^{n+1} A(0)$$

- When $\mathcal{R}e\,(\mu_m) \leq 0$ the exact solution $A(t) = A(0)e^{\mu t}$ can decays exponentially fast in time. And $|A| \leq |A(0)|$.

Does this property satisfy by the Euler-Forward scheme ?
$|\tilde{A}^{n+1}| \leq |A(0)| \quad \forall n$

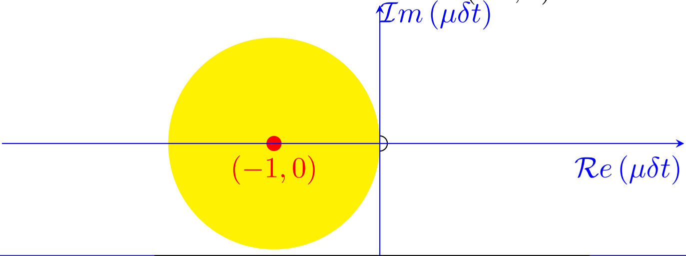
Euler-Forward : Stability Region (yellow) for $\mathcal{F}(A) = \mu A$

For a given $\tilde{A}^0 = A(0)$, Euler-Forward scheme gives :

$$\tilde{A}^{n+1} = (1 + \mu\delta t)^{n+1} A(0)$$

$$|\tilde{A}^{n+1}| \leq |A(0)| \quad \forall n \Longleftrightarrow |1 + \mu\delta t| < 1$$

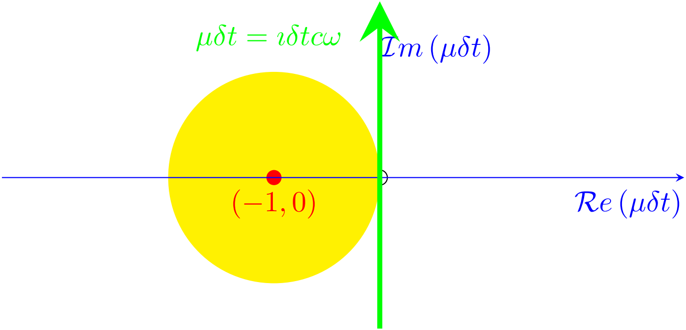
The region of the complex plane which satisfies this condition is the interior of the unit circle centered at $(-1, 0)$



Euler-Forward scheme applied to the Fourier transform of the advection equation : always Unstable

Advection equation for the periodic interval has $\mu = \imath \omega c$ which is purely imaginary and

$$|1 + \imath \omega c \delta t| > 1 \quad \forall \delta t > 0 \quad \text{if } \omega \neq 0, \quad c \neq 0$$

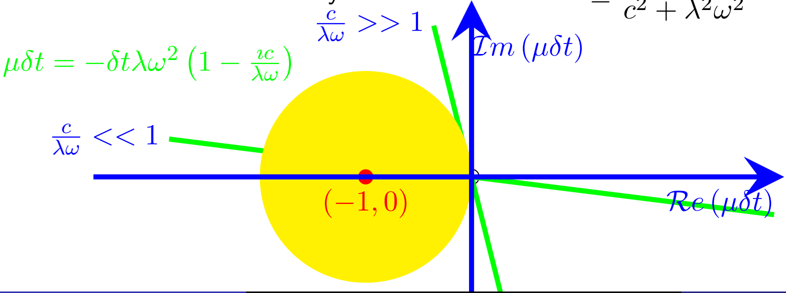


Euler-Forward scheme applied to the Fourier transform of the advection-diffusion equation : stable under condition

Advection-diffusion equation for the periodic interval has $\mu = \imath\omega c - \lambda\omega^2 = -\lambda\omega^2\left(1 - \imath\frac{c}{\lambda\omega}\right)$. Then for given ω, c and λ

$$\left(1-\lambda\omega^2\delta t\right)^2 + (\omega c\delta t)^2 \le 1 \Longleftrightarrow \delta t\omega^2\left(\delta t c^2 + \delta t\lambda^2\omega^2 - 2\lambda\right) \le 0$$

The stability is obtain when $\quad \delta t \le \dfrac{2\lambda}{c^2+\lambda^2\omega^2}$



Can we find schemes with better properties ?

Integrating the ODE on the time interval $[t^n, t^n + \delta t)$

$$\tilde{A}(t^n + \delta t) = \tilde{A}(t^n) + \int_{t^n}^{t^n+\delta t} \mathcal{F}(\tilde{A}(t))dt$$

- "Euler Forward " Explicit : $\mathcal{F}(\tilde{A}(t)) \simeq \mathcal{F}(\tilde{A}^n)$
- "Euler Backward " Implicit : $\mathcal{F}(\tilde{A}(t)) \simeq \mathcal{F}(\tilde{A}^{n+1})$
- Semi-Implicit scheme :
  $\mathcal{F}(\tilde{A}(t)) =\simeq \theta\mathcal{F}(\tilde{A}^n) + (1-\theta)\mathcal{F}(\tilde{A}^{n+1})$
- Adams-Bashford scheme : (linear approximation of $\mathcal{F}$)

$$\mathcal{F}(\tilde{A}) \simeq \mathcal{F}(\tilde{A}^n) + \frac{t - t^n}{\delta t}\left(\mathcal{F}(\tilde{A}^n) - \mathcal{F}(\tilde{A}^{n-1})\right)$$

Then

$$\int_{t^n}^{t^n+\delta t} \mathcal{F}(\tilde{A}(t))dt \simeq \delta t\left(\frac{3}{2}\mathcal{F}(\tilde{A}^n) - \frac{1}{2}\mathcal{F}(\tilde{A}^{n-1})\right)$$

Euler-Backward scheme applied to the Fourier transform of the advection equation : always stable

$$\tilde{A}^{n+1} - \delta t \mathcal{F}(\tilde{A}^{n+1}) = \tilde{A}^n \Longrightarrow \tilde{A}^{n+1} = \frac{1}{1-\mu\delta t}\tilde{A}^n$$

Advection equation for the periodic interval has $\mu = \imath\omega c$ which is purely imaginary and

$$\left|\frac{1}{1-\mu\delta t}\right| < 1 \quad \forall \delta t > 0 \quad \text{if } \omega \neq 0, \quad c \neq 0$$

What about the accuracy of this scheme ?

Stability of the Adams-Bashford scheme $\mathcal{F}(A) = \mu A$

$$\begin{cases} \tilde{A}^{n+1} - \left(1 + \dfrac{3\mu\delta t}{2}\right)\tilde{A}^{n} + \dfrac{\mu\delta t}{2}\tilde{A}^{n-1} = 0 \\ \tilde{A}^{0} = A(0), \quad \tilde{A}^{-1} = A(-\delta t) \end{cases}$$

Let us defined $\mathcal{V}^{n+1} = \begin{pmatrix} \tilde{A}^{n+1} \\ \tilde{A}^{n} \end{pmatrix}$ and $\mathcal{V}_0 = \begin{pmatrix} A(0) \\ A(-\delta t) \end{pmatrix}$. Then

$$\begin{cases} \mathcal{V}^{n+1} = \mathcal{M}\mathcal{V}^{n} \\ \mathcal{V}^{0} = \mathcal{V}_0 \end{cases} \quad \text{where} \quad \mathcal{M} = \begin{pmatrix} 1 + \frac{3\mu\delta t}{2} & -\frac{\mu\delta t}{2} \\ 1 & 0 \end{pmatrix}$$

Von Neumann Stability

The scheme is VN stable if $\mathcal{M}$ is diagonalizable and

$$\mathcal{P}(z) = \det\left(\mathcal{M} - zId\right) = z^2 - \left(1 + \frac{3\mu\delta t}{2}\right)z + \frac{\mu\delta t}{2}$$

have all roots (r_ℓ) satisfying $|r_\ell| \leq 1$.

Miller Theorem

Let us consider a polynomial $\mathcal{P}(z) = \sum_{\ell=0}^{n} \alpha_\ell z^\ell$ where $\alpha_\ell \in \mathbb{C}$, $\alpha_0 \neq 0$ and $\alpha_{\ell_n} \neq 0$. The we define the conjugate polynomial $\tilde{\mathcal{P}}(z)$ and the reduce polynomial $\mathcal{R}(z)$ (of degree $\leq n-1$) as :

$$\tilde{\mathcal{P}}(z) = \sum_{\ell=0}^{n} \overline{\alpha}_{n-\ell} z^\ell, \quad \mathcal{R}(z) = \frac{1}{z}\left[\mathcal{P}(z)\tilde{\mathcal{P}}(0) - \mathcal{P}(0)\tilde{\mathcal{P}}(z)\right]$$

Definition A Von Neumann polynomial is a polynomial that all roots (r_ℓ) are such as $|r_\ell| \leq 1$.

Theorem

$\mathcal{P}(z)$ is a Von Neumann polynomial If and only If one of this tow point is satisfied :

- $|\tilde{\mathcal{P}}(0)| > |\mathcal{P}(0)|$ and $\mathcal{R}(z)$ is a Von Neumann polynomial.
- $\mathcal{R}(z) \equiv 0$ and $\frac{d\mathcal{P}}{dz}$ is a Von Neumann polynomial.

Miller Th. for $\mathcal{P}(z) = z^2 - (1+3\nu)\,z + \nu$ with $\nu = \frac{\mu\delta t}{2}$

$$\tilde{\mathcal{P}}(z) = \overline{\nu} z^2 - (1+3\overline{\nu})\,z + 1$$

$$\begin{aligned} \mathcal{R}(z) &= \frac{1}{z}\left(\mathcal{P}(z) - \nu\tilde{\mathcal{P}}(z)\right) = z - (1+3\nu) - |\nu|^2 z + \nu\,(1+3\overline{\nu}) \\ &= \left(1-|\nu|^2\right) z - 1 + 3|\nu|^2 - 2\nu \end{aligned}$$

When ν is imaginary (advection case), the root of $\mathcal{R}$ satisfy

$$|r|^2 = \frac{\left(1-3|\nu|^2\right)^2 + 4|\nu|^2}{\left(1-|\nu|^2\right)^2} = \frac{\left(1-|\nu|^2\right)^2 + 8|\nu|^4}{\left(1-|\nu|^2\right)^2} \geq 1$$

- $|\tilde{\mathcal{P}}(0)| > |\mathcal{P}(0)|$ if $\frac{|\mu|\delta t}{2} < 1$. But $\mathcal{R}$ is not a VN polynomial.

The tow levels Adams-Bashford scheme, applied to the Fourier transform of the advection equation, is not VN stable. Exercise : Obtain the same result by computing the eigenvalues of $\mathcal{M}$.

Some definitions

Let consider a scheme defined by the following operator

$$\tilde{A}(t+\delta t) = \tilde{\mathcal{L}}(\tilde{A}(t)) = \sum_{\ell=0}^{\ell_{max}} \alpha_\ell \tilde{A}^{n-\ell} + \sum_{\ell=0}^{\ell_{max}} \beta_\ell \mathcal{F}(\tilde{A}^{n-\ell})$$

- Truncation error :

$$\mathcal{E}(t+\delta t) = \frac{\mathcal{L}(A) - \tilde{\mathcal{L}}(A)}{\delta t} = \frac{A(t+\delta t) - \tilde{\mathcal{L}}(A(t))}{\delta t}$$

- Local error :

$$e(t+\delta t) = A(t+\delta t) - \tilde{A}(t+\delta t)$$

- Consistency and Accuracy : A scheme is consistent of p'th order accurate (with $p > 0$) if

$$\|\mathcal{E}(t+\delta t)\| = O(\delta t^p)$$

Some definitions

$$e(t+\delta t) = A(t+\delta t) - \tilde{A}(t+\delta t) = \tilde{\mathcal{L}}(A(t)) - \tilde{\mathcal{L}}(\tilde{A}(t)) + \delta t \mathcal{E}(t+\delta t)$$

If $\tilde{\mathcal{L}}$ is linear then $e(t+\delta t) = \tilde{\mathcal{L}}(e(t)) + \delta t \mathcal{E}(t+\delta t)$ and

$$e^{n+1} = \tilde{\mathcal{L}}^{n+1}(e^0) + \delta t \sum_{p=1}^{n+1} \tilde{\mathcal{L}}^{n+1-p}(\mathcal{E}^{(p)})$$

- Linear stability : A scheme is linear-stable for the norm $\|.\|$ if for any time t_*, $\forall \delta t$ and for $n\delta t \leq t_*$, $\exists C > 0$ such as

  $$\|\tilde{\mathcal{L}}^n\| \leq C$$

  For example the linear stability is achived when $\|\tilde{\mathcal{L}}\| \leq 1$
- Convergence : The scheme converge when :

  $$\lim_{\delta t \to 0} \|\tilde{A}(t) - A(t)\| = 0 \quad \text{uniformly for all } t \in [0, t_*]$$

Equivalence Theorem

Theorem : assume the initial error $\|e^0\| < \delta t^p$, p acurecy order

A linear multistep scheme is convergent if and only if it is consistent and stable.

Demonstration of : consistent and stable $\Longrightarrow$ Convergent

$$
\begin{aligned}
\|e^{n+1}\| &\leq \|\tilde{\mathcal{L}}^{n+1}(e^0)\| + \delta t \sum_{s=1}^{n+1} \|\tilde{\mathcal{L}}^{n+1-s}(\mathcal{E}^{(s)})\| \\
&\leq \|\tilde{\mathcal{L}}^{n+1}\|\|e^0\| + \delta t \sum_{s=1}^{n+1} \|\tilde{\mathcal{L}}^{n+1-s}\|\|\mathcal{E}^{(s)}\| \\
&\leq C\|e^0\| + C\delta t \sum_{s=1}^{n+1} \|\mathcal{E}^{(s)}\| \text{ stability used} \\
&\leq C\left(\|e^0\| + (n+1)\delta t^{1+p}\right) \text{ consistency used} \\
&\leq C(1+T)\delta t^p \text{ convergence obtained}
\end{aligned}
$$

Taylor's expansion

Assuming that $A(t)$ is sufficiently smooth (has m bounded derivatives). Then we can evaluate $A(t+\delta t)$ by a linear sum of $A(t)$ its derivatives at the time t :

$$A(t+\delta t) = A(t)+\delta t\frac{dA}{dt}(t)+\frac{\delta t^2}{2}\frac{d^2A}{dt^2}(t)+...+\frac{\delta t^m}{m!}\frac{d^mA}{dt^m}(t)+R_m(t)$$

The residual $R_m = 0(\delta t^{m+1}$ takes various form.
Then we use the fact that $\frac{dA}{dt}(t) = \mathcal{F}(A)$ to obtain

$$A(t+\delta t) = A(t)+\delta t\mathcal{F}(A(t))+\frac{\delta t^2}{2}\frac{d^2A}{dt^2}(t)+...+\frac{\delta t^m}{m!}\frac{d^mA}{dt^m}(t)+R_m(t)$$

Truncation error

Euler Forward : $\tilde{\mathcal{L}}(A(t)) = A(t) + \delta t \mathcal{F}(A(t))$

$$\mathcal{E}(t+\delta t) = \frac{A(t+\delta t) - \tilde{\mathcal{L}}(A(t))}{\delta t} = C\delta t$$

This scheme is first order accurate.

2 levels AB : $\tilde{\mathcal{L}}(A(t)) = A(t) + \delta t \frac{3}{2}\mathcal{F}(A(t)) - \delta t \frac{1}{2}\mathcal{F}(A(t-\delta t))$

$$\mathcal{F}(A(t-\delta t)) = \frac{dA}{dt}(t-\delta t) = \frac{dA}{dt}(t) - \delta t \frac{d^2A}{dt^2}(t) + C\delta t^2$$

$$\text{Then } \tilde{\mathcal{L}}(A(t)) = A(t) + \delta t \mathcal{F}(A(t)) + \frac{\delta t^2}{2}\frac{d^2A}{dt^2}(t) + C\delta t^3$$

And finally $\mathcal{E}(t+\delta t) = \dfrac{A(t+\delta t) - \tilde{\mathcal{L}}(A(t))}{\delta t} = B\delta t^2$

This scheme is second order accurate.

Accurate one step Runge-Kutta (RKp) methods

Given the difficulties inherent in starting the higher order (AB) schemes we are encouraged to look for one-step methods which only require $\tilde{A}^n$ to accurately evalute $\tilde{A}^{n+1}$.

- They require many evaluations $\mathcal{F}$
- They will be for some p'th order accurate.
- They only need one starting value.

Modified Euler (RK2)

$$\begin{aligned} \tilde{A}^{n+\frac{1}{2}} &= \tilde{A}^n + \frac{\delta t}{2}\mathcal{F}(\tilde{A}^n) \\ \tilde{A}^{n+1} &= \tilde{A}^n + \delta t \mathcal{F}\left(\tilde{A}^{n+\frac{1}{2}}\right) \end{aligned}$$

Accurate one step Runge-Kutta (RKp) methods

$$\begin{aligned}\tilde{A}^{n+\frac{1}{2}} &= \tilde{A}^n + \tfrac{\delta t}{2}\mathcal{F}(\tilde{A}^n)\\ \tilde{A}^{n+1} &= \tilde{A}^n + \delta t \mathcal{F}\left(\tilde{A}^{n+\frac{1}{2}}\right)\end{aligned}$$

$$\Longrightarrow \tilde{A}^{n+1} = \tilde{A}^n + \delta t \mathcal{F}\left(\tilde{A}^n + \frac{\delta t}{2}\mathcal{F}(\tilde{A}^n)\right)$$

$$\begin{aligned}\mathcal{F}\left(A(t) + \tfrac{\delta t}{2}\mathcal{F}(A(t))\right) &= \mathcal{F}\left(A(t)\right) + \frac{\delta t}{2}\mathcal{F}(A(t))\mathcal{F}'\left(A(t)\right) + O(\delta t^2)\\ &= \frac{dA}{dt} + \frac{\delta t}{2}\frac{d^2A}{dt^2} + O(\delta t^2)\end{aligned}$$

Therefore $\tilde{\mathcal{L}}(A(t)) = A(t) + \delta t\frac{dA}{dt} + \frac{\delta t^2}{2}\frac{d^2A}{dt^2} + O(\delta t^3)$ and

$$\mathcal{E}(t+\delta t) = \frac{A(t+\delta t) - \tilde{\mathcal{L}}(A(t))}{\delta t} = O\left(\delta t^2\right)$$

One step Runge-Kutta methods : RK3 family

$$A^{n+1} = A^n + \delta t \alpha_0 \mathcal{F}\left(\tilde{A}^n\right) + \delta t \alpha_1 \mathcal{F}\left(\tilde{A}^n + \delta t \theta_0 \mathcal{F}\left(\tilde{A}^n + \delta t \theta_1 \mathcal{F}(A^n)\right)\right)$$

Exercice

- Find α_0, α_1, θ_0 and θ_1 such as to obtain a tird's order accurate method.
- For a set of parapeters that gives a tird's order accurate method, chek the stability (advection and advection-difusion).

One step Runge-Kutta methods : RK3 family

$$A^{n+1} = A^n + \delta t \alpha_0 \mathcal{F}\left(\tilde{A}^n\right) + \delta t \alpha_1 \mathcal{F}\left(\tilde{A}^n + \delta t \theta_0 \mathcal{F}\left(\tilde{A}^n + \delta t \theta_1 \mathcal{F}(A^n)\right)\right)$$

$$\begin{aligned}
&\mathcal{F}\left(A + \theta_0 \delta t \mathcal{F}\left(A + \theta_1 \delta t \mathcal{F}\left(A\right)\right)\right) \\
&= \mathcal{F}\left(A\right) + \theta_0 \delta t \mathcal{F}\left(A + \theta_1 \delta t \mathcal{F}\left(A\right)\right) \mathcal{F}'\left(A\right) \\
&+ \frac{\theta_0^2 \delta t^2}{2}\left[\mathcal{F}\left(A + \theta_1 \delta t \mathcal{F}\left(A\right)\right)\right]^2 \mathcal{F}''\left(A\right) + O(\delta t^3) \\
&= \frac{dA}{dt} + \theta_0 \delta t \frac{d^2 A}{dt^2} + \theta_0 \theta_1 \delta t^2 \left[\mathcal{F}'\right]^2 \mathcal{F} + \frac{\theta_0^2 \delta t^2}{2}\left[\mathcal{F}\right]^2 \mathcal{F}'' + O(\delta t^3)
\end{aligned}$$

$$\begin{aligned}
\tilde{\mathcal{L}}(A(t)) \quad &= A(t) + \delta t \left(\left(\alpha_0 + \alpha_1\right) \frac{dA}{dt} + \alpha_1 \theta_0 \delta t \frac{d^2 A}{dt^2} \right) \\
&\delta t \alpha_1 \left(\theta_0 \theta_1 \delta t^2 \left[\mathcal{F}'\right]^2 \mathcal{F} + \frac{\theta_0^2 \delta t^2}{2}\left[\mathcal{F}\right]^2 \mathcal{F}'' \right) + O(\delta t^4)
\end{aligned}$$

Accurate one step Runge-Kutta

$$\begin{aligned}\tilde{\mathcal{L}}(A(t)) \quad &= A(t) + \delta t \left((\alpha_0 + \alpha_1) \frac{dA}{dt} + \alpha_1 \theta_0 \delta t \frac{d^2 A}{dt^2} \right) \\ &\delta t \alpha_1 \left(\theta_0 \theta_1 \delta t^2 \left[\mathcal{F}' \right]^2 \mathcal{F} + \frac{\theta_0^2 \delta t^2}{2} \left[\mathcal{F} \right]^2 \mathcal{F}'' \right) + O(\delta t^4)\end{aligned}$$

Condition for third order accurate :

$$\alpha_0 + \alpha_1 = 1, \quad \alpha_1 \theta_0 = \frac{1}{2}, \quad \theta_1 = \frac{\theta_0}{2}, \quad \alpha_1 \theta_0^2 = \frac{1}{3},$$

Then we obtain the Heun's third order formula with

$$\theta_0 = \frac{2}{3}, \quad \theta_1 = \frac{1}{3}, \quad \alpha_1 = \frac{3}{4}, \quad \alpha_0 = \frac{1}{4},$$

Accurate one step Runge-Kutta methods : simple RKp family

$\tilde{A}^* = \tilde{A}^n$

For m=0, p-1

$$\tilde{A}^* = \tilde{A}^n + \frac{\delta t}{p-m}\mathcal{F}\left(\tilde{A}^*\right)$$

End

$A^{n+1} = \tilde{A}^*$

Back to the PDE with non periodic Boundaries

- We can't use the Fourier transform any more.

The next lecture consider a problen that is defined by the boundary conditions.
The Poisson equation (elliptic) is a Boundary Value Problem (BVP)

Plan

Plan

Plan

Plan

Plan

Plan