Lecture 3

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Numerical Methods for PDEs

Outline of Lecture 3

- exercises of Lecture 2
- method of horizontal/vertical lines
- time-integration methods
- local truncation error & consistency & zero stability
- absolute stability & stability regions
- boundary locus
- outlook to Lecture 4

Method of Lines [1]

time-dependent PDE: $\frac{\partial u}{\partial t} = \mathcal{L}(u)$ ← spatial operator

The spatial ("x") and temporal ("t") discretization are done separately (in two steps)

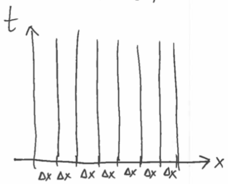
Option 1: method of vertical Lines ("the" method of lines)

1) spatial approximation of $\mathcal{L}(u)$ ⇝ $\frac{d}{dt}\vec{u}(t) = \vec{L}(\vec{u}(t))$ a system of ordinary differential equations (ODEs)

2) time integration

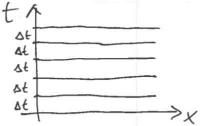
⇓

fully discrete approximation



Method of Lines [2]

<u>Option 2</u>:



method of horizontal lines ("Rothe's method")

1) time integration ⇝ $\vec{F}(\vec{u}^{\,n}, \vec{u}^{\,n+1}) = \vec{0}$ a system of (non)linear "stationary" PDEs

2) numerical (non)linear algebra ⇝ fully discrete approximation.

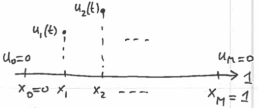
We will use <u>option 1</u> "MoL"

<u>example 1</u> the heat equation $u_t = k \cdot u_{xx}$ ($k>0$), $x \in (0,1)$, $t>0$

IC: $u(x,0) = \sin(\pi x)$, $x \in [0,1]$ $\qquad u(x,t) =$?

(homogeneous Dirichlet) BCs: $u(0,t) = u(1,t) = 0$, $t>0$

(step 1 in MoL): $u_i(t) \approx u(x_i,t)$



Method of lines [3]

$$x_i = \frac{i}{M}, \quad i = 0, \dots, M \leftarrow \text{number of spatial grid points}$$

$$\Rightarrow \quad x_{i+1} - x_i = \frac{i+1}{M} - \frac{i}{M} = \frac{1}{M} \underset{\text{def}}{=} \Delta x \quad \forall i \quad (\text{constant}$$

BCs: $u_0 = 0 \ \forall t$, $u_M = 0 \ \forall t$ IC: $u_i(0) = \sin(\pi x_i)$ $i = 1, \dots, M-1$

How to obtain OD equations for $u_i(t)$, $t > 0$?

$\rightsquigarrow$ approximate $u_{xx}(x_i, t)$ in terms of the $u_i(t)$:

$$u_{xx}(x_i, t) \approx \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{(\Delta x)^2}, \quad i = 1, \dots, M-1, \quad t > 0$$

$\Rightarrow$ system of $M-1$ coupled ODEs: $\dot{\vec{u}}(t) = \kappa \cdot D_{2c} \, \vec{u}(t)$

with $\vec{u}(t) = (u_1(t), u_2(t), \dots, u_{M-1}(t))^T$

and $D_{2c} = \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 1 & & \Theta \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ \Theta & & 1 & -2 \end{pmatrix}$ a tri-diagonal matrix with $\lambda \in \mathbb{R}^-$

Method of lines [4]

Step 2 in MoL: numerically integrate the ODE system

example: use Euler Forward (EF): $\frac{\vec{U}^{n+1} - \vec{U}^{n}}{\Delta t} = \kappa \cdot D_{2c} \vec{U}^{n}$ $n = 0, 1, 2, \ldots, N-1$

$$\Rightarrow \begin{cases} \vec{U}^{n+1} = (I + \kappa \Delta t D_{2c}) \vec{U}^{n} \\ \vec{U}^{0} \text{ given by IC} \end{cases}$$

with $U_i^N \approx u(x_i, T)$ (T: final time)

$\Delta t = \frac{T}{N}$

$t^n = n \cdot \Delta t$, $n = 0, 1, \ldots, N$

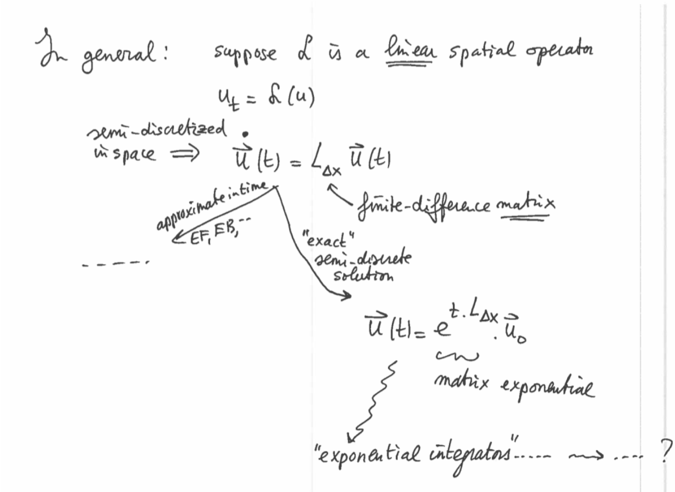
$U_i^n \approx u(x_i, t^n)$

or Euler Backward (EB): $\frac{\vec{U}^{n+1} - \vec{U}^{n}}{\Delta t} = \kappa \cdot D_{2c} \vec{U}^{n+1}$

$$\Rightarrow \begin{cases} \vec{U}^{n+1} = (I - \kappa \Delta t D_{2c})^{-1} \vec{U}^{n} \\ \vec{U}^{0} \text{ given by IC} \end{cases}$$

or ------ many options ---

Method of lines [5]



Method of lines [6]

example 2 the advection equation

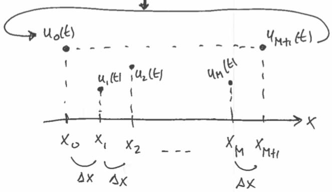
$$\begin{cases} u_t + a u_x = 0 & , x \in [0,1], t>0 \\ u(x,0) = u_0(x) & , x \in [0,1], t>0 \end{cases}$$

(exact solution: $u(x,t) = u_0(x-at)$)

if $a>0$, then we need a BC at $x=0$ ("the inflow boundary")
in that case $x=1$ is the "outflow boundary".

if $a<0$; BC at $x=1$, etcetera

consider periodic BCs: $u(0,t)=u(1,t)$, $t>0$
("whatever flows at the outflow boundary flows back in at the inflow boundary)
in that case: $u_0(t) = u_{M+1}(t)$



$$\vec{U}(t) = \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_{M+1}(t) \end{pmatrix}$$

Method of lines [7]

$$u_x(x_i,t) \approx \frac{u_{i+1}(t) - u_{i-1}(t)}{2\Delta x}, \quad i = 2, 3, \dots, M$$

↑ Central FDs (example)

$\Rightarrow$ ODE system (semi-discrete): $\dot{u}_i(t) = -\frac{a}{2\Delta x}\left(u_{i+1}(t) - u_{i-1}(t)\right), \quad i = 2, \dots, M$

with $\dot{u}_1(t) = -\frac{a}{2\Delta x}\left(u_2(t) - u_0(t)\right)$

$(u_0 = u_{M+1})$ $\quad = -\frac{a}{2\Delta x}\left(u_2(t) - u_{M+1}(t)\right)$

and $\dot{u}_{M+1}(t) = -\frac{a}{2\Delta x}\left(u_{M+2}(t) - u_M(t)\right)$

$(u_1 = u_{M+2})$ $\quad = -\frac{a}{2\Delta x}\left(u_1(t) - u_M(t)\right)$

$\Rightarrow \dot{\vec{u}}(t) = a D_{1c}\, \vec{u}(t)$ with $D_{1c} = \frac{1}{2\Delta x}\begin{pmatrix} 0 & -1 & 0 & \cdots & 1 \\ & \ddots & \ddots & & 0 \\ -1 & & & & \end{pmatrix}$ a circulant skew-symmetric matrix $(D_{1c}^T = -D_{1c})$

$\Rightarrow \lambda \in i\mathbb{R}$

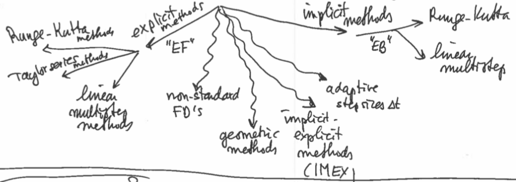
Method of lines [8]

In general, we obtain, after one step in MoL:

$$\begin{cases} \dot{\vec{u}}(t) = M\,\vec{u}(t) \\ \vec{u}(0) = \vec{u}_0 \end{cases}$$

the eigenvalues of the matrix M are going to play an important role in step 2 of MoL.

In step 2, we need to apply a time-integration method:

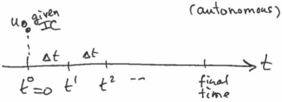


- accuracy ?
- stability ?
- efficiency ?

!

Time-integration methods [1]

Consider the scalar ODE : $u' = f(u)$
(autonomous)



$t^n = n . \Delta t, \; n \geq 0$

$u^n \approx u(t^n)$

Forward Euler (EF, Explicit Euler) : $u^{n+1} = u^n + \Delta t \, f(u^n)$

Backward Euler (EB, Implicit Euler) : $u^{n+1} = u^n + \Delta t \, f(u^{n+1})$

Trapezoidal method (implicit): $\dfrac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}\left[f(u^n) + f(u^{n+1})\right]$

Midpoint method ("leapfrog") explicit : $\dfrac{u^{n+1} - u^{n-1}}{2\Delta t} = f(u^n)$

BDF_2 (implicit) : $\dfrac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = f(u^{n+1})$

etcetera ....

Time-integration methods [2]

(Local) truncation error: (example: midpoint)

LTE: $$\tau^n \overset{\text{def}}{=} \frac{u(t^{n+1}) - u(t^{n-1})}{2\Delta t} - f(u(t^n))$$

Taylor expansion:

$$= \left[u'(t^n) + \frac{1}{6}(\Delta t)^2 u'''(t^n) + O((\Delta t)^4)\right] - u'(t^n)$$

$$= \frac{1}{6}(\Delta t)^2 u'''(t^n) + O((\Delta t)^4)$$

(note that the $O((\Delta t)^3)$ term drops out by "symmetry")

[similar for other methods]

Taylor series methods:

$$u(t^{n+1}) \approx u(t^n) + \Delta t\, u'(t^n) + \frac{1}{2}(\Delta t)^2 u''(t^n) + \dots + \frac{1}{p!}(\Delta t)^p u^{(p)}(t^n)$$

we know: $u' = f(u) \Rightarrow u'' = \frac{df}{du}\cdot u' = \frac{df}{du}\cdot f(u)$ etcetera for u''', ...

Time-integration methods [3]

Runge-Kutta methods

two-stage (explicit)

$$\begin{cases} k_1 = u^n + \frac{1}{2}\Delta t\, f(u^n) \\ u^{n+1} = u^n + \Delta t\, f(k_1) \end{cases}$$

← intermediate value to approximate $u(t^{n+\frac{1}{2}})$ using EF

$\Longrightarrow$ local error $\tau^n = O((\Delta t)^3)$ ("second order")

global error: $O((\Delta t)^2)$

four-stage (explicit)

$$\begin{cases} k_1 = u^n \\ k_2 = u^n + \frac{1}{2}\Delta t\, f(k_1) \\ k_3 = u^n + \frac{1}{2}\Delta t\, f(k_2) \\ k_4 = u^n + \Delta t\, f(k_3) \\ u^{n+1} = u^n + \frac{\Delta t}{6}\left[f(k_1) + 2f(k_2) + 2f(k_3) + f(k_4)\right] \end{cases}$$

("fourth-order")

global error: $O((\Delta t)^4)$

Can be generalized
- → r-stage
- → implicit
- → many variants

Time-integration methods [4]

Linear multistep methods (LMM)

k-step LMM: $$\sum_{j=0}^{k} \alpha_j u^{n+j} = \Delta t \sum_{j=0}^{k} \beta_j f(u^{n+j})$$

if $\beta_k = 0$, then explicit (otherwise: implicit)

Example: Adams methods: $$u^{n+k} = u^{n+k-1} + \Delta t \sum_{j=0}^{k} \beta_j f(u^{n+j})$$

$$(\alpha_k = 1,\ \alpha_{k-1} = 1,\ \alpha_j = 0 \quad j < k-1)$$

3-step explicit: $$u^{n+3} = u^{n+2} + \frac{\Delta t}{12}\left[5 f(u^n) - 16 f(u^{n+1}) + 23 f(u^{n+2})\right]$$

2-step implicit: $$u^{n+2} = u^{n+1} + \frac{\Delta t}{2}\left[-f(u^n) + 8 f(u^{n+1}) + 5 f(u^{n+2})\right]$$

Time-integration methods [5]

LTE $\tau^{n+r} = \frac{1}{\Delta t}\left(\sum_{j=0}^{r} \alpha_j u(t^{n+j}) - \Delta t \sum_{j=0}^{r} \beta_j \underbrace{u'(t^{n+j})}_{= f(u^{n+j})} \right)$

consistency: $\tau \to 0$ as $\Delta t \to 0$

$\iff \sum_{j=0}^{r} \alpha_j = 0$ & $\sum_{j=0}^{r} j \alpha_j = \sum_{j=0}^{r} \beta_j$

Characteristic polynomials: $\rho(\zeta) = \underbrace{\sum_{j=0}^{r} \alpha_j \zeta^j}_{\text{degree} = r}$ & $\sigma(\zeta) = \underbrace{\sum_{j=0}^{r} \beta_j \zeta^j}_{\text{degree} = r \text{ (if implicit), otherwise degree} < r}$

note: $\rho(1) = \sum_{j=0}^{r} \alpha_j$ & $\rho'(\zeta) = \sum_{j=1}^{r} j \alpha_j \zeta^{r-1}$

consistency $\iff$ $\rho(1) = 0$ AND $\rho'(1) = \sigma(1)$

Zero stability [1]

Example of a consistent LMM that does not converge

$$u^{n+2} - 3u^{n+1} + 2u^n = -\Delta t\, f(u^n) \quad \boxed{*}$$

LTE $\tau^n = \frac{1}{\Delta t}\left[u(t^{n+2}) - 3u(t^{n+1}) + 2u(t^n)\right] + u'(t^n)$

$---= \frac{5}{2}\Delta t\, u''(t^n) + O((\Delta t)^2) \quad \to 0$ for $\Delta t \to 0$

$\Rightarrow$ method is consistent and first order accurate

What happens with the global error?

Check with the "trivial" ODE $\begin{cases} u'(t) = 0 \\ u(0) = 0 \end{cases}$ $(\Rightarrow u(t) = 0 \ \forall t \geq 0 !)$

Apply LMM $\boxed{*}$: $u^{n+2} - 3u^{n+1} + 2u^n = 0 \quad \boxed{**}$

we need two starting values, say $u^0 = u^1 = 0 \Longrightarrow u^n = 0 \ \forall n \geq 0$ (solves the "ODE" exactly!)

However, in general, some perturbation must be added,

say $u^0 = 0$, $u^1 = \Delta t$ (small!!) $\overset{----}{\Longrightarrow} u^{20} = O(10^4)$ blows-up

Explanation: solve $\boxed{**}$ explicitly $\Rightarrow u^n = 2u^0 - u^1 + 2^n(u^1 - u^0)$ (check!!)

We know that $u(t) = 0 \ \forall t \geq 0 \Rightarrow$ global error $= u^n - \underbrace{u(t^n)}_{=0} = u^n = ?$

Zero stability [2]

factor 2^n magnifies the global error $\Rightarrow$ no convergence for $n \to \infty$!

"Root condition": the roots of $\rho(\zeta)$ are all inside the unit circle in $\mathbb{C}$ (those on the circle : simple roots)

A method is zero stable $\Longleftrightarrow$ it satisfies the root condition

---

Theorem: (without proof) method is convergent $\Longleftrightarrow$ it is consistent AND zerostable

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Note: zero-stability $\Longleftrightarrow$ the origin $z=0 \in \mathbb{C}$ lies in the (absolute) stability region

follows

Stability regions [1]

Define the stability polynomial $\pi(\zeta;z)=\rho(\zeta)-z\cdot\sigma(\zeta)$

The region of (absolute) stability ("stability region") $\Leftrightarrow$ "A-stability" of a method

$$= \{ z\in\mathbb{C} \mid \pi(\zeta;z) \text{ satisfies the "root condition"} \}$$

EF: $\pi=\zeta-(1+z)$, a single root: $\zeta_1 = 1+z$

$|\zeta_1| = |1+z| < 1$ inside a circle

EB: $\pi=(1-z)\zeta-1$, a single root: $\zeta_1=(1-z)^{-1}$

$|\zeta_1| = |(1-z)^{-1}| < 1$ outside another circle

Stability regions [2]

Absolute stability in the MoL ~ stability properties of the ODE methods in step 2 of MoL and the properties of the semi-discrete matrices M

A method is (absolutely) stable, or A-stable, if $\lambda \Delta t \overset{\text{def}}{=} z \in \mathbb{C}$, $\in S$ ← stability region of the ODE method

where λ (an eigenvalue) $\in$ spectrum of the matrix M

Consider the (scalar) "test" ODE: $\begin{cases} u' = \lambda u \\ u(0) = u_0 \end{cases}$ and $\lambda \in \mathbb{C}$

and the "perturbed" ODE: $\begin{cases} v' = \lambda v \\ v(0) = u_0 + \delta \end{cases}$ ← small perturbation

As an example, apply EF:

$$\begin{cases} u^{n+1} = (1+\lambda\Delta t)u^n \\ \quad = \cdots = (1+\lambda\Delta t)^{n+1} u^0 \\ v^{n+1} = (1+\lambda\Delta t)v^n \\ \quad = \cdots = (1+\lambda\Delta t)^{n+1}(u^0+\delta) \end{cases}$$

Stability regions [3]

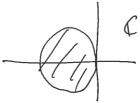
$$\Rightarrow \underbrace{v^{n+1} - u^{n+1}}_{?\ \text{small}\ ??} = \underbrace{(1+\lambda\Delta t)^{n+1}}_{\text{amplification factor}} \cdot \underbrace{\delta}_{\text{small}}$$

amplification factor: $|\cdot| > 1$ or $|\cdot| < 1$?

If $|1+\lambda\Delta t| = |1+z| < 1$, the $|v^{n+1} - u^{n+1}| < 1$ and the initial small perturbation won't affect the numerical solution.

EF is stable, if $|1+z| < 1$ with $z = \lambda \Delta t$ (λ from ODE, Δt from numerical method)

$$S_{EF} = \{ z \in \mathbb{C} \mid |1+z| < 1 \}$$



$$R(z) = 1 + z \approx 1 + z + \tfrac{1}{2} z^2 + \dots = e^z$$

$R(z)$ is called the "stability function" of the method

Note: solutions of the ODE are "stable" for $\lambda \in \mathbb{C}^-$

$\Rightarrow$ EF is conditionally stable, accuracy $O(\Delta t)$

Stability regions [4]

For Euler-Backward (EB): $S_{EB} = \{ z \in \mathbb{C} \mid |1-z| > 1 \}$

$$R(z) = \frac{1}{1-z} = 1+z+z^2+z^3+\dots \approx 1+z+\frac{1}{2}z^2+\frac{1}{6}z^3+\dots = e^z$$

Since $S_{EB} \supset \mathbb{C}^-$, EB is unconditionally stable.

Accuracy: $O(\Delta t)$

Trapezoïdal method: $S_{TM} = \mathbb{C}^-$

unconditionally stable

accuracy: $O((\Delta t)^2)$

$$R(z) = \frac{1+\frac{1}{2}z}{1-\frac{1}{2}z} = (1+\tfrac{1}{2}z)(1+\tfrac{1}{2}z+\dots) = 1+z+\dots \approx e^z$$

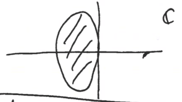
Stability regions [5]

p-th order Taylor method : $R(z) = 1 + z + \frac{1}{2!}z^2 + \dots + \frac{1}{p!}z^p \approx e^z$

conditionally stable
accuracy : $O((\Delta t)^p)$
explicit

Runge-Kutta 4 (RK4) : $R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 \approx e^z$

conditionally stable
accuracy : $O((\Delta t)^4)$
explicit



NOTE: $R(z)$ is a rational function or polynomial in z

Theorem : The boundary locus (= curve in ℂ defined by $|R(z)| = 1$) is symmetric around the real axis in the complex plane : $R(\bar{z}) = \overline{R(z)}$

AND

the angle at $z = 0 \in \mathbb{C}$ between the boundary locus and the real axis in the complex plane is $90°$: $\arg(R(0)) = \frac{\pi}{2}$

Boundary locus [1]

how to find the region of (absolute) stability?

$z \in$ stability region S, if the stability polynomial $\pi(\zeta; z)$ satisfies the "root condition" for this $z \in \mathbb{C}$.

If $z \in \partial S$, then $\pi(\zeta; z)$ must have at least one root ζ_j with $|\zeta_j| = 1$.

this ζ_j must have the form: $\zeta_j = e^{i\varphi}$ for some $\varphi \in [0, 2\pi]$.

$\Rightarrow \pi(e^{i\varphi}; z) = 0$ for this φ, z combination

$\Leftrightarrow \rho(e^{i\varphi}) - z\,\sigma(e^{i\varphi}) = 0$

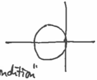
$$\Leftrightarrow \quad z = \frac{\rho(e^{i\varphi})}{\sigma(e^{i\varphi})} \qquad (\text{from } \varphi \text{ follows } z \in \partial S)$$

Each point on ∂S must be of this form! (for some value of $\varphi \in [0, 2\pi]$)

$\Rightarrow$ "simply" plot the parametrized curve $z = \dfrac{\rho(e^{i\varphi})}{\sigma(e^{i\varphi})}$, $\varphi \in [0, 2\pi]$

example 1: EF $\begin{cases} \rho(\zeta) = \zeta - 1 \\ \sigma(\zeta) = 1 \end{cases} \Rightarrow z(\varphi) = \dfrac{e^{i\varphi} - 1}{1} = e^{i\varphi} - 1$

this function maps $[0, 2\pi]$ to the unit circle centered at $z = -1$.



* Evaluate at some "random" point z on the inside or outside of the curve and see if the polynomial satisfies the "root condition"

Boundary locus [2]

example 2 BDF$_2$ method $u^{n+2} - \frac{4}{3}u^{n+1} + \frac{1}{3}u^n = \frac{2}{3}\Delta t\, f(u^{n+2})$

$$\begin{cases} \rho(\zeta) = \zeta^2 - \frac{4}{3}\zeta + \frac{1}{3} \\ \sigma(\zeta) = \frac{2}{3}\zeta^2 \end{cases} \Rightarrow \pi(\zeta; z) = \left(1 - \frac{2}{3}z\right)\zeta^2 - \frac{4}{3}\zeta + \frac{1}{3}$$

$$\Rightarrow z = \frac{e^{2i\varphi} - \frac{4}{3}e^{i\varphi} + \frac{1}{3}}{\frac{2}{3}e^{2i\varphi}} = \frac{3}{2} - 2e^{-i\varphi} + \frac{1}{2}e^{-2i\varphi}, \quad z \in \partial S$$

set $z = x + iy$, $\begin{cases} x = x(\varphi) \\ y = y(\varphi) \end{cases}$ $\Rightarrow x + iy = \frac{3}{2} - 2(\cos(-\varphi) + i\sin(-\varphi)) + \frac{1}{2}(\cos(-2\varphi) + i\sin(-2\varphi))$

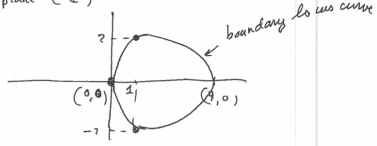
$$= \frac{3}{2} - 2\cos(\varphi) + \frac{1}{2}\cos(2\varphi) + i\left(2\sin(\varphi) - \frac{1}{2}\sin(2\varphi)\right)$$

$$\Rightarrow \begin{cases} x(\varphi) = \frac{3}{2} - 2\cos(\varphi) + \frac{1}{2}\cos(2\varphi) \\ y(\varphi) = 2\sin(\varphi) - \frac{1}{2}\sin(2\varphi) \end{cases}$$

this is a curve in the x-y-plane ("$\mathcal{C}$")

Table:

φ	x	y
0	0	0
$\pi/2$	1	2
π	4	0
$3\pi/2$	1	-2
2π	0	0



Boundary locus [3]

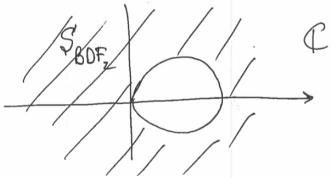
stability region $\mathcal{S}$: inside or outside closed curve ?
(need to check one point)

Recall $\pi(\zeta;z) = (1 - \frac{2}{3}z)\zeta^2 - \frac{4}{3}\zeta + \frac{1}{3} \Rightarrow \pi(\zeta; -\frac{3}{2}) = 2\zeta^2 - \frac{4}{3}\zeta + \frac{1}{3}$

has roots: $\zeta_{1,2} = \dfrac{\frac{4}{3} \pm \sqrt{(-\frac{4}{3})^2 - 4 \cdot 2 \cdot \frac{1}{3}}}{2 \cdot 2} = \frac{1}{3} \pm \frac{i}{4}\frac{\sqrt{8}}{3}$

and $|\zeta|^2 = \frac{1}{9} + \frac{8}{16 \cdot 9} = \frac{1}{9} + \frac{1}{18} = \frac{3}{18} \Rightarrow |\zeta| < 1$

$\Rightarrow \mathcal{S}$ outside $\partial\mathcal{S}$



Outlook to Lecture 4

- prepare exercises of Lecture 3 (see webpage!)
- the heat equation
- semi-discretization
- time-integration
- space-time discretizations
- higher dimensions