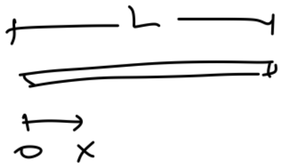
Numerics for the heat equation

* Heat equation: $\dfrac{\partial u}{\partial t} = c^2 \dfrac{\partial^2 u}{\partial x^2}$, $\underbrace{u(x,0) = f(x)}_{\text{IC}}$



* Some common boundary conditions:
  - → Prescribed temperature: $u(x,t) = g(t)$ at $x=0$ and/or $x=L$ (Dirichlet BC)
  - → Prescribed heat flux: $-c^2 \dfrac{\partial u}{\partial x} = q(t)$ at $x=0$ and/or $x=L$ (Neumann BC)
  - → Mixed condition: $\beta u + \dfrac{\partial u}{\partial x} = r(t)$ at $x=0$ and/or $x=L$ (Robin BC)

• Finite differences

* Spatial derivative: $\dfrac{\partial^2 u}{\partial x^2}(x,t) = \dfrac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$

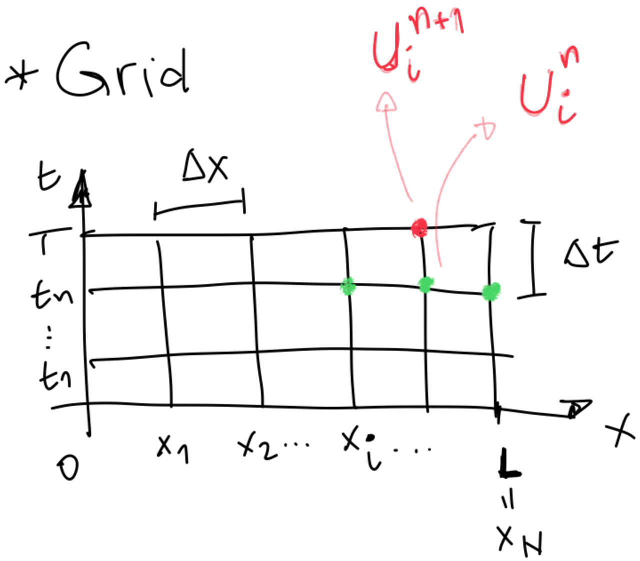
* For the temporal (first-order) derivative, we have different options:

• Backward: $\dfrac{\partial u}{\partial t}(x,t) = \dfrac{u(x,t) - u(x,t-\Delta t)}{\Delta t} + \mathcal{O}(\Delta t)$

• Forward: $\dfrac{\partial u}{\partial t}(x,t) = \dfrac{u(x,t+\Delta t) - u(x,t)}{\Delta t} + \mathcal{O}(\Delta t)$

• Central: $\frac{\partial u}{\partial t}(x,t) = \frac{u(x,t+\Delta t) - u(x,t-\Delta t)}{2\Delta t} + O(\Delta t^2)$

* Grid



Forward: $\frac{U_i^{n+1} - U_i^n}{\Delta t} = c^2\left(\frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Delta x^2}\right)$

$$\to U_i^{n+1} = U_i^n + \underbrace{\frac{\Delta t c^2}{\Delta x^2}}_{=\alpha}\left(U_{i+1}^n - 2U_i^n + U_{i-1}^n\right)$$

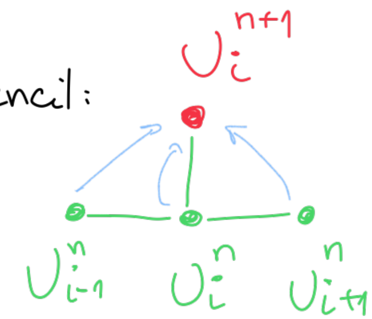
• The explicit scheme (forward Euler method)

$$U_i^{n+1} = \underbrace{\alpha U_{i-1}^n + (1-2\alpha)U_i^n + \alpha U_{i+1}^n}_{\text{past time step}}, \quad \boxed{\alpha = \frac{c^2 \Delta t}{\Delta x^2}}$$

$\downarrow$ next step (unknown)

past time step (we already have these values!)

Stencil:



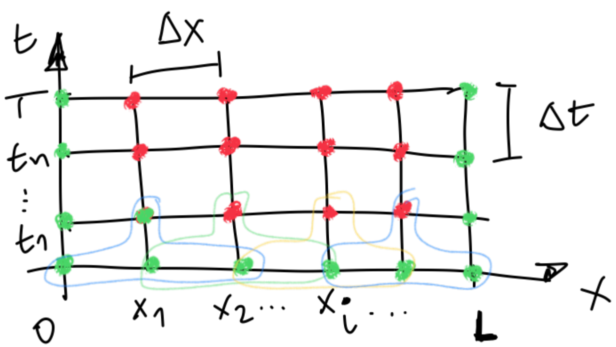
* Initial condition

first time step

$\rightarrow u(x,0) = f(x) \Rightarrow U_i^0 = f(x_i)$

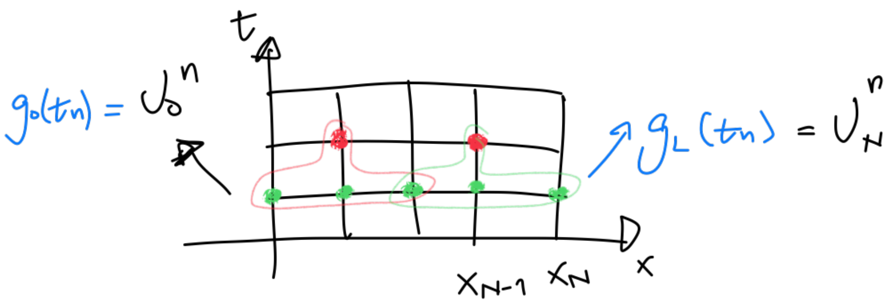
$$* n=0 : \quad U_i^1 = \alpha \underbrace{U_{i-1}^0}_{f(x_{i-1})} + (1-2\alpha)\underbrace{U_i^0}_{f(x_i)} + \alpha \underbrace{U_{i+1}^0}_{f(x_{i+1})}$$

a general point x_i in space



* Dirichlet case

$\rightarrow u(0,t) = \underbrace{g_0(t)}_{\text{given}} , \quad u(L,t) = \underbrace{g_L(t)}_{\text{given}}$



$\rightarrow i=1 : \quad U_1^{n+1} = \alpha \underbrace{U_0^n}_{g_0(t_n)} + (1-2\alpha) \underbrace{U_1^n}_{\checkmark} + \underbrace{U_2^n}_{\checkmark}$

$\rightarrow i=N-1 : \quad U_{N-1}^{n+1} = \alpha U_{N-2}^n + (1-2\alpha) U_{N-1}^n + \alpha \underbrace{U_N^n}_{g_L(t_n)}$

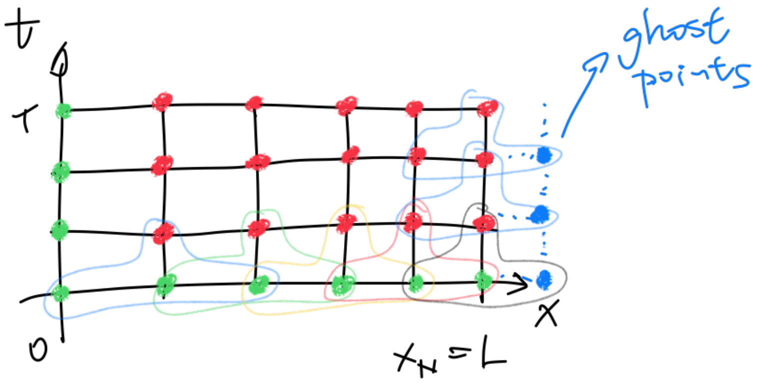
* Neumann or Robin BCs

$\beta u + \frac{\partial u}{\partial x} = r(t)$ at $x=0$ or $x=L$, $\beta \in \mathbb{R}$ (usually a constant)

→ if $\beta = 0$, we call this a Neumann BC

– Consider, for instance, the following BCs:

$$\begin{cases} u = g(t) & \text{at } x=0 \quad \text{(Dirichlet on the left)} \\ \beta u + \frac{\partial u}{\partial x} = r(t) & \text{at } x=L \quad \text{(Robin on the right)} \end{cases}$$



$$U_N^{n+1} = \alpha U_{N-1}^n + (1-2\alpha) U_N^n + \alpha U_{N+1}^n$$

→ doesn't exist! (off the grid)

– Robin/Neumann BC: $\beta u(L,t) + \left.\frac{\partial u}{\partial x}\right|_{x=L} \overset{\text{given}}{=} r(t) \xRightarrow[\text{FD}]{\text{central}} \beta U_N^n + \frac{U_{N+1}^n - U_{N-1}^n}{2\Delta x} = r_n$

FD

$:= r(t_n)$

$$\Rightarrow \boxed{U_{N+1}^n = U_{N-1}^n - 2\Delta x \beta U_N^n + 2\Delta x\, r_n} \checkmark$$

• Numerical stability

* Explicit Euler: $\boxed{U_i^{n+1} = \boxed{\alpha} U_{i-1}^n + \boxed{(1-2\alpha)} U_i^n + \boxed{\alpha} U_{i+1}^n}$

– At a certain time t_{n+1}, we can compute all U_i^{n+1}, $i=1,2,\dots,N-1$ at once, using vectors and matrices. Considering zero Dirichlet BCs ($g_0(t)=g_L(t)=0$), for simplicity, we can write:

All values of U in space, at time t_{n+1}

$$\underbrace{\begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ U_3^{n+1} \\ \vdots \\ U_{N-1}^{n+1} \end{pmatrix}}_{\underline{U}_{n+1}} = \underbrace{\begin{pmatrix} 1-2\alpha & \alpha & 0 & 0 & \cdots & 0 & 0 & 0 \\ \boxed{\alpha} & \boxed{1-2\alpha} & \boxed{\alpha} & 0 & \cdots & 0 & 0 & 0 \\ 0 & \alpha & 1-2\alpha & \alpha & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \alpha & 1-2\alpha \end{pmatrix}}_{\underline{\underline{Q}}} \underbrace{\begin{pmatrix} U_1^n \\ U_2^n \\ U_3^n \\ \vdots \\ U_{N-1}^n \end{pmatrix}}_{\underline{U}_n}$$

$$\rightarrow \underline{U}_{n+1} = \underbrace{\left(\underline{\underline{I}} + \alpha \underline{\underline{A}}\right)}_{\underline{\underline{Q}}} \underline{U}_n, \quad \underline{\underline{I}} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}; \quad \underline{\underline{A}} = \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 \end{pmatrix}$$

$\underline{\underline{I}}$: $(N-1)\times(N-1)$ identity matrix

$$\to \underline{U}_{n+1} = \underline{\underline{Q}}\,\underline{U}_n = \underline{\underline{Q}}\left(\underline{\underline{Q}}\,\underline{U}_{n-1}\right) = \underline{\underline{Q}}^{2}\,\underline{U}_{n-1} = \underline{\underline{Q}}^2\left(\underline{\underline{Q}}\,\underline{U}_{n-2}\right) = \underline{\underline{Q}}^3\,\underline{U}_{n-2} = \cdots =$$

$$= \underline{\underline{Q}}^{n+1}\,\underline{U}_0 \implies \boxed{\underline{U}_{n+1} = \underline{\underline{Q}}^{n+1}\,\underline{f}}\ ; \quad \underline{f} = \begin{pmatrix} f(0) \\ f(x_1) \\ \vdots \\ f(L) \end{pmatrix}$$

$\to$ exponent! $\to$ exponent!

$\underline{U}_0$: initial condition

– If the entries of $\underline{\underline{Q}}$ are "too large" (in some sense), then the solution $\underline{U}_n$ will grow "exponentially" as n grows (i.e., as we go forward in time) $\to$ non-physical!

– This exponential growth will happen if the largest eigenvalue (in absolute value) of $\underline{\underline{Q}}$ is larger than 1. It is possible to prove that this can be avoided if, and only if, we take $\alpha \le 1/2$, that is:

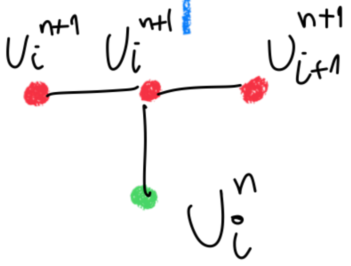
$$\frac{c^2\Delta t}{\Delta x^2} \le \frac{1}{2} \implies \boxed{\Delta t \le \frac{\Delta x^2}{2c^2}}$$

$\to$ a parabolic CFL condition!

$\to$ the explicit Euler method is only conditionally stable!

– This is a severe restriction. For example, if we double the spatial resolution ($\Delta x \to \Delta x/2$), then we have to quadruple the temporal resolution ($\Delta t \to \Delta t/4$).

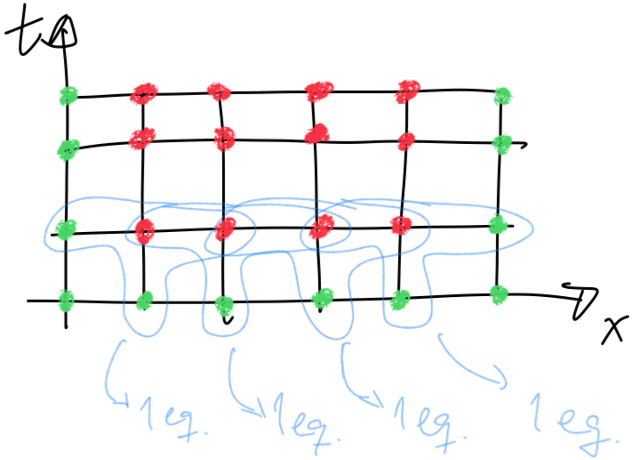
• Implicit scheme (backward Euler method)



$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} \Rightarrow \frac{U_i^{n+1} - U_i^n}{\Delta t} = c^2 \left(\frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{\Delta x^2} \right)$$

$$\hookrightarrow \boxed{-\alpha U_{i-1}^{n+1} + (1+2\alpha) U_i^{n+1} - \alpha U_{i+1}^{n+1} = U_i^n}$$

↳ we have more than 1 unknown to find from this equation ...



Shortcoming: need to solve a linear system!

"stiffness matrix"

Matrix form: $(\underline{\underline{I}} - \alpha \underline{\underline{A}}) \underline{U}_{n+1} = \underline{U}_n \Rightarrow \underline{\underline{K}}\, \underline{U}_{n+1} = \underline{U}_n$

$$\hookrightarrow \underline{U}_{n+1} = \underline{\underline{K}}^{-1} \underline{U}_n = \underline{\underline{\tilde{Q}}}\, \underline{U}_n$$

↓

$\underline{\underline{\tilde{Q}}}$ has all eigenvalues less than 1 (in absolute value), regardless of α → unconditional stability!

• Semi-implicit scheme (Crank-Nicolson)

* Explicit Euler: $\underline{\underline{I}}\,\underline{U}_{n+1} = (\underline{\underline{I}} + \alpha \underline{\underline{A}})\,\underline{U}_n$
* Implicit Euler: $(\underline{\underline{I}} - \alpha \underline{\underline{A}})\,\underline{U}_{n+1} = \underline{\underline{I}}\,\underline{U}_n$

→ Mean: $\left(\underline{\underline{I}} - \frac{\alpha}{2}\underline{\underline{A}}\right)\underline{U}_{n+1} = \left(\underline{\underline{I}} + \frac{\alpha}{2}\underline{\underline{A}}\right)\underline{U}_n \quad (CN)$

Important: CN is also unconditionally stable, but it is $\mathcal{O}(\Delta t^2)$, while the other two schemes are $\mathcal{O}(\Delta t)$.