

Lecture 3

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Numerical Methods for Time-Dependent PDEs, Spring 2024

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

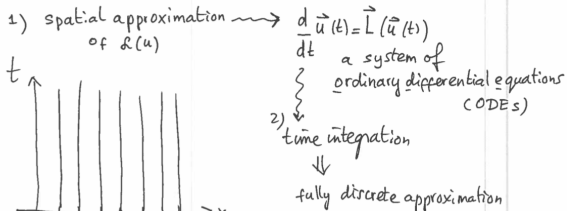
Method of Lines [1]

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

\swarrow
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)



Method of Lines [2]



- 1) time integration $\rightarrow \vec{F}(\vec{u}^n, \vec{u}^{n+1}) = \vec{0}$ a system of (non)linear "stationary" PDEs
- 2) numerical (non)linear algebra \rightarrow fully discrete approximation.

We will use option 1 "MOL"

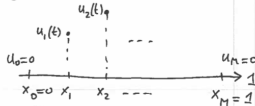
example 1 the heat equation $u_t = \underset{\substack{\text{or} \\ k > 0}}{k} \cdot u_{xx}, x \in (0,1), t > 0$

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

$u(x,t) = ?$

(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]

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

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

$$\text{BCs: } u_0 = 0 \quad \forall t \\ u_M = 0 \quad \forall t$$

$$\text{IC: } u_i(0) = \sin(\pi x_i) \quad i=1, \dots, M-1$$

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

\rightarrow 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: $\dot{\vec{u}}(t) = \kappa \mathcal{D}_{2c} \vec{u}(t)$

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

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

Method of lines [4]

step 2 in MoL: numerically integrate the ODE system

example: use Euler Forward (EF): $\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = \kappa \cdot \mathcal{D}_{2c} \vec{u}^n$
 $n=0, 1, \dots, N-1$

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

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

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

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

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

⊙ Euler Backward (EB): $\frac{\vec{u}^{n+1} - \vec{u}^n}{\Delta t} = \kappa \cdot \mathcal{D}_{2c} \vec{u}^{n+1}$

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

⊙ ----- many options -----

Method of lines [5]

In general: suppose \mathcal{L} is a linear spatial operator

$$u_t = \mathcal{L}(u)$$

semi-discretized
in space $\Rightarrow \vec{u}(t) = L_{\Delta x} \vec{u}(t)$

approximate in time
EF, EB, ...

finite-difference matrix
"exact" semi-discrete solution

$$\vec{u}(t) = e^{t \cdot L_{\Delta x}} \vec{u}_0$$

matrix exponential

"exponential integrators" ... ?

Method of lines [6]

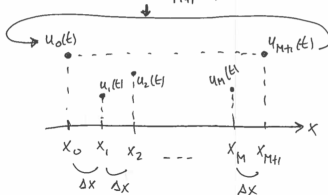
example 2 the advection equation
$$\begin{cases} u_t + au_x = 0, & x \in [0, 1], t > 0 \\ u(x, 0) = u_0(x), & x \in [0, 1], t > 0 \end{cases}$$

(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)

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

with $\dot{u}_1(t) = -\frac{a}{2\Delta x} (u_2(t) - u_0(t))$
 $(u_0 = u_{M+1}) \Rightarrow = -\frac{a}{2\Delta x} (u_2(t) - u_{M+1}(t))$

and $\dot{u}_{M+1}(t) = -\frac{a}{2\Delta x} (u_{M+2}(t) - u_M(t))$
 $(u_1 = u_{M+2}) \Rightarrow = -\frac{a}{2\Delta x} (u_1(t) - u_M(t))$

$$\Rightarrow \dot{\vec{u}}(t) = \mathcal{D}_{1c} \vec{u}(t) \quad \text{with} \quad \mathcal{D}_{1c} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & -1 & & & \\ & 0 & 1 & & \\ & & & \ddots & \\ & & & & -1 \\ & & & & & 0 \end{pmatrix}$$

a circulant skew-symmetric matrix
 $(\mathcal{D}_{1c}^T = -\mathcal{D}_{1c})$

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

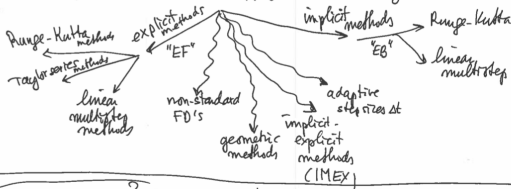
Method of lines [8]

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

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

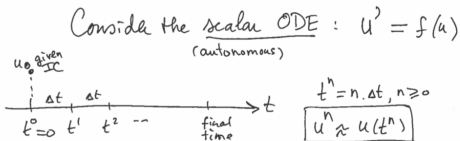
the eigenvalues of the matrix M are going to play an important role in step 2 of MOL.

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



- accuracy ?
- stability ?
- efficiency ?

Time-integration methods [1]



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

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

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

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

explicit

BSDF₂ : $\frac{3u^{n+1} - 4u^n + u^{n-1}}{2 \Delta t} = f(u^{n+1})$
(implicit)

et cetera ...

Time-integration methods [2]

(local) truncation error: (example: midpoint)

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

Taylor expansion \Rightarrow

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

(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

\Rightarrow LTE $\tau^n = O((\Delta t)^2)$ ("second order")

four-stage (explicit) $\begin{cases} k_1 = u^n \\ k_2 = u^n + \frac{1}{2} \Delta t f(k_1) \\ k_3 = u^n + \frac{1}{2} \Delta t f(k_2) \\ k_4 = u^n + \Delta t f(k_3) \\ u^{n+1} = u^n + \frac{\Delta t}{6} [f(k_1) + 2f(k_2) + 2f(k_3) + f(k_4)] \end{cases}$ ("fourth-order")

can be generalized $\begin{cases} \rightarrow r\text{-stage} \\ \rightarrow \text{implicit} \\ \rightarrow \text{many variants} \end{cases}$

Time-integration methods [4]

Linear multistep methods (LMM)

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

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

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

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

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

Time-integration methods [5]

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

consistency $\Rightarrow \tau \rightarrow 0 \text{ as } \Delta t \rightarrow 0$

$$\Leftrightarrow \sum_{j=0}^n \alpha_j = 0 \quad \& \quad \sum_{j=0}^n j \alpha_j = \sum_{j=0}^n \beta_j$$

Characteristic polynomials

$$\rho(\zeta) = \sum_{j=0}^n \alpha_j \zeta^j$$

degree = n

$$\sigma(\zeta) = \sum_{j=0}^n \beta_j \zeta^j$$

degree = n (if implicit)
otherwise degree < n

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

consistency $\Leftrightarrow \rho(1) = 0 \text{ AND } \rho'(1) = \sigma(1)$

Zero stability [1]

Example of a consistent LMM that does not converge

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

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

$$\approx \frac{5}{2} \Delta t u''(t^n) + O(\Delta t^2) \quad \rightarrow 0 \text{ for } \Delta t \rightarrow 0$$

\Rightarrow method is consistent and first order accurate

What happens with the global error?

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

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

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

However, in general, some perturbation must be added,

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

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

We know that $u(t) = 0 \quad \forall t \geq 0 \Rightarrow \text{global error} = u^n - \underbrace{u(t^n)}_0 = u^n = \tau^n$

Zero stability [2]

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

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

A method is zero stable \Leftrightarrow it satisfies the root condition

Theorem: method is convergent \Leftrightarrow it is consistent
(without proof) AND zero stable

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

follows \rightarrow

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 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 \sim 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 $\lambda \Delta t \stackrel{\text{def}}{=} z \in \mathcal{S}$
where λ is an eigenvalue \in spectrum of the matrix M \mathcal{S} = stability region of the ODE method

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

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

As an example, apply EF: $\begin{cases} u^{n+1} = (1 + \lambda \Delta t) u^n \\ \quad \quad \quad = \dots = (1 + \lambda \Delta t)^{n+1} u^0 \\ v^{n+1} = (1 + \lambda \Delta t) v^n \\ \quad \quad \quad = \dots = (1 + \lambda \Delta t)^{n+1} (u^0 + \delta) \end{cases}$

Stability regions [3]

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

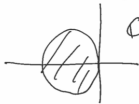
? small?? small

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 $z = \lambda \Delta t$

from ODE from numerical method

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



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

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: $\mathcal{O}(\Delta t)$



Trapezoidal method: $S'_{TM} = \mathbb{C}^-$

unconditionally stable
accuracy: $\mathcal{O}(\Delta t^2)$

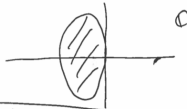
$$R(z) = \frac{1+\frac{1}{2}z}{1-\frac{1}{2}z} = (1+\frac{1}{2}z)(1+\frac{1}{2}z+\dots) = 1+z+\dots \approx e^z$$



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 (= curve in \mathbb{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 curve 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 $\varphi \in [0, 2\pi]$.

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

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

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

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

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

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

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 BDF₂ method $u^{n+2} - \frac{4}{3}u^{n+1} + \frac{1}{3}u^n = \frac{2}{3} \Delta t f(u^{n+2})$

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

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

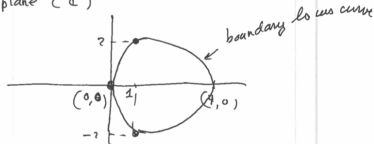
let $z = x + iy$, $\begin{cases} x = x(\varphi) \\ y = y(\varphi) \end{cases} \Rightarrow x + iy = \frac{3}{2} - 2(\cos(-\varphi) + i\sin(-\varphi)) + \frac{1}{2}(\cos(-2\varphi) + i\sin(-2\varphi))$

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

this is a curve in the x-y-plane ("a")

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]

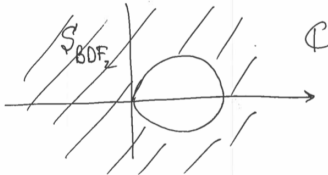
stability region S : inside or outside closed curve?
(need to check one point)

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

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

$$\text{and } |z|^2 = \frac{1}{9} + \frac{8}{169} = \frac{1}{9} + \frac{1}{18} = \frac{3}{18} \Rightarrow |z| < 1$$

$\Rightarrow S$ outside ∂S



Outlook to Lecture 4

⌋ prepare exercises of Lecture 3 (see webpage!)

⌋ the heat equation

⌋ semi-discretization

⊖ time-integration

≠ space-time discretizations

⌋ higher dimensions