Parabolic Equations - Explicit Methods

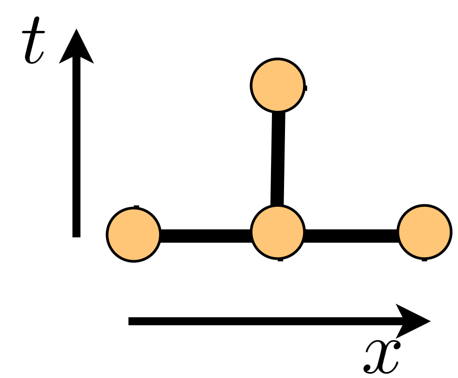
$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common explicit methods

FTCS

$$\varphi_i^{n+1} = \varphi_i^n + \frac{\alpha \Delta t}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$

stencil:



- truncation errors: $O(\Delta t)$ in time, $O(\Delta x^2)$ in space
- stable for $\dfrac{\alpha \Delta t}{\Delta x^2} \leq 1$

Richardson Method

Idea: Why not go 2[nd]-order in time?

From Taylor series in time: $$\left.\frac{\partial \varphi_i}{\partial t}\right|^n = \frac{\varphi_i^{n+1} - \varphi_i^{n-1}}{2\Delta t} + O(\Delta t^2)$$

Parabolic Equations - Explicit Methods

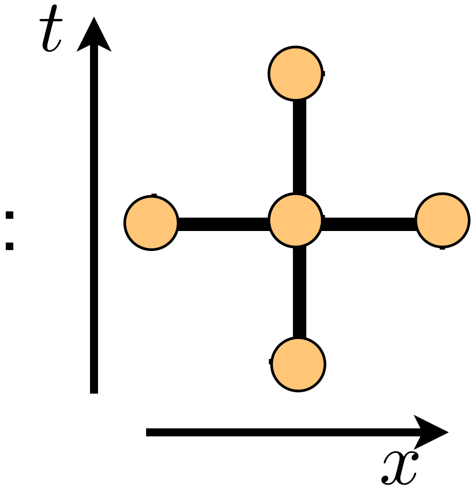
$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common explicit methods

Richardson Method

$$\varphi_i^{n+1} = \varphi_i^{n-1} + 2\alpha \frac{\Delta t}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$

stencil:



- truncation errors: $O(\Delta t^2)$ in time, $O(\Delta x^2)$ in space

BUT: turns out to be ***always*** unstable

Du-Fort-Frankel fix Richardson method

$$\frac{\varphi_i^{n+1} - \varphi_i^{n-1}}{2\Delta t} = +\frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2\overline{\varphi_i^n} + \varphi_{i-1}^n\right) \quad \text{with} \quad \overline{\varphi_i^n} = \frac{1}{2}\left(\varphi_i^{n+1} + \varphi_i^{n-1}\right)$$

$$\frac{\varphi_i^{n+1} - \varphi_i^{n-1}}{2\Delta t} = +\frac{\alpha}{h^2}\left(\varphi_{i+1}^n - \varphi_i^{n-1} - \varphi_i^{n+1} + \varphi_{i-1}^n\right)$$

Is this now implicit?

let's rearrange

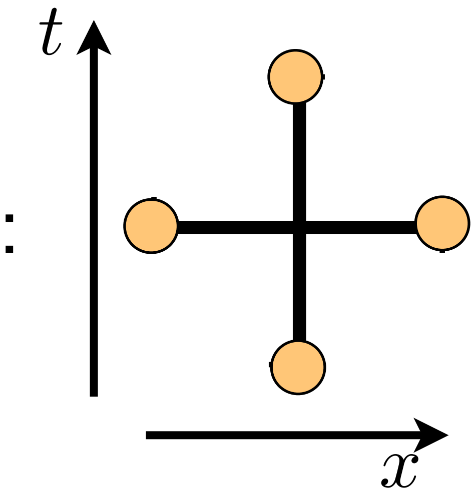
Parabolic Equations - Explicit Methods

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common explicit methods

Du-Fort-Frankel

stencil:



$$\left(1 + 2\alpha \frac{\Delta t}{h^2}\right) \varphi_i^{n+1} = \left(1 - 2\alpha \frac{\Delta t}{h^2}\right) \varphi_i^{n-1} + 2\alpha \frac{\Delta t}{h^2} \left(\varphi_{i+1}^n + \varphi_{i-1}^n\right)$$

$\Rightarrow$ still explicit

But, does the averaging in time impact the accuracy in time? TS in time!

$$\varphi_i^{n+1} = \varphi_i^n + \Delta t \left.\frac{\partial \varphi_i}{\partial t}\right|^n + \frac{\Delta t^2}{2} \left.\frac{\partial^2 \varphi_i}{\partial t^2}\right|^n + \ldots$$

$$+ \quad \varphi_i^{n-1} = \varphi_i^n - \Delta t \left.\frac{\partial \varphi_i}{\partial t}\right|^n + \frac{\Delta t^2}{2} \left.\frac{\partial^2 \varphi_i}{\partial t^2}\right|^n + \ldots$$

$$\varphi_i^{n+1} + \varphi_i^{n-1} = 2\varphi_i^n + \Delta t^2 \left.\frac{\partial^2 \varphi_i}{\partial t^2}\right|^n + \ldots$$

$$\varphi_i^n = \frac{\varphi_i^{n+1} + \varphi_i^{n-1}}{2} + O(\Delta t^2)$$

$\Rightarrow$ still 2nd order in time

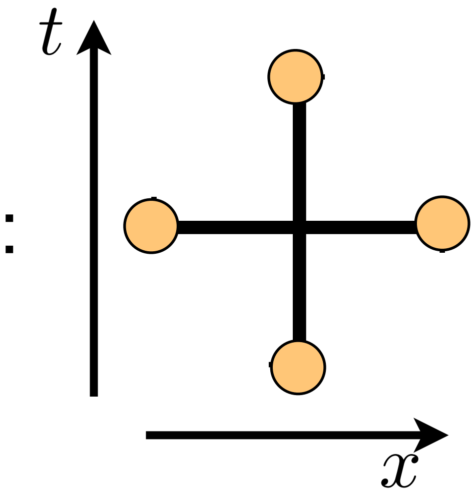
Parabolic Equations - Explicit Methods

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common explicit methods

Du-Fort-Frankel

stencil:



$$\left(1 + 2\alpha\frac{\Delta t}{h^2}\right)\varphi_i^{n+1} = \left(1 - 2\alpha\frac{\Delta t}{h^2}\right)\varphi_i^{n-1} + 2\alpha\frac{\Delta t}{h^2}\left(\varphi_{i+1}^n + \varphi_{i-1}^n\right)$$

$\Rightarrow$ still explicit

But, does the averaging in time impact the accuracy in time?

- truncation errors: $O(\Delta t^2)$ in time, $O(\Delta x^2)$ in space
- Stability? turns out to be always stable!

But, there are some issues:

- must store 3 time levels: $n\text{-}1$, n, $n+1$ data
- startup problem: cannot use for $n=0$, since there is no $n=-1$ data!
  fix: start with lower order scheme, e.g. FTCS or BTCS for 1 time step

$$\varphi^0 \xrightarrow{\text{FTCS}} \varphi^1 \xrightarrow{\text{DF}} \varphi^2 \xrightarrow{\text{DF}} \varphi^3 \quad \ldots.$$

Consistency of Du-Fort Frankel

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Recap: Consistency ≜ numerical approximation approaches PDE

Du-Fort Frankel

$$\left(1 + 2\alpha \frac{\Delta t}{\Delta x^2}\right) \varphi_i^{n+1} = \left(1 - 2\alpha \frac{\Delta t}{\Delta x^2}\right) \varphi_i^{n-1} + 2\alpha \frac{\Delta t}{\Delta x^2} \left(\varphi_{i+1}^n + \varphi_{i-1}^n\right)$$

- Question: Does this approach the PDE, as $\Delta x, \Delta t \rightarrow 0$?

Substitute Taylor series into finite difference form

$$\left(1+2\alpha\frac{\Delta t}{\Delta x^2}\right)\varphi_i^{n+1}=\left(1-2\alpha\frac{\Delta t}{\Delta x^2}\right)\varphi_i^{n-1}+2\alpha\frac{\Delta t}{\Delta x^2}\left(\varphi_{i+1}^n+\varphi_{i-1}^n\right)$$

$$\frac{\partial\varphi}{\partial t}=\alpha\frac{\partial^2\varphi}{\partial x^2}$$

Write Taylor series for each term in the finite difference form

$$\varphi_i^{n+1}=\varphi_i^n+\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n+\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)$$

$$\varphi_i^{n-1}=\varphi_i^n-\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n-\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)$$

$$\varphi_{i+1}^n=\varphi_i^n+\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i+\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)$$

$$\varphi_{i-1}^n=\varphi_i^n-\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i-\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)$$

Substitute Taylor series into FTCS

$$\left(1+2\alpha\frac{\Delta t}{\Delta x^2}\right)\left(\varphi_i^n+\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n+\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)\right)=$$

$$\left(1-2\alpha\frac{\Delta t}{\Delta x^2}\right)\left(\varphi_i^n-\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n-\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)\right)$$

$$+2\alpha\frac{\Delta t}{\Delta x^2}\left(\varphi_i^n+\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i+\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)\right.$$

$$\left.+\varphi_i^n-\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i-\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)\right)$$

$$\left(1+2\alpha\frac{\Delta t}{\Delta x^2}\right)\left(\varphi_i^n+\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n+\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)\right)=$$

$$\left(1-2\alpha\frac{\Delta t}{\Delta x^2}\right)\left(\varphi_i^n-\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+\frac{\Delta t^2}{2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n-\frac{\Delta t^3}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)\right)$$

$$+2\alpha\frac{\Delta t}{\Delta x^2}\left(\varphi_i^n+\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i+\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)\right.$$

$$\left.+\varphi_i^n-\Delta x\left.\frac{\partial\varphi}{\partial x}\right|_i+\frac{\Delta x^2}{2}\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i-\frac{\Delta x^3}{6}\left.\frac{\partial^3\varphi}{\partial x^3}\right|_i+\frac{\Delta x^4}{24}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+O(\Delta x^5)\right)$$

$$2\Delta t\left.\frac{\partial\varphi}{\partial t}\right|^n+2\alpha\frac{\Delta t^3}{\Delta x^2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n+\frac{\Delta t^3}{3}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^4)=\ 2\alpha\Delta t\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i+2\alpha\Delta t\frac{\Delta x^2}{12}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+2\alpha\frac{\Delta t}{\Delta x^2}O(\Delta x^5)$$

$$\left.\frac{\partial\varphi}{\partial t}\right|^n+\alpha\frac{\Delta t^2}{\Delta x^2}\left.\frac{\partial^2\varphi}{\partial t^2}\right|^n+\frac{\Delta t^2}{6}\left.\frac{\partial^3\varphi}{\partial t^3}\right|^n+O(\Delta t^3)=\alpha\left.\frac{\partial^2\varphi}{\partial x^2}\right|_i+\alpha\frac{\Delta x^2}{12}\left.\frac{\partial^4\varphi}{\partial x^4}\right|_i+\alpha\frac{1}{\Delta x^2}O(\Delta x^5)$$

$$\frac{\partial\varphi}{\partial t}=\alpha\frac{\partial^2\varphi}{\partial x^2}-\alpha\frac{\Delta t^2}{\Delta x^2}\frac{\partial^2\varphi}{\partial t^2}-\frac{\Delta t^2}{6}\frac{\partial^3\varphi}{\partial t^3}+\alpha\frac{\Delta x^2}{12}\frac{\partial^4\varphi}{\partial x^4}+O(\Delta x^3)+O(\Delta t^3)$$

Consistency of Du-Fort Frankel

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Recap: Consistency ≜ numerical approximation approaches PDE

Du-Fort Frankel

$$\left(1 + 2\alpha \frac{\Delta t}{\Delta x^2}\right) \varphi_i^{n+1} = \left(1 - 2\alpha \frac{\Delta t}{\Delta x^2}\right) \varphi_i^{n-1} + 2\alpha \frac{\Delta t}{\Delta x^2} \left(\varphi_{i+1}^n + \varphi_{i-1}^n\right)$$

Modified equation:

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2} - \alpha \frac{\Delta t^2}{\Delta x^2} \frac{\partial^2 \varphi}{\partial t^2} - \frac{\Delta t^2}{6} \frac{\partial^3 \varphi}{\partial t^3} + \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \varphi}{\partial x^4} + O(\Delta x^3) + O(\Delta t^3)$$

- Question: Does this approach the PDE, as $\Delta x, \Delta t \rightarrow 0$?

⇒ consistent only if as $\Delta x \rightarrow 0, \Delta t \rightarrow 0,$ **AND** $\Delta t/\Delta x \rightarrow 0$

if $\Delta t/\Delta x = const = C,$ then the PDE that is solved is

$$\frac{\partial \varphi}{\partial t} + \alpha C \frac{\partial^2 \varphi}{\partial t^2} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Parabolic Equations - Explicit Methods

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common explicit methods

Runge-Kutta (RK)

Idea: use intermediate time levels between n and n+1 to get a better estimate for the right hand side

$$\frac{d\varphi_i}{dt} = \frac{\alpha}{h^2}\left(\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}\right) = f_i$$

Example: 4th-order RK (RK-4):

i) $\varphi_i^{\left(n+\frac{1}{2}\right)^*} = \varphi_i^n + \frac{\Delta t}{2} f_i^n$

ii) $\varphi_i^{\left(n+\frac{1}{2}\right)^{**}} = \varphi_i^n + \frac{\Delta t}{2} f_i^{\left(n+\frac{1}{2}\right)^*}$ use results of i) to evaluate f_i

iii) $\varphi_i^{(n+1)^{***}} = \varphi_i^n + \frac{\Delta t}{2} f_i^{\left(n+\frac{1}{2}\right)^{**}}$ use results of ii) to evaluate f_i

iv) combine: $\varphi_i^{n+1} = \varphi_i^n + \frac{\Delta t}{6}\left(f_i^n + 2 f_i^{\left(n+\frac{1}{2}\right)^*} + 2 f_i^{\left(n+\frac{1}{2}\right)^{**}} + f_i^{(n+1)^{***}}\right)$

Parabolic Equations - Implicit Methods

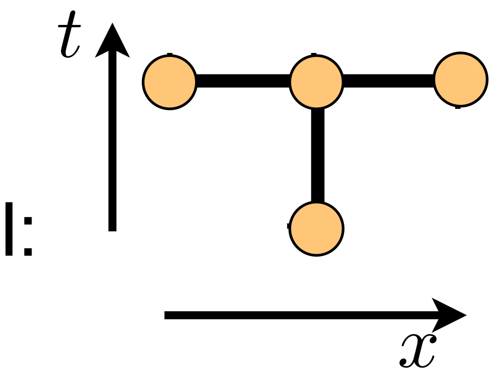
$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common **implicit** methods (usually preferred for parabolic equations)

Backward time / Laasonen Method (BTCS)

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}\right)$$

stencil:

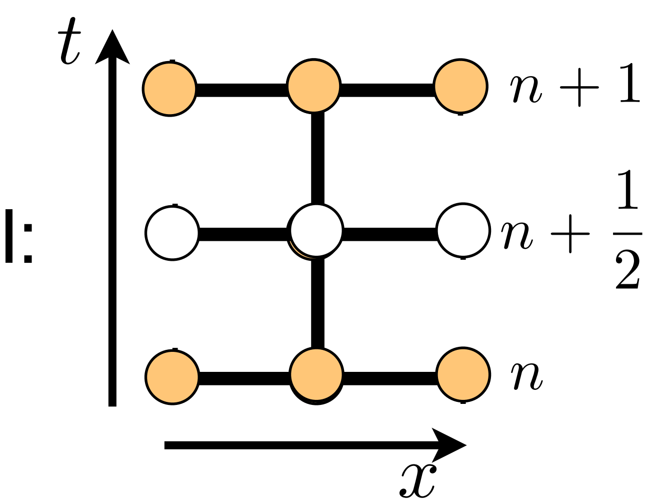


- truncation errors: $O(\Delta t)$ in time, $O(\Delta x^2)$ in space
- always stable

Crank-Nicolson

(very common)

stencil:



Idea: average the right hand side in time to $n+1/2$

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \frac{1}{2}\left(f_i^{n+1} + f_i^n\right) = \frac{\alpha}{2}\left(\frac{\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}}{h^2} + \frac{\varphi_{i+1}^{n} - 2\varphi_i^{n} + \varphi_{i-1}^{n}}{h^2}\right)$$

- same as average of FTCS and BTCS
- truncation errors: $O(\Delta t^2)$ in time, $O(\Delta x^2)$ in space

lhs: central difference @ n+1/2
rhs: midpoint average

Parabolic Equations - Implicit Methods

$$\frac{\partial \varphi}{\partial t} = \alpha \frac{\partial^2 \varphi}{\partial x^2}$$

Common **implicit** methods (usually preferred for parabolic equations)

Crank-Nicolson

Often, Crank-Nicolson is implemented in a 2-step process:

step 1: $$\frac{\varphi_i^{n+\frac{1}{2}} - \varphi_i^n}{\frac{\Delta t}{2}} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n\right)$$ explicit

step 2: $$\frac{\varphi_i^{n+1} - \varphi_i^{n+\frac{1}{2}}}{\frac{\Delta t}{2}} = \frac{\alpha}{h^2}\left(\varphi_{i+1}^{n+1} - 2\varphi_i^{n+1} + \varphi_{i-1}^{n+1}\right)$$ implicit

Beta-Formulation

Idea: don't just do arithmetic average of n and $n+1$, but use weighted average

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\Delta t} = \beta f_i^{n+1} + (1-\beta) f_i^n$$

$\beta = 0$: FTCS
$\beta = 0.5$: Crank-Nicholson
$\beta = 1$: BTCS

$0 \leq \beta \leq 0.5$
conditionally stable

$0.5 \leq \beta \leq 1$
always stable

Parabolic Equations with Source Terms

What changes when we add a source term q to the PDE?

$$\frac{\partial \varphi}{\partial t} = \alpha \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right) + q(x, y, t)$$

- need to evaluate source term q at time t consistent with the chosen method, e.g.,
  - FTCS: evaluate q at t^n
  - BTCS: evaluate q at t^{n+1}
  - Crank-Nicholson: evaluate q at $t^{n+1/2}$ or as average of q evaluated at t^n and t^{n+1}
  - Beta-Formulation: evaluate q as beta average of q evaluate at t^n and t^{n+1}

What changes for 2D vs 1D problems?

- additional finite difference terms for the y-direction derivate
- different stability constraint for time step for explicit methods
- implicit methods are no longer tridiagonal. Thus Gaussian elimination not a good choice. Use iterative method (Gauss Seidel, better V-cycle multigrid)