

Practical Course: Modeling, Simulation, Optimization

Week 3

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- 3.B** Spatial discretization
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3.A Time-dependent problems



Motivating example: Diffusion of mass

$$\frac{\partial \rho}{\partial t}(t, \mathbf{x}) = -\nabla \cdot \phi(t, \mathbf{x}) \quad \left(\frac{\partial \rho}{\partial t}(t, x, y) = -\frac{\partial \phi_x}{\partial x}(t, x, y) - \frac{\partial \phi_y}{\partial y}(t, x, y) \right).$$

To complete the model, we need a *constitutive relation* that relates the mass flux $\phi(t, \mathbf{x})$ to the mass density $\rho(t, \mathbf{x})$.

We could for example use.

Fick's law

$$\phi(t, \mathbf{x}) = -D \nabla \rho(t, \mathbf{x}) \quad \left(\begin{bmatrix} \phi_x(t, x, y) \\ \phi_y(t, x, y) \end{bmatrix} = -D \begin{bmatrix} \frac{\partial \rho}{\partial x}(t, x, y) \\ \frac{\partial \rho}{\partial y}(t, x, y) \end{bmatrix} \right).$$

The coefficient D [m^2/s] is called the diffusivity.

'Mass flows from locations with high concentrations to locations with low concentrations'

We then obtain

$$\frac{\partial \rho}{\partial t}(t, \mathbf{x}) = -D \Delta \rho(t, \mathbf{x}), \quad \left(\frac{\partial \rho}{\partial t}(t, x, y) = -D \frac{\partial^2 \rho}{\partial x^2}(t, x, y) - D \frac{\partial^2 \rho}{\partial y^2}(t, x, y) \right)$$

Motivating example: Heat conduction

$$\frac{\partial \rho_u}{\partial t}(t, \mathbf{x}) = -H \nabla \cdot \mathbf{q}(t, \mathbf{x}) + Q(t, \mathbf{x}).$$

We again need constitutive relations to complete the model.

Fourier's law of heat conduction in 2-D

$$\mathbf{q}(t, \mathbf{x}) = -k \nabla T(t, \mathbf{x}).$$

The coefficient k^* [W/m/K] is the thermal conductivity and $T(t, \mathbf{x})$ [K] is the temperature. 'Heat flows from locations with high temperatures to locations with low temperatures'

Internal energy in 2-D

$$\rho_u(t, \mathbf{x}) = cHT(t, \mathbf{x}).$$

The coefficient c [J/K/m³] heat capacity per unit volume.

We thus obtain

$$cH \frac{\partial T}{\partial t}(t, \mathbf{x}) = kH \Delta T(t, \mathbf{x}) + Q(t, \mathbf{x}). \quad (1)$$

3.B Spatial discretization



Spatial discretization / Method of Lines (MOL) / Semi-discretization

Suppose we want to approximate the solution $u(t, x)$ of the initial value problem

$$\begin{aligned} \frac{\partial u}{\partial t}(t, x) &= \kappa \frac{\partial^2 u}{\partial x^2}(t, x) + f(t, x), & (t, x) &\in (0, T) \times (0, L), \\ u(t, 0) &= 0, & \frac{\partial u}{\partial x}(t, L) &= 0, & u(0, x) &= u_0(x). \end{aligned}$$

Introduce an M -point grid in the interval $[0, L]$ with a grid spacing $\Delta x = L/(M - 1)$



Also introduce $f_m(t) = f(t, x_m)$ and the approximations $u_m(t) \approx u(t, x_m)$.

Finite difference discretization (implicit BCs):

$$\begin{aligned} \frac{du_m}{dt}(t) &= \kappa \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + f_m(t), & m &= 1, 2, \dots, M, \\ u_1(t) &= 0, & \frac{u_{M+1}(t) - u_{M-1}(t)}{2\Delta x} &= 0, & u_m(0) &= u_0(x_m). \end{aligned}$$

Implicit or explicit implementation of the boundary conditions

Finite difference discretization (implicit BCs):

$$\frac{du_m}{dt}(t) = \kappa \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + f_m(t), \quad m = 1, 2, \dots, M,$$

$$u_1(t) = 0, \quad \frac{u_{M+1}(t) - u_{M-1}(t)}{2\Delta x} = 0, \quad u_m(0) = u_0(x_m).$$

This is a system of Differential Algebraic Equations (DAEs)

$$\frac{d}{dt} \begin{bmatrix} \mathbf{u}_1(t) \\ 0 \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \mathbf{u}_1(t) \\ \mathbf{u}_2(t) \end{bmatrix} + \begin{bmatrix} \mathbf{f}(t) \\ 0 \end{bmatrix}.$$

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Finite difference discretization (explicit BCs):

$$\frac{du_m}{dt}(t) = \kappa \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + f_m(t), \quad m = 2, 3, \dots, M - 1,$$

$$\frac{du_M}{dt}(t) = \kappa \frac{-2u_M(t) + 2u_{M-1}(t)}{\Delta x^2} + f_M(t), \quad u_m(0) = u_0(x_m),$$

where we should remember that $u_1(t) = 0$.

This is a system of Ordinary Differential Equations (ODEs) for the free DOFs $\mathbf{u}_f(t)$

$$\dot{\mathbf{u}}_f(t) = \mathbf{A}_{ff} \mathbf{u}_f(t) + \mathbf{f}_f(t).$$

The explicit implementation of the BCs is preferred in time-dependent problems.

3.C Temporal discretization



Linear ODEs

Consider the following system of linear ODEs:

$$\frac{d\mathbf{u}}{dt}(t) = \mathbf{A}\mathbf{u}(t) + \mathbf{f}(t), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

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$$\frac{d\mathbf{u}}{dt}(t) = \mathbf{A}\mathbf{u}(t) + \mathbf{f}(t), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

- ▶ Choose a uniform time grid t_0, t_1, t_2, \dots with $t_k = k\Delta t$.
- ▶ Define $\mathbf{f}^k := \mathbf{f}(t_k)$ and introduce the approximations $\mathbf{u}^k \approx \mathbf{u}(t_k)$.

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By Taylor's theorem

$$\mathbf{u}(t_{k+1}) = \mathbf{u}(t_k + \Delta t) = \mathbf{u}(t_k) + \Delta t \frac{d\mathbf{u}}{dt}(t_k) + \frac{\Delta t^2}{2} \frac{d^2\mathbf{u}}{dt^2}(\tau),$$

for some $\tau \in [t_k, t_{k+1}]$. Rearranging, we find

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = \frac{d\mathbf{u}}{dt}(t_k) + O(\Delta t).$$

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$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = \frac{d\mathbf{u}}{dt}(t_k) + O(\Delta t).$$

We thus find the following scheme.

Forward Euler

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \mathbf{A}\mathbf{u}^k + \mathbf{f}^k, \quad \mathbf{u}^0 = \mathbf{u}_0.$$

Backward Euler

Instead of making a Taylor series expansion of $\mathbf{u}(t_{k+1})$ around $t = t_k$, we can also expand $\mathbf{u}(t_k)$ in a Taylor series around $t = t_{k+1}$:

$$\mathbf{u}(t_k) = \mathbf{u}(t_{k+1} - \Delta t) = \mathbf{u}(t_{k+1}) - \Delta t \frac{d\mathbf{u}}{dt}(t_{k+1}) + \frac{\Delta t^2}{2} \frac{d^2\mathbf{u}}{dt^2}(\tau),$$

for some $\tau \in [t_k, t_{k+1}]$. Rearranging, we find

$$\frac{d\mathbf{u}}{dt}(t_{k+1}) = \frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} + O(\Delta t).$$

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Updates with forward and backward Euler:

$$\mathbf{u}^{k+1} = \mathbf{u}^k + \Delta t(\mathbf{A}\mathbf{u}^k + \mathbf{f}^k), \quad \mathbf{u}^{k+1} = (\mathbf{I} - \Delta t\mathbf{A})^{-1}(\mathbf{u}^k + \Delta t\mathbf{f}^{k+1}).$$

In backward Euler we need to solve a system of linear equations in every time step. Forward Euler is an *explicit scheme*, backward Euler is an *implicit scheme*.

θ -schemes

From the previous two slides, we have

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = \frac{d\mathbf{u}}{dt}(t_k) + O(\Delta t),$$

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = \frac{d\mathbf{u}}{dt}(t_{k+1}) + O(\Delta t).$$

Take a convex combination (with $\theta \in [0, 1]$)

$$(1 - \theta + \theta) \frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = (1 - \theta) \frac{d\mathbf{u}}{dt}(t_k) + \theta \frac{d\mathbf{u}}{dt}(t_{k+1}) + O(\Delta t).$$

θ -scheme

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = (1 - \theta) (\mathbf{A}\mathbf{u}^k + \mathbf{f}^k) + \theta (\mathbf{A}\mathbf{u}^{k+1} + \mathbf{f}^{k+1}), \quad \mathbf{u}^0 = \mathbf{u}_0.$$

For $\theta = 1/2$, we find the Crank-Nicolson scheme.

Crank-Nicolson

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \frac{1}{2} (\mathbf{A}\mathbf{u}^k + \mathbf{f}^k) + \frac{1}{2} (\mathbf{A}\mathbf{u}^{k+1} + \mathbf{f}^{k+1}), \quad \mathbf{u}^0 = \mathbf{u}_0.$$

Convergence analysis

Two ingredients:

1) ODE with continuous solution $u(t)$.

$$F(\mathbf{u}(t)) = 0.$$

2) Discrete numerical scheme

$$\mathbf{F}_{\Delta t}((\mathbf{u}^k)_k) = 0.$$

Theorem (Lax)

The numerical scheme is convergent if it is both

- ▶ *consistent and*
- ▶ *stable.*

Definition (Consistent numerical scheme)

The numerical scheme is consistent iff $\mathbf{F}_{\Delta t}((\mathbf{u}(t_k))_k) = O((\Delta t)^p)$ for some $p > 0$.

Definition (Stable numerical scheme)

The numerical scheme is stable iff there exists a constant K independent of Δt such that $\|\mathbf{u}^k - \mathbf{u}(t_k)\| \leq K \|\mathbf{F}_{\Delta t}((\mathbf{u}(t_k))_k)\|$

Consistency

The computations on the previous slide already show that

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = (1 - \theta) (\mathbf{A}\mathbf{u}(t_k) + \mathbf{f}^k) + \theta (\mathbf{A}\mathbf{u}(t_{k+1}) + \mathbf{f}^{k+1}) + O(\Delta t).$$

But for the Crank-Nicolson scheme ($\theta = \frac{1}{2}$) we can do better

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = \frac{1}{2} (\mathbf{A}\mathbf{u}(t_k) + \mathbf{f}^k) + \frac{1}{2} (\mathbf{A}\mathbf{u}(t_{k+1}) + \mathbf{f}^{k+1}) + O((\Delta t)^2).$$

(Exercise: check this using Taylor series expansions)

Proving stability (1/2)

We have

$$\frac{\mathbf{u}(t_{k+1}) - \mathbf{u}(t_k)}{\Delta t} = (1 - \theta) (\mathbf{A}\mathbf{u}(t_k) + \mathbf{f}^k) + \theta (\mathbf{A}\mathbf{u}(t_{k+1}) + \mathbf{f}^{k+1}) + \mathbf{r}_k.$$

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where the residues \mathbf{r}_k are $O(\Delta t)$ (or $O((\Delta t)^2)$ if $\theta = \frac{1}{2}$).

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where the residues \mathbf{r}_k are $O(\Delta t)$ (or $O((\Delta t)^2)$ if $\theta = \frac{1}{2}$).

Introduce $\mathbf{e}^k := \mathbf{u}^k - \mathbf{u}(t_k)$ and subtract the first equation from the second:

$$\frac{\mathbf{e}^{k+1} - \mathbf{e}^k}{\Delta t} = (1 - \theta)\mathbf{A}\mathbf{e}^k + \theta\mathbf{A}\mathbf{e}^{k+1} - \mathbf{r}_k, \quad \mathbf{e}^0 = 0.$$

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Rearranging shows that

$$\begin{aligned} (\mathbf{I} - \theta\Delta t\mathbf{A})\mathbf{e}^{k+1} &= (1 - \theta)\Delta t\mathbf{A}\mathbf{e}^k - \mathbf{r}_k \\ \mathbf{e}^{k+1} &= \mathbf{B}\mathbf{e}^k - \Delta t\mathbf{b}_k, \quad \mathbf{e}^0 = 0, \end{aligned}$$

where

$$\mathbf{B} = (\mathbf{I} - \theta\Delta t\mathbf{A})^{-1} (\mathbf{I} + (1 - \theta)\Delta t\mathbf{A}), \quad \mathbf{b}_k = (\mathbf{I} - \theta\Delta t\mathbf{A})^{-1} \mathbf{r}_k.$$

Note that $\mathbf{b}_k = O(\Delta t)$ (or $O((\Delta t)^2)$ if $\theta = 1/2$).

Proving stability (2/2)

$$\mathbf{e}^{k+1} = \mathbf{B}\mathbf{e}^k - \Delta t \mathbf{b}_k, \quad \mathbf{e}^0 = 0,$$

When $\|\mathbf{B}\| > 1$, the scheme is clearly unstable.

Assume that $\|\mathbf{B}\| \leq 1$, then

$$|\mathbf{e}^{k+1}| \leq |\mathbf{e}^k| + \Delta t |\mathbf{b}_k|, \quad \Rightarrow \quad |\mathbf{e}^k| \leq \Delta t \sum_{k=0}^{k-1} |\mathbf{b}_k| \leq Ck(\Delta t)^2,$$

where it was used that \mathbf{b}_k is $O(\Delta t)$, i.e. there exists a C such that $|\mathbf{b}_k| \leq C\Delta t$.

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where it was used that \mathbf{b}_k is $O(\Delta t)$, i.e. there exists a C such that $|\mathbf{b}_k| \leq C\Delta t$.

So the error after a *fixed number of k time-steps* is of $O((\Delta t)^2)$.

However, the error at a fixed time-instant T , i.e. the error after $K = T/\Delta t$ is

$$|\mathbf{e}^K| = CK(\Delta t)^2 = CT\Delta t = O(\Delta t).$$

Stability regions

Recall that

$$\mathbf{B} = (\mathbf{I} - \theta\Delta t\mathbf{A})^{-1} (\mathbf{I} + (1 - \theta)\Delta t\mathbf{A}).$$

Suppose that ν is an eigenvalue of \mathbf{A} , i.e. that $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$. Then also

$$\mathbf{B}\mathbf{v} = \frac{1 + (1 - \theta)\lambda\Delta t}{1 - \theta\lambda\Delta t}\mathbf{v}.$$

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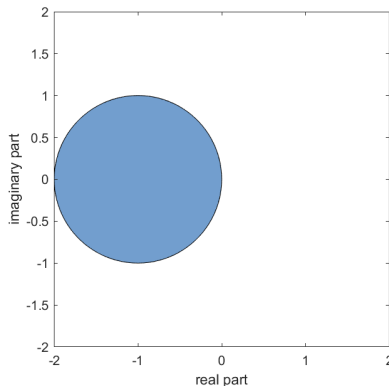
$$\mathbf{B}\mathbf{v} = \frac{1 + (1 - \theta)\lambda\Delta t}{1 - \theta\lambda\Delta t}\mathbf{v}.$$

The scheme is thus stable when

$$\left| \frac{1 + (1 - \theta)\lambda\Delta t}{1 - \theta\lambda\Delta t} \right| \leq 1, \quad \text{for all } \lambda \in \sigma(\mathbf{A}).$$

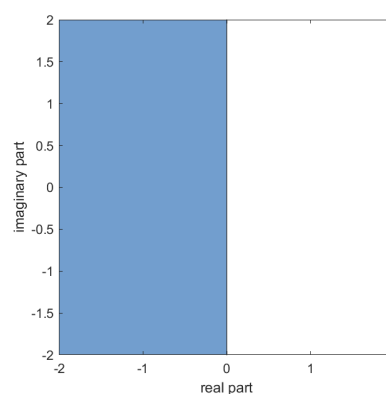
Forward Euler ($\theta = 0$)

$$|1 + \lambda\Delta t| \leq 1$$



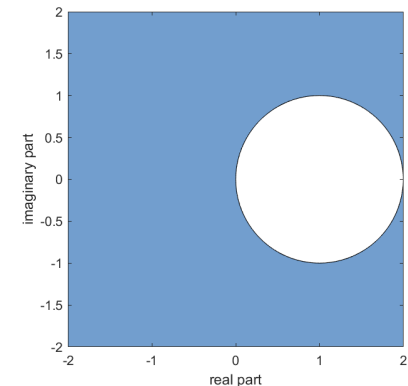
Crank-Nicolson ($\theta = \frac{1}{2}$)

$$\left| 1 + \frac{1}{2}\lambda\Delta t \right| \leq \left| 1 - \frac{1}{2}\lambda\Delta t \right|$$



Backward Euler ($\theta = 1$)

$$|1 - \lambda\Delta t| \geq 1$$



Summary

$$\frac{d\mathbf{u}}{dt}(t) = \mathbf{A}\mathbf{u}(t) + \mathbf{f}(t), \quad \mathbf{u}(0) = \mathbf{u}_0.$$

θ -scheme

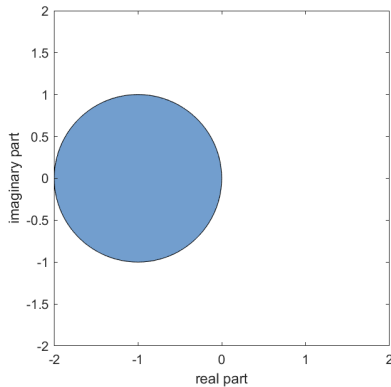
$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = (1 - \theta) (\mathbf{A}\mathbf{u}^k + \mathbf{f}^k) + \theta (\mathbf{A}\mathbf{u}^{k+1} + \mathbf{f}^{k+1}), \quad \mathbf{u}^0 = \mathbf{u}_0.$$

The scheme is stable iff

$$|1 + (1 - \theta)\lambda\Delta t| \leq |1 - \theta\lambda\Delta t|, \quad \text{for all } \lambda \in \sigma(\mathbf{A}).$$

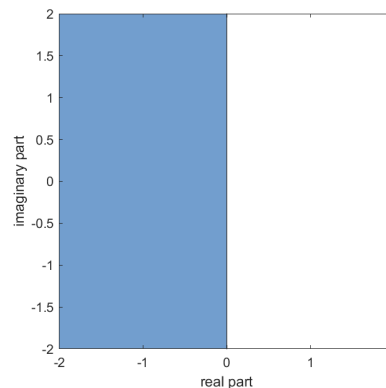
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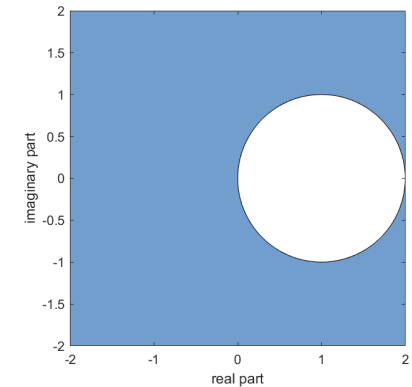
Crank-Nicolson ($\theta = \frac{1}{2}$)

$$|1 + \frac{1}{2}\lambda\Delta t| \leq |1 - \frac{1}{2}\lambda\Delta t|$$



Backward Euler ($\theta = 1$)

$$|1 - \lambda\Delta t| \geq 1$$



3.D Back to the spatial discretization



Returning to our original problem

Suppose we want to approximate the solution $u(t, x)$ of the initial value problem

$$\begin{aligned} \frac{\partial u}{\partial t}(t, x) &= \kappa \frac{\partial^2 u}{\partial x^2}(t, x) + f(t, x), & (t, x) &\in (0, T) \times (0, L), \\ u(t, 0) &= 0, & \frac{\partial u}{\partial x}(t, L) &= 0, & u(0, x) &= u_0(x). \end{aligned}$$

Introduce an M -point grid in the interval $[0, L]$ with a grid spacing $\Delta x = L/(M - 1)$



Also introduce $f_m(t) = f(t, x_m)$ and the approximation $u_m(t) \approx u(t, x_m)$.

Finite difference discretization (explicit BCs):

$$\begin{aligned} \frac{du_m}{dt}(t) &= \kappa \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + f_m(t), & m &= 2, 3, \dots, M - 1, \\ \frac{du_M}{dt}(t) &= \kappa \frac{-2u_M(t) + 2u_{M-1}(t)}{\Delta x^2} + f_M(t), & u_m(0) &= u_0(x_m), \end{aligned}$$

where we should remember that $u_1(t) = 0$.

Returning to our original problem

Finite difference discretization (explicit BCs):

$$\begin{aligned} \frac{du_m}{dt}(t) &= \kappa \frac{u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)}{\Delta x^2} + f_m(t), & m = 2, 3, \dots, M-1, \\ \frac{du_M}{dt}(t) &= \kappa \frac{-2u_M(t) + 2u_{M-1}(t)}{\Delta x^2} + f_M(t), & u_m(0) = u_0(x_m), \end{aligned}$$

where we should remember that $u_1(t) = 0$.

This is a system of Ordinary Differential Equations (ODEs) for the free DOFs $\mathbf{u}_f(t)$

$$\dot{\mathbf{u}}_f(t) = \mathbf{A}_{\text{ff}} \mathbf{u}_f(t) + \mathbf{f}_f(t).$$

$$\mathbf{A}_{\text{ff}} = \frac{\kappa}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & & 0 & 0 & 0 \\ 1 & -2 & 1 & & 0 & 0 & 0 \\ 0 & 1 & -2 & & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & & -2 & 1 & 0 \\ 0 & 0 & 0 & & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 2 & -2 \end{bmatrix}.$$

Note: \mathbf{A}_{ff} depends on Δx ,

The stability of the numerical scheme may thus depend on Δt and Δx !

A first observation

Claim: All eigenvalues of A_{ff} are nonpositive.

We will prove this claim next week.

Conclusion:

The Crank-Nicolson and Backward Euler scheme are stable (for all Δx and Δt).

What about Forward Euler?

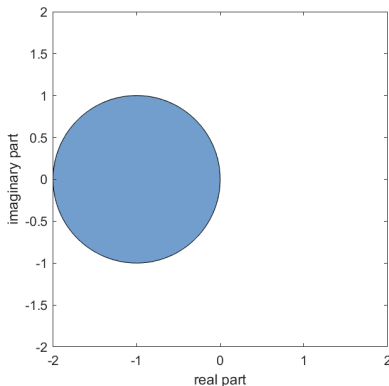
In the lecture next week, we will see how we can prove that

$$\sigma(\mathbf{A}_{\text{ff}}) \subset \left[\frac{-4\kappa}{(\Delta x)^2}, 0 \right]$$

The Forward Euler scheme is stable when

Forward Euler ($\theta = 0$)

$$|1 + \lambda \Delta t| \leq 1$$



$$\left| 1 + \frac{-4\kappa}{(\Delta x)^2} \Delta t \right| \leq 1$$

$$1 + \frac{-4\kappa}{(\Delta x)^2} \Delta t \leq 1, \quad \text{and} \quad - \left(1 + \frac{-4\kappa}{(\Delta x)^2} \Delta t \right) \leq 1$$

$$\frac{-4\kappa}{(\Delta x)^2} \Delta t \leq 0, \quad \text{and} \quad \frac{4\kappa}{(\Delta x)^2} \Delta t \leq 2$$

Conclusion:

The Forward Euler scheme is stable when

$$\Delta t \leq \frac{1}{2\kappa} (\Delta x)^2$$

A nice trick for Finite Differences with Forward Euler

We consider

$$\frac{\partial u}{\partial t}(t, x) = \kappa \frac{\partial^2 u}{\partial x^2}(t, x).$$

Finite differences+Forward Euler:

$$\frac{u_m^{k+1} - u_m^k}{\Delta t} = \kappa \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{(\Delta x)^2}$$

This scheme is of $O(\Delta t + (\Delta x)^2)$.

However, when we check the consistency error we see that

$$\begin{aligned} \frac{u(t_{k+1}, x_m) - u(t_k, x_m)}{\Delta t} &= \frac{\partial u}{\partial t}(t_k, x_m) + \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2}(t_k, x_m) + O((\Delta t)^2) \\ \kappa \frac{u(t_k, x_{m+1}) - 2u(t_k, x_m) + u(t_k, x_{m-1}))}{(\Delta x)^2} &= \kappa \frac{\partial^2 u}{\partial x^2}(t_k, x_m) + \kappa \frac{(\Delta x)^2}{12} \frac{\partial^4 u}{\partial x^4}(t_k, x_m) + O((\Delta x)^4) \end{aligned}$$

Note that $\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}$ and $\frac{\partial^2 u}{\partial t^2}(t_k, x_m) = \kappa^2 \frac{\partial^4 u}{\partial x^4}(t_k, x_m)$.

When $\Delta t = \frac{1}{6\kappa} (\Delta x)^2$ we get $O((\Delta t)^2 + (\Delta x)^4)$!

(But you need to discretize the BCs with the same rates...)