Computer-Assisted Problem-Solving / Numerical Methods

Partial Differential Equations

version: October 16th, 2017

Legend: Method, Theory, Example, Advanced, Appendix

Theory

Parabolic PDEs

Describe e.g. heat conduction (temperature), diffusion, time-dependence of concentrations, viscous effects, etc.

1D diffusion equation for variable $u = u(x,t)$

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

Diffusion coefficient $D > 0$

Variable u is e.g. temperature, concentration, velocity, etc.

Remark: if u is temperature $\Longrightarrow D = \lambda/(\rho C_p)$, with heat conduction coefficient λ, density ρ, specific heat C_p

Initial condition at $t = 0$: $u(x,0) = \phi(x)$, with ϕ given function of x

Spatial coordinate $x \in [0, L]$

Boundary conditions at $x = 0$ and $x = L$:

$$u(0,t) = U_L(t) \qquad\qquad u(L,t) = U_R(t)$$

Method

Spatial Discretization

Approximation of second derivative $\dfrac{\partial^2 u}{\partial x^2}$
via relations between u-values at mesh points

Meshing of interval $[0, L]$:
M **equidistant intervals:** $\Delta x := L/M$
$M+1$ **mesh points** $x_m = m\Delta x,\ m{=}1, ..., M{+}1$
2 boundary points: $m = 1$ **en** $m = M+1$
$M-1$ **internal mesh points** $x_m,\ m = 2, .., M$

Taylor-expansions:

$$
\begin{aligned}
u(x_{m+1}, t) = u(x_m, t) \ &+ \ \Delta x \frac{\partial u}{\partial x}(x_m, t) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_m, t) \\
&+ \ \frac{\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3}(x_m, t) + \mathcal{O}(\Delta x^4) \\
u(x_{m-1}, t) = u(x_m, t) \ &- \ \Delta x \frac{\partial u}{\partial x}(x_m, t) + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x_m, t) \\
&- \ \frac{\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3}(x_m, t) + \mathcal{O}(\Delta x^4)
\end{aligned}
$$

Combine and divide by $\Delta x^2 \Longrightarrow$

$$
\frac{\partial^2 u}{\partial x^2}(x_m, t) = \frac{u(x_{m+1}, t) - 2u(x_m, t) + u(x_{m-1}, t)}{\Delta x^2} + \mathcal{O}(\Delta x^2)
$$

In short-hand notation:

$$\frac{\partial^2 u}{\partial x^2}(m,t) = \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

Neglect $\mathcal{O}(\Delta x^2)$ **term** $\Longrightarrow$
2nd-order accurate approximation of $\frac{\partial^2 u}{\partial x^2}$ **in all internal points** $m = 2, .., M$

Substitution in PDE $\Longrightarrow$ **approximation** $u_m(t)$**, which satisfies the ODE**

$$\frac{du_m}{dt}(t) = D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2}$$

The functions $u_m(t)$ **have to satisfy the initial condition (at** $t = 0$**):** $u_m(t = 0) = \phi(x_m)$

At the boundaries:
$u_1(t) = U_L(t)$, $u_{M+1}(t) = U_R(t)$ **for every time** t

System of coupled ODEs for the unknowns $u_m(t)$, $m = 2, \cdots M$, **with initial conditions.**

Can be solved with methods for ODEs:
Euler (explicit, implicit), Heun, Runge-Kutta, Trapezoidal rule, ...

Method

Explicit Time Discretization

Approximate time variable of ODE system:

steps with size $\Delta t > 0$, starting at $t = 0$

Approximation $u_m(t)$ at time $t{=}n\Delta t$: u_m^n

The solution at $t = 0$ is given by: $u_m^0 = \phi(x_m)$

At each time $t = (n+1)\Delta t$ we can approximate the solution of

$$\begin{aligned} \frac{du_m}{dt}(t) &= D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} \\ &=: f(u_{m-1}, u_m, u_{m+1}) \end{aligned}$$

using explicit Euler:

$$u_m^{n+1} = u_m^n + \Delta t f(u_{m-1}^n, u_m^n, u_{m+1}^n)$$

This does not give the exact solution

$$u(m\Delta x, (n+1)\Delta t),$$

but an approximation u_m^{n+1} satisfying

$$u_m^{n+1} = r u_{m-1}^n + (1-2r)u_m^n + r u_{m+1}^n,$$

with

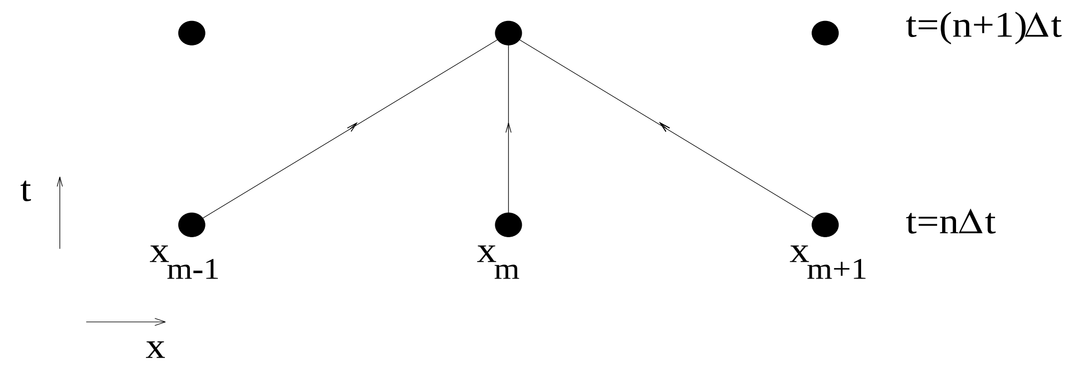
$$r := \frac{\Delta t D}{\Delta x^2}, \text{ and } m = 1, 2, .., M$$

Difference equation

$$u_m^{n+1} = ru_{m-1}^n + (1-2r)u_m^n + ru_{m+1}^n$$

Working of algorithm:

- **1st time line** $t = 1\Delta t$
  - internal u_m **from** u_{m-1}, u_m, u_{m+1} **at** $t = 0$
  - boundary points u_1 **and** u_{M+1} **from bouco**
- **2nd time line** $t = 2\Delta t$
  - internal u_m **from** u_{m-1}, u_m, u_{m+1} **at** $t=1\Delta t$
  - boundary points u_1 **and** u_{M+1} **from bouco**
- **general:**
  time line $n+1$ **follows from time line** n



- **continue until** $t = n\Delta t = T_{end}$

Theory

Consistency

Definition:
the discretization is *consistent* **with the PDE when the difference between difference eqn. and PDE** $\to 0$ **for** $\Delta x \to 0$ **and** $\Delta t \to 0$

Local truncation error $=$
difference between difference eqn. and PDE

$$T(m\Delta x, n\Delta t) = \mathcal{O}(\Delta t, \Delta x^2),$$

since:
$\mathcal{O}(\Delta x^2)$ **thrown away for approximation of** $\frac{\partial^2 u}{\partial x^2}$
$\mathcal{O}(\Delta t)$ **thrown away with (explicit) Euler for** $\frac{\partial u}{\partial t}$

Remark:
this does not necessarily mean that $u_m^n \to u(x,t)$ **for** $\Delta x \to 0$ **and** $\Delta t \to 0$

But if this is the case $\Longrightarrow$ *convergence*

Stability

Stability: errors in initial and boundary conditions should not grow too fast

Consider the difference equation

$$u_m^{n+1} = r u_{m-1}^n + (1 - 2r) u_m^n + r u_{m+1}^n$$

Physics: increase of u (e.g. temperature) in point must lead to increase (not decrease!) in neighbouring points.

Coefficients must be of equal sign $\Longrightarrow$

$$0 \leq r \leq \frac{1}{2}$$

So choose Δx and Δt such that $r = \frac{\Delta t D}{\Delta x^2} \leq 1/2$

Necessary condition, but also sufficient?
Yes! This follows from "practical stability"

Theory

Practical Stability

Practical stability:
- something in between stability and accuracy
- in terms of Fourier analysis:
no Fourier component of the numerical solution should grow faster than the fastest possible growth of the exact solution

Fourier expansion of exact solution $u(x,t)$:

$$u(x,t) = \sum_{j=0}^{\infty} f_j(t) e^{ib_j x}$$

Consider arbitrary j-th term in the series:

$$f(t)e^{ibx}$$

Substitution in PDE $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \Longrightarrow$

$$f'(t)e^{ibx} = -Db^2 f(t)e^{ibx} \Longrightarrow$$

$$f'(t) = -Db^2 f(t) \Longrightarrow$$

$$f(t) = ce^{-Db^2t}, \textbf{ with } c = f(0) \textbf{ constant}$$

Since $D > 0 \Longrightarrow f(t)/f(0) = e^{-Db^2t}$ decreases (when $t \to \infty$)

Fourier expansion of numerical approx. u_m^n:

$$u_m^n = \sum_{j=0}^{\infty} f_j^n e^{ib_j m\Delta x}$$

Consider arbitrary j-th term in the series:

$$f^n e^{ibm\Delta x}$$

Substitution in difference scheme $\Longrightarrow$

$$\begin{aligned} f^{n+1} &= \left(re^{-ib\Delta x} + 1 - 2r + re^{ib\Delta x}\right) f^n \\ &= \left(1 - 2r + 2r\cos b\Delta x\right) f^n \\ &= \left(1 - 4r\sin^2\frac{b\Delta x}{2}\right) f^n \end{aligned}$$

In the last step, $\cos x = 1 - 2\sin^2(x/2)$ **was used**

Since $f(t)/f(0) \downarrow \Longrightarrow f^n/f^0$ **may not increase**

This leads to the condition

$$|1 - 4r\sin^2\frac{b\Delta x}{2}| \leq 1 \; (\forall b) \; ,$$

which is satisfied if $r \leq 1/2$

In other words: $0 \leq r \leq 1/2$ **is necessary and sufficient for stability**

Advanced

Convergence and Stability

Explicit scheme:

$$u_m^{n+1} = ru_{m-1}^n + (1-2r)u_m^n + ru_{m+1}^n$$

Definition: a scheme is called convergent if the error $\epsilon_m^n := u_m^n - u(m\Delta x, n\Delta t)$ **goes to 0, when** $\Delta x \to 0$ **en** $\Delta t \to 0$

An unstable scheme may give unrealistic (physically unacceptable) results u_m^n**, even if** Δx **and** Δt **are very small**

Hence: convergence requires stability

Consequence:
explicit scheme requires $r \leq 1/2$ **for convergence**

Equivalence theorem of Lax:

If scheme consistent: stability $\iff$ **convergence**

Consequence:
explicit scheme convergent $\iff r \leq 1/2$

Theorem: $r \leq 1/2 \implies$
Global Error Explicit scheme 1st order in Δt**, 2nd order in** Δx **(see Appendix A for proof)**

Advanced

Domain of Influence

Analytic solution of PDE $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$

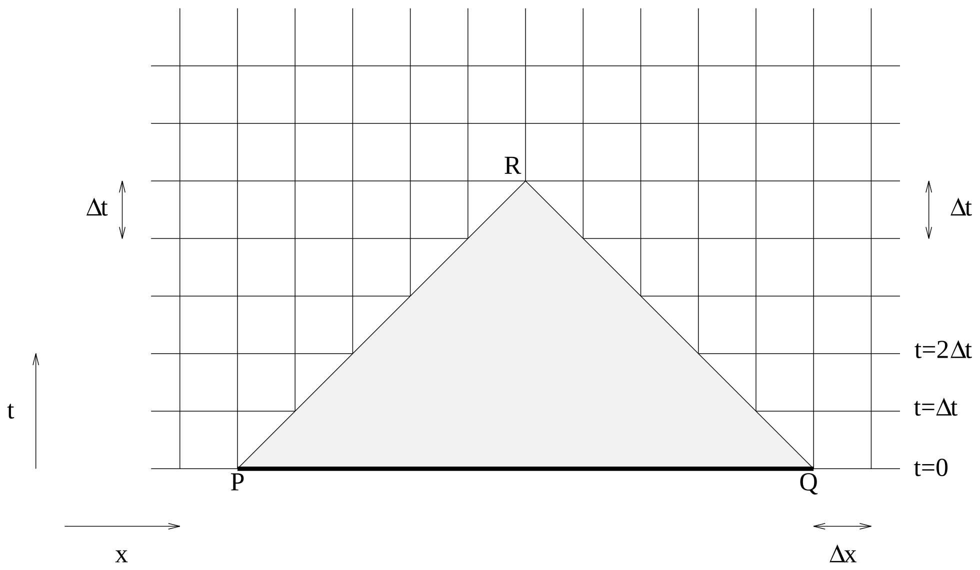
with initial profile $u(x, t = 0) = \phi(x)$

$$u(x,t) = \int_{-\infty}^{\infty} \phi(\xi)v(x-\xi,t)d\xi \quad \text{with} \quad v(y,t) = \frac{e^{\frac{-y^2}{4D\,t}}}{\sqrt{4\pi Dt}}$$

Analytic solution:

- **Every location** x **contains information of** $\phi(x)$**, directly after** $t = 0$
- **Information of initial profile** $\phi(x)$ **is spread infinitely fast, everywhere in** xt**-plane**

Explicit Euler:



Value of u_m^n **in point** R **only determined by segment** PQ **of initial profile** $\phi(x)$

Triangle is called Domain of Influence of PQ

Stability restriction ($r < \frac{1}{2}$):

- **For fixed Δt: Δx should be large enough**
- **Angle at top of PQR should be large enough**
- **Numerical information transfer must be sufficiently fast**

For infinitely fast information transfer:

- **angle $= 180^o$**
- **direct information transfer required between u_m^{n+1} and neighbours u_{m-1}^{n+1} , u_{m+1}^{n+1}**

$\Longrightarrow$ **Implicit methods**

Method

Implicit Time Discretization

At each time line $t=(n+1)\Delta t$ we can solve

$$\frac{du_m}{dt}(t) = D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2}$$

approximately using implicit Euler:

$$u_m^{n+1} = u_m^n + \Delta t D\frac{u_{m+1}^{n+1} - 2u_m^{n+1} + u_{m-1}^{n+1}}{\Delta x^2}$$

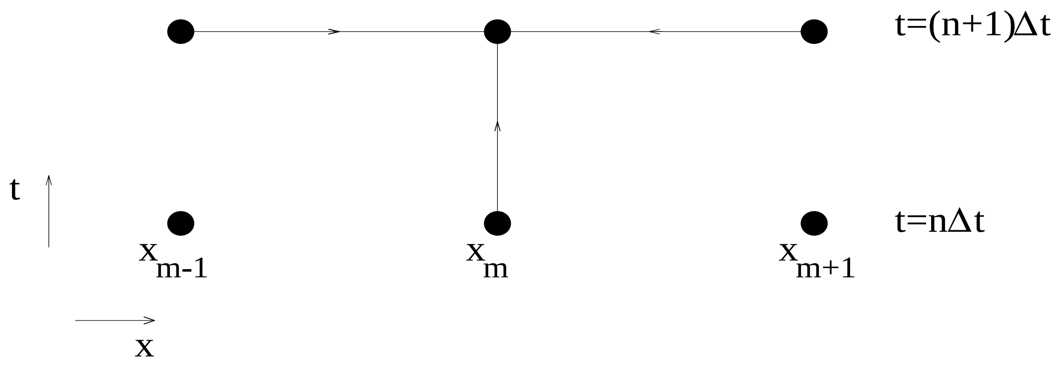
This leads to the difference scheme

$$-ru_{m-1}^{n+1} + (1+2r)u_m^{n+1} - ru_{m+1}^{n+1} = u_m^n,$$

with (similar to explicit Euler)

$$r := \frac{\Delta t D}{\Delta x^2}, \quad \textbf{and } m = 1, 2, .., M$$

There are 3 unknown u-values (at time line $n+1$) related to 1 "old" u-value at $t = n\Delta t$



Truncation error of implicit scheme has same order as explicit scheme:
1st order in Δt and 2nd order in Δx

So implicit scheme is also consistent

Stability: Fourier component of u_m^n

$$f^n e^{ibm\Delta x}$$

substitution in implicit difference scheme $\Longrightarrow$

$$\begin{aligned} f^{n+1} &= \frac{f^n}{-re^{-ib\Delta x} + 1 + 2r - re^{ib\Delta x}} \\ &= \frac{f^n}{1 + 2r - 2r\cos\left(b\Delta x\right)} \\ &= \frac{f^n}{1 + 4r\sin^2\left(b\Delta x/2\right)} \end{aligned}$$

The amplification factor

$$\frac{1}{1 + 4r\sin^2\left(b\Delta x/2\right)}$$

is smaller than 1 for all $r > 0 \Longrightarrow$
implicit scheme is unconditionally stable

Equivalence theorem of Lax $\Longrightarrow$
implicit scheme convergent

Theory

Solution Scheme

Implicit Euler $\Longrightarrow$ difference scheme

$$-ru_{m-1}^{n+1} + (2r+1)u_m^{n+1} - ru_{m+1}^{n+1} = u_m^n,$$

with $$r := \frac{\Delta t D}{\Delta x^2}, \text{ **en** } m = 1, 2, .., M$$

Divide by r $\Longrightarrow$

$$-u_{m-1}^{n+1} + (2 + \frac{1}{r})u_m^{n+1} - u_{m+1}^{n+1} = \frac{1}{r}u_m^n$$

For each time $t = (n+1)\Delta t$:

- system of $M+1$ coupled (linear) eqns.

- boundary conditions $u_1 = U_L(t)$, $u_{M+1} = U_R(t)$

Linear system:

$$\begin{pmatrix} 1 & 0 & & & & & \\ -1 & 2+\frac{1}{r} & -1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -1 & 2+\frac{1}{r} & -1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -1 & 2+\frac{1}{r} & -1 \\ & & & & & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_m^{n+1} \\ \vdots \\ u_M^{n+1} \\ u_{M+1}^{n+1} \end{pmatrix} = \begin{pmatrix} U_L(t) \\ \frac{1}{r}u_2^n \\ \vdots \\ \frac{1}{r}u_m^n \\ \vdots \\ \frac{1}{r}u_M^n \\ U_R(t) \end{pmatrix}$$

Solve with LU (TDMA), SOR, PCG, ...

Method

Crank-Nicolson

Implicit Euler is only $\mathcal{O}(\Delta t) \Longrightarrow$ small Δt necessary for accuracy (not for stability)

Higher accuracy with e.g. Crank-Nicolson

$$\begin{aligned}\frac{du_m}{dt}(t) &= D\frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} \\ &=: f(u_{m-1}, u_m, u_{m+1})\end{aligned}$$

Trapezoidal rule $\Longrightarrow$

$$\frac{u_m^{n+1} - u_m^n}{\Delta t} = \frac{\left\{f(u_{m-1}^{n+1}, u_m^{n+1}, u_{m+1}^{n+1}) + f(u_{m-1}^n, u_m^n, u_{m+1}^n)\right\}}{2}$$

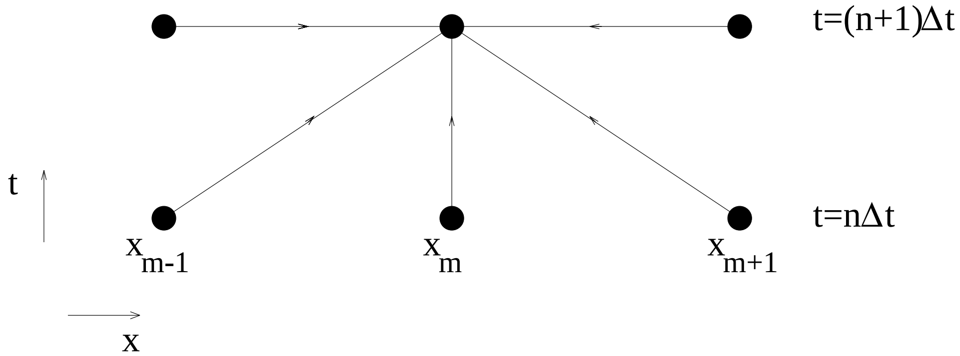
Corresponding difference equation

$$-ru_{m-1}^{n+1}+(2+2r)u_m^{n+1}-ru_{m+1}^{n+1} = ru_{m-1}^n+(2-2r)u_m^n+ru_{m+1}^n$$

with $r = \Delta t D/\Delta x^2$ (similar to Euler)

Truncation error: 2nd order in both Δx and Δt

Calculation scheme in the xt-plane:



Divide difference equation by $r \Longrightarrow$

$$-u_{m-1}^{n+1} + (2+\frac{2}{r})u_m^{n+1} - u_{m+1}^{n+1} = u_{m-1}^n + (-2+\frac{2}{r})u_m^n + u_{m+1}^n$$

Linear system:

$$\begin{pmatrix} 1 & 0 & & & & & \\ -1 & 2+\frac{2}{r} & -1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -1 & 2+\frac{2}{r} & -1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -1 & 2+\frac{2}{r} & -1 \\ & & & & & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_m^{n+1} \\ \vdots \\ u_M^{n+1} \\ u_{M+1}^{n+1} \end{pmatrix} = \begin{pmatrix} U_L(t) \\ u_1^n + (-2+\frac{2}{r})u_2^n + u_3^n \\ \vdots \\ u_{m-1}^n + (-2+\frac{2}{r})u_m^n + u_{m+1}^n \\ \vdots \\ u_{M-1}^n + (-2+\frac{2}{r})u_M^n + u_{M+1}^n \\ U_R(t) \end{pmatrix}$$

Computational work per time-line similar to implicit Euler.

Larger Δt possible because of 2nd order accuracy $\Longrightarrow$ faster method.

Appendix A: Global Error Explicit Scheme

Error $\epsilon_m^n = u_m^n - u(m\Delta x, n\Delta t) \to 0$ **if** $\Delta x, \Delta t \to 0$

Question: how fast?

At the boundaries $m = 1$ **and** $m = M{+}1$**:** $\epsilon_m^{n+1} = 0$
Substitution of $u_m^n = \epsilon_m^n + u(m\Delta x, n\Delta t)$ **in the explicit scheme**

$$u_m^{n+1} = ru_{m-1}^n + (1-2r)u_m^n + ru_{m+1}^n$$

gives $M-1$ **equations for internal points**

$$\begin{aligned}\epsilon_m^{n+1} + u(x_m, (n{+}1)\Delta t) &= r\epsilon_{m-1}^n + (1{-}2r)\epsilon_m^n + r\epsilon_{m+1}^n \\ &+ ru(x_{m-1}, n\Delta t) + (1{-}2r)u(x_m, n\Delta t) \\ &\quad +ru(x_{m+1}, n\Delta t)\end{aligned}$$

Local (truncation) error $=$ $|$**difference eqn - PDE**$|$**:**

$$T(m\Delta x, n\Delta t) = \mathcal{O}(\Delta t, \Delta x^2),$$

This gives

$$\epsilon_m^{n+1} = r\epsilon_{m-1}^n + (1{-}2r)\epsilon_m^n + r\epsilon_{m+1}^n + \Delta t T(m\Delta x, n\Delta t)$$

Define for the n-th time line $t = n\Delta t$

$$\begin{aligned}E^n &:= \max_m |\epsilon_m^n| \\ T^n &:= \max_m |T(m\Delta x, n\Delta t)|\end{aligned}$$

Use these to estimate $|\epsilon_m^{n+1}|$

$$\left|\epsilon_m^{n+1}\right| \le (r + |1-2r| + r)E^n + \Delta t T^n$$

Stability restriction $r \leq 1/2 \Longrightarrow$

$1 - 2r > 0 \Longrightarrow r + |1 - 2r| + r = 1 \Longrightarrow$

$$\left|\epsilon_m^{n+1}\right| \leq E^n + \Delta t T^n$$

This holds for $m\!=\!2, ..., M$**, hence also for** m **with maximum** $|\epsilon_m^{n+1}|$**:**

$$E^{n+1} := \max_m \left|\epsilon_m^{n+1}\right| \leq E^n + \Delta t T^n$$

Now estimate the (absolute) largest error for time line $t = (n+1)\Delta t$**, with induction**

$$\begin{aligned} E^{n+1} &\leq E^n + \Delta t T^n \\ &\leq E^{n-1} + \Delta t(T^n + T^{n-1}) \\ &\leq ... \\ &\leq E^0 + \Delta t(T^n + T^{n-1} + ... + T^0) \end{aligned}$$

Define $\quad T := \max_{0 \leq j \leq n} T^j,$

then we obtain

$$E^{n+1} \leq E^0 + \Delta t(n+1)T \sim E^0 + tT$$

Besides initial error E^0**, the error** $\sim tT$
The latter is 1st order in Δt**, 2nd order in** Δx