Ch. 4 Stiff Equations

Key Points:

- Examples of stiff ODEs
- A central problem $y' = \lambda y$ for understanding numerical stability
  - Euler, Backward Euler, Trapezoid, ...
  - Runge-Kutta Methods
  - Multi-step Methods

... see also Heath, p. 401-404

K.E. Atkinson "An Introduction to Numerical Analysis" (2nd Edition) ch. 6

EXAMPLE (aka Competitive Lotka Volterra Equations)

Consider the 3-species Lotka-Volterra system

$$\begin{cases} \dfrac{dx}{dt} = ax - bxy \\[2ex] \dfrac{dy}{dt} = -cy + dxy - eyz \\[2ex] \dfrac{dz}{dt} = -fz + gyz \end{cases}$$

$a, b, c, d, e, f, g > 0$

Ref: "A Lotka-Volterra Three-Species food chain"
E. Chauvet
J. E. Paullet
J. Walls
Math Mag. 75 (4) Oct. 2002
243-255

(x, y, z) : (mouse, snake, owl)
(vegetation, hare, lynx)
(worm, robin, falcon)

I.C. $x(0) = x_0$, $y(0) = y_0$, $z(0) = z_0$

2 equilibrium solutions $\frac{dx}{dt} = \frac{dy}{dt} = \frac{dz}{dt} = 0$. (assume $\frac{a}{b} \neq \frac{f}{g}$)

$\underline{x=0}$ $\qquad$ $\underline{y = a/b}$

$(x, y, z) = (0, 0, 0)$

$\underline{y=0}$ $\quad$ $z = \cancel{\frac{c}{e}}$ $\qquad$ $c = dx + ez$

$\left(\frac{c}{d}, \frac{a}{b}, 0\right)$

$\underline{z=0}$ $\qquad$ $z=0$ $\quad$ $\underline{x = \frac{c}{d}}$

Jacobian:

$$J = \begin{bmatrix} a & -bx & 0 \\ dy & -c + dx - ez & -ey \\ 0 & gz & -f + gy \end{bmatrix}$$

Before trying to analyze this system let's just try to solve it numerically using Euler's Method...

see
euler_system.m + feuler_system.m

Here I've set

$a = b = d = e = 1$

$c = 2 \quad f = 100 \quad g = 0.1$

$\boxed{\begin{array}{l} x_0 = 0.5 \\ y_0 = 1 \\ z_0 = 2 \end{array}}$

c: fast decay of y (snakes)

f: very fast decay of z (owls)

mice grow slowly if left alone but... then the nonlinear terms start to matter...

Numerical Experiment #1

- set $t_F = 5$ ... increase nk for 'sufficient resolution'

nk = 1000 seems quite good $\quad h = \frac{5}{1000} = 0.005$

observe: $z \to 0$ quickly
x, y : some dynamics

- lets run things longer to observe the x, y dynamics by increasing t_F but keeping nk fixed (– not necessarily a good idea since this causes $h = \frac{t_F}{nk}$ to increase)

- set $t_f = 10$ ... seems OK ... observe
  repeating motion in xy ... $z \sim 0$ (no owls)

- set $t_f = 20$ ... z behaving strangely...
  (large +/- oscillations)

Note: $\frac{dz}{dt} = -fz + gyz = -\boxed{(f-gy)}\,z$

$f = 100$ $\quad y \in [0,5]$
$g = 0.1$

so $f - gy > 0$
why isn't z decaying
rapidly to zero?

- set $t_f = 40$ ... code crashes...

⋮

more reasonable-looking results restored by increasing nk
(nk = 4000, ...)

even here you should be asking if we
are ...
correctly solving this problem.

Numerical Experiment #2

same a, b, c, d, e, f, g as in N.E. #1
x_0, y_0, z_0

- set $\begin{cases} t_F = 0.5 \\ \cancel{nk = 100} \end{cases}$ ... ~~looks ok relative to~~ $\begin{cases} \cancel{t_F = 0.5} \\ \cancel{nk = 100} \end{cases}$

these look OK...

$\boxed{\cancel{h = 0.005}}$ x grows, y decays, z decays fast

- set $\begin{cases} t_F = 1.0 \\ \cancel{nk = 100} \end{cases}$ $\boxed{h = 0.01}$ - seems OK ~~more of the same~~ x, y, z trends

- set $\begin{cases} \cancel{t_F = 1.5} \\ \cancel{nk = 100} \end{cases}$ ← $\boxed{h = 0.015}$ some initial oscillations in z but they die out. x, y ~~behave as before.~~

- set $\begin{cases} \cancel{t_F = 2.0} \\ nk = 100 \end{cases}$ ← $\boxed{h = 0.02}$ z has major oscillations between −2 and 2 ~~... not good~~

- set $\begin{cases} t_F = 2.01 \\ nk = 100 \end{cases}$ ← $\boxed{h > 0.02}$ - z has growing oscillations

Again observe $\frac{dz}{dt} = -\underbrace{(f - gy)}_{\approx 100}\, z$

≈ 100 since $f = 100$, $g = 0.1$ and $0 < y < 1$

Why is z not ~~decaying~~?

- set $\begin{cases} \cancel{t_F = 2.05} \\ nk = 100 \end{cases}$ ← $\boxed{h > 0.02}$ - now x, y 'blow up'
z - oscillates badly...

This is a fairly 'rich' mathematical system that ~~we can easily have trouble with if we are not careful.~~

What's going on?

The presence of multiple "timescales" such as the widely different decay rates a, c and f ~~makes the~~ not to mention the other oscillatory dynamics makes this a 'stiff' system (see also Iserles, p.56)

Consider the system of linear differential equations

$$\begin{cases} \vec{y}\,' = A\vec{y} & A = \text{constant } m\times m \text{ matrix} \\ \vec{y}(0) = y_0 \end{cases}$$

Assume A is diagonalizable (has a full set of linearly-independent eigenvectors) so $A = VDV^{-1}$ is its spectral factorization (D = diagonal matrix with eigenvalues λ_j $j=1,2,\ldots,m$ of A along the diagonal and V = matrix whose columns are the linearly-independent eigenvectors).

This problem has exact solution

$$\vec{y}_{ex} = V e^{Dt} V^{-1} \vec{y}_0 \quad \text{where}$$

$\vec{x}_j$ are multipliers related to V, $\vec{y}_0$.

$$e^{Dt} = \begin{bmatrix} e^{\lambda_1 t} & & 0 \\ & e^{\lambda_2 t} & \\ 0 & & \ddots \; e^{\lambda_m t} \end{bmatrix} \quad \text{or} \quad \vec{y}_{ex} = e^{\lambda_1 t}\vec{x}_1 + \ldots + e^{\lambda_m t}\vec{x}_m$$

What happens if we apply Euler's method to this problem?

$$\vec{y}_{n+1} = \vec{y}_n + hA\vec{y}_n = (I + hA)\vec{y}_n$$

so

$$\vec{y}_1 = (I + hA)\vec{y}_0$$

$$\vec{y}_2 = (I + hA)\vec{y}_1 = (I + hA)^2\vec{y}_0$$

$$\boxed{\vec{y}_n = (I + hA)^n \vec{y}_0} \quad n = 0,1,2,\ldots$$

Note: $A = VDV^{-1}$

$$(I + hA)(I + hA)$$
$$= I + 2hA + h^2 A^2$$
$$= I + 2hVDV^{-1} + h^2(VDV^{-1})(VDV^{-1})$$
$$= I + 2hVDV^{-1} + h^2(VD^2V^{-1})$$
$$= VIV^{-1} + 2hVDV^{-1} + h^2(VD^2V^{-1})$$
$$= V\left(I + 2hD + h^2D^2\right)V^{-1}$$
$$= V(I + hD)^2 V^{-1}$$

etc. so

$$(I + hA)^n = V(I + hD)^n V^{-1}$$

and then

$$\boxed{\vec{y}_n = V(I + hD)^n V^{-1} \vec{y}_0}$$

but also note

$$I + hD = \begin{bmatrix} 1+h\lambda_1 & & & \\ & 1+h\lambda_2 & & \\ & & 1+h\lambda_3 & \\ & & & \ddots \end{bmatrix}$$

so

$$(I + hD)^n = \begin{bmatrix} (1+h\lambda_1)^n & & & 0 \\ & (1+h\lambda_2)^n & & \\ & & \ddots & \\ 0 & & & (1+h\lambda_m)^n \end{bmatrix}$$

so $$\vec{y}_n = V \begin{bmatrix} (1+h\lambda_1)^n & & \\ & \ddots & \\ & & (1+h\lambda_m)^n \end{bmatrix} V^{-1} \vec{y}_0$$

$$\boxed{\vec{y}_n = (1+h\lambda_1)^n \vec{x}_1 + (1+h\lambda_2)^n \vec{x}_2 + \dots + (1+h\lambda_m)^n \vec{x}_m}$$

again, ~~[illegible]~~ recall exact solution...

$$\boxed{\vec{y}_{ex} = e^{\lambda_1 t}\vec{x}_1 + e^{\lambda_2 t}\vec{x}_2 + \dots + e^{\lambda_m t}\vec{x}_m}$$

<u>EXAMPLE</u> (Iserles, p. 53-54)

$$A = \begin{bmatrix} -100 & 0 \\ 0 & -\frac{1}{10} \end{bmatrix} \quad \text{so} \quad A = D : \quad \begin{array}{l} \lambda_1 = -100 \\ \lambda_2 = -\frac{1}{10} \end{array}$$

$$\vec{y}_n = (1-100h)^n \vec{x}_1 + (1-\tfrac{1}{10}h)^n \vec{x}_2$$

$$\vec{y}_{ex} = e^{-100t}\vec{x}_1 + e^{-\frac{1}{10}t}\vec{x}_2$$

<u>Comments</u>

- the exact solution has $\vec{y}_{ex} \to 0$ as $t \to \infty$ for any initial conditions.
- Does Euler's solution have this property? (i.e. $\vec{y}_n \to 0$ as $n \to \infty$ for fixed h?)

  ↳ Not necessarily...

- $(1-100h)^n \to 0$ as $n \to \infty$ for fixed h if

$$|1-100h| < 1$$

$$-1 < 1-100h < 1$$

$$\underbrace{-2 < \underbrace{-100h < 0}_{\substack{\text{always true} \\ \text{for } h>0}}}$$

here we need $\boxed{h < \frac{2}{100}}$ ← step size restriction!

- we also need $(1-\frac{1}{10}h)^n \to 0$ so

$$|1-\tfrac{1}{10}h| < 1$$

$$-1 < 1-\tfrac{1}{10}h < 1$$

$$\underbrace{-2 < -\tfrac{1}{10}h} < 0$$

↳ here we need $\boxed{h < \frac{2}{(1/10)} = 20}$ ← step size restriction (but probably not a very restrictive one).

Iserles (Fig. 4.1) shows what happens if you violate the first one of these (i.e. they use $h = \frac{1}{10}$ and

$$\frac{2}{100} < \frac{1}{10} < 20).$$

Everything looks ok for a while in this example until the $(1-100h)^n$ terms start getting large!

The above examples and discussion highlight the idea of a 'stiff' differential equation: $\boxed{\vec{y}\,' = \vec{f}(t,\vec{y})}$ $\boxed{\vec{y}(t_0) = \vec{y}_0}$

Some characteristics of stiff differential equations

- some numerical methods for solving these equations require a significant reduction in step size — maybe far beyond that expected necessary for accuracy — to avoid instability.

- the equations contain modes or describe physical phenomena that are associated with a broad range of time scales (e.g. we saw exponential decay rates of 100 and $\frac{1}{10}$ in the Iserles example). Fast dynamics and slow dynamics both present.
- the equations have associated with them a large 'stiffness ratio' = ratio of largest to smallest eigenvalue (in modulus) of the Jacobian $\frac{\partial f_i}{\partial y_j}$ matrix.

* stiffness is in general a relative concept

- depends on method used (Euler, Backward Euler, ...)
- " " accuracy required
- length of interval (i.e. t_{Final})

i.e. the consequences of stiffness are not always apparent

(see discussion in Heath, p. 401)

* stiff systems of ODEs often arise from a semidiscretization of a PDE (e.g. using the method of lines ...)

Many of the key concepts associated with stiff equations and the stability of numerical methods can be understood by examining a very simple linear, scalar ODE

$$
* \quad \begin{cases} y' = \lambda y & \lambda \in \mathbb{C} \quad (\text{complex } \lambda) \\ y(0) = y_0 \end{cases}
$$

where we are focused here on the case with $Re(\lambda) < 0$ so that $y \to 0$ as $t \to \infty$ in the <u>exact</u> solution.

Note:

- we saw the $\lambda_1, \lambda_2, \ldots, \lambda_m$ come out of the analysis in our linear system $\vec{y}' = A\vec{y}$ (so think in terms of the worst case scenario... largest $|\lambda_i|$).
- In a nonlinear system we still have interest in the eigenvalues of the Jacobian $\frac{\partial \vec{f}}{\partial \vec{y}}$ where again an understanding of equation * is central.

Linear Stability Domain + A-stability

Consider
$$\begin{cases} y' = \lambda y & \lambda \in \mathbb{C} \\ y(0) = 1 & (y_0 = 1 \text{ for simplicity}) \end{cases}$$

$Re(\lambda) < 0$, so $y \to 0$ as $t \to \infty$ is a feature of the exact sol.

Euler

$$Y_{n+1} = Y_n + h\lambda y_n = (1+h\lambda) y_n$$

$$\Rightarrow \quad Y_n = (1+h\lambda)^n \qquad n = 0, 1, 2, \ldots$$

so for $Y_n \to 0$ as $n \to \infty$ require

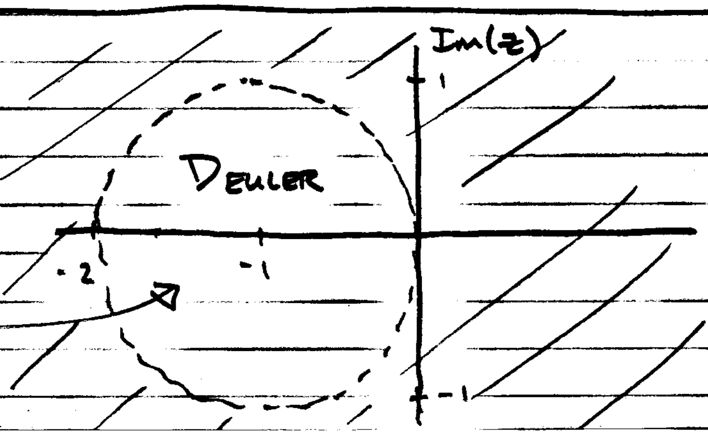
$$|1 + h\lambda| < 1 \qquad \longleftarrow \text{time step restriction}$$

Let $z \equiv h\lambda \in \mathbb{C}$.

Define the <u>linear stability domain</u> D to be the set of all $h\lambda$ $(=z)$ such that $Y_n \to 0$ as $n \to \infty$. So

$$\boxed{D_{EULER} = \{ z \in \mathbb{C} \mid |1+z| < 1 \}}$$

linear stability domain for Euler



λh must stay in here

.. so if $|\lambda|$ is big then h may need to be quite small...

Backward Euler

$$y_{n+1} = y_n + h\lambda y_{n+1}$$

$$(1-h\lambda)y_{n+1} = y_n$$

assume $1-h\lambda \neq 0$

$$y_{n+1} = \frac{1}{(1-h\lambda)} y_n$$

$$y_n = \frac{1}{(1-h\lambda)^n} \quad \text{for } n=0,1,2,\ldots$$

So for $y_n \to 0$ as $n \to \infty$ for fixed h require

$$\frac{1}{|1-h\lambda|} < 1$$

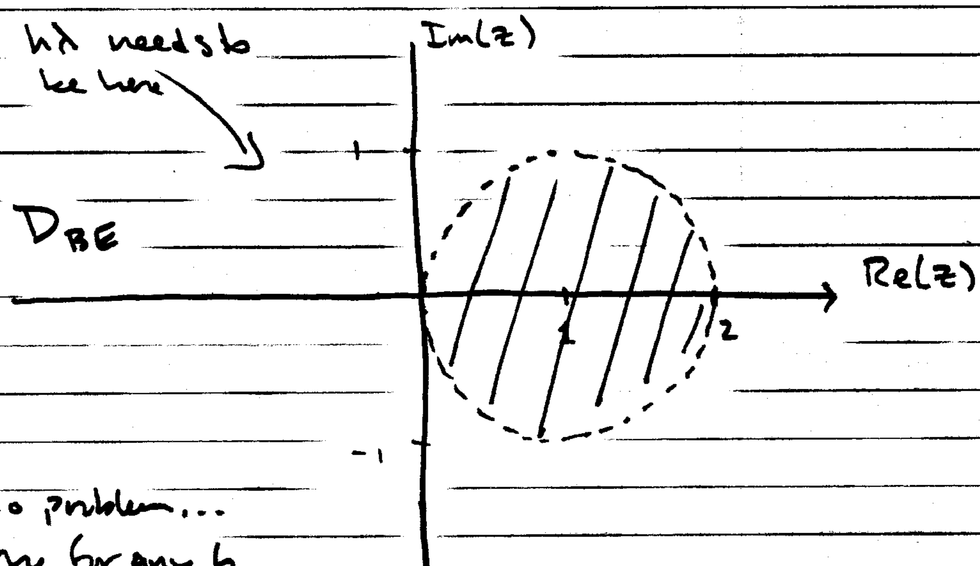
no time step restriction for $Re(\lambda) < 0$.

~~Recall that Real~~

So, assuming $1-h\lambda \neq 0$ require

$$|1-h\lambda| > 1$$

Let $z = h\lambda \implies |1-z| > 1$



(no problem... true for any h with $Re(\lambda)<0$)

Trapezoid Method

$$y_{n+1} = y_n + \tfrac{1}{2}h(\lambda y_n + \lambda y_{n+1})$$

$$(1-\tfrac{1}{2}h\lambda)\,y_{n+1} = (1+\tfrac{1}{2}h\lambda)\,y_n$$

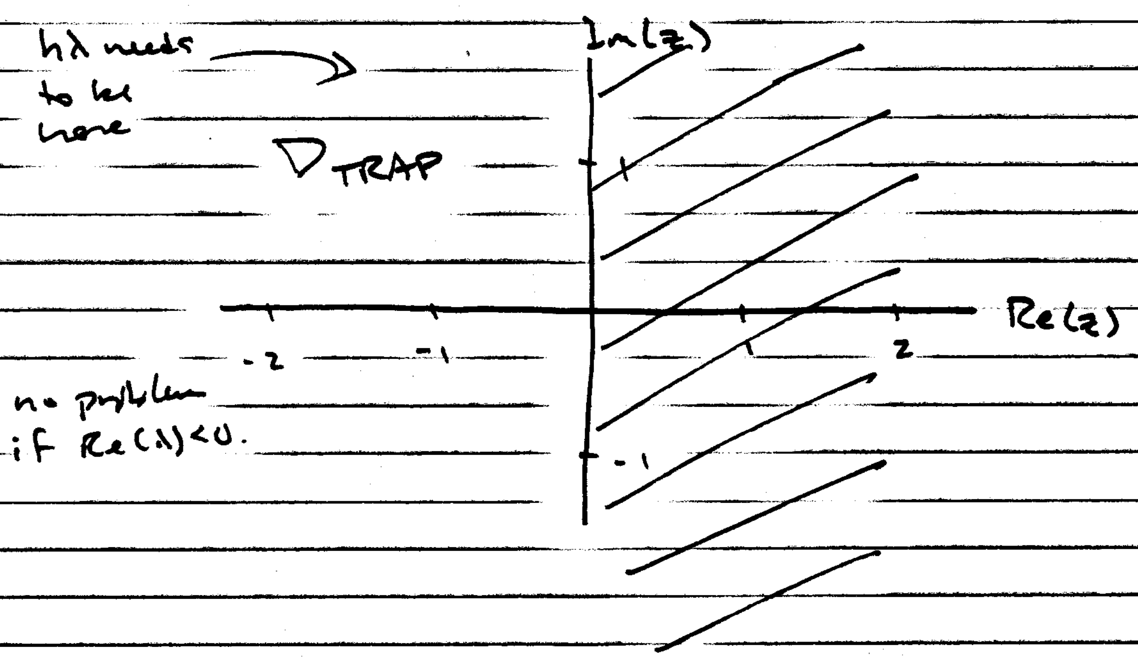
$1-\frac{1}{2}h\lambda \neq 0.$

$$y_{n+1} = \frac{(1+\frac{1}{2}h\lambda)}{(1-\frac{1}{2}h\lambda)}\,y_n$$

$$y_n = \left[\frac{1+\frac{1}{2}h\lambda}{1-\frac{1}{2}h\lambda}\right]^n$$

Here we require $\left|\dfrac{1+\frac{1}{2}h\lambda}{1-\frac{1}{2}h\lambda}\right| < 1$ ← no restriction on ~~h~~ h if $Re(\lambda) < 0$.

i.e. $\left|\dfrac{1+\frac{1}{2}z}{1-\frac{1}{2}z}\right| < 1$ ← always ~~true~~ true if $Re(z) < 0$
always false if $Re(z) > 0$



For Heun's Method see Homework...

Midpoint Rule (Implicit)

$$y_{n+1} = y_n + h\vec{f}\left(t_n + \tfrac{1}{2}h,\ \tfrac{1}{2}(y_n + y_{n+1})\right)$$

see Iserles p. 12

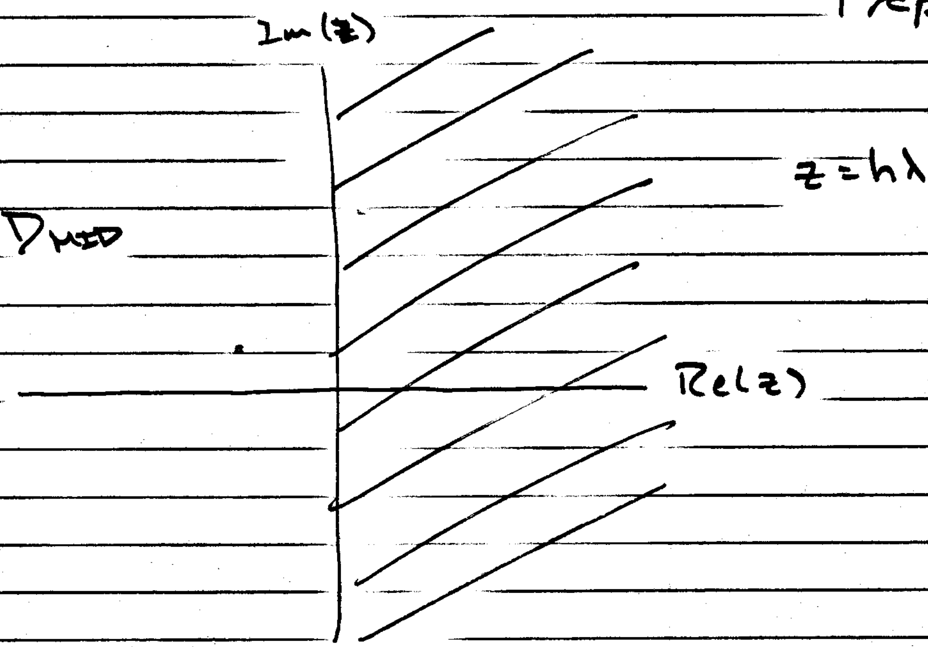
for $y' = \lambda y$ this reduces to

$$y_{n+1} = y_n + h\left(\lambda \cdot \tfrac{1}{2}(y_n + y_{n+1})\right)$$

$$\left(1 - \tfrac{1}{2}h\lambda\right) y_{n+1} = \left(1 + \tfrac{1}{2}h\lambda\right) y_n$$

← same result for this problem as we saw for Trapezoid

So



The ideas we've been using in these examples are captured in the following Lemma

<u>Lemma 4.2</u> (Iserles, p. 60)

Suppose the application of a numerical method to the problem

$$\begin{cases} y' = \lambda y \\ y(0) = 1 \end{cases}$$

leads to the geometric solution sequence

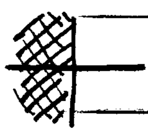
$$Y_n = \left[r(h\lambda) \right]^n \qquad n = 0, 1, 2, \dots$$

Then, the linear stability domain D is

$$D = \left\{ z \in \mathbb{C} \mid |r(z)| < 1 \right\}$$

Def: A-stable (i.e. a numerical method is A-stable when...)

We say that a numerical method if

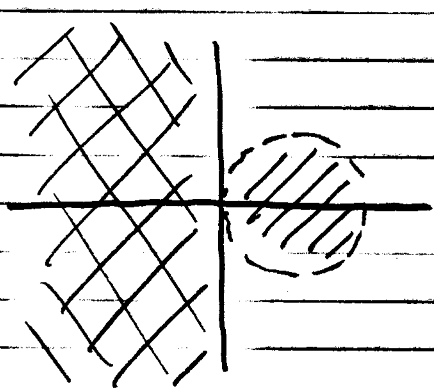
 $= \mathbb{C}^- \equiv \{ z \in \mathbb{C} \mid \mathrm{Re}(z) < 0 \} \subseteq D$

where D is the linear stability domain in terms of $z \equiv h\lambda$, where $y' = \lambda y$

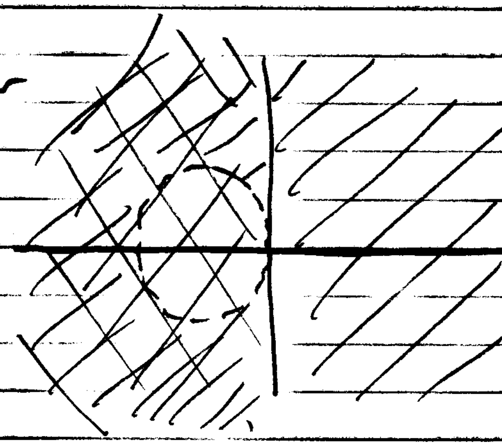
So for the previously discussed methods, we have

<u>A-stable</u>	<u>not A-stable</u>
Backward Euler	Euler
Trapezoid	Heun (see HW)
Implicit Midpoint	

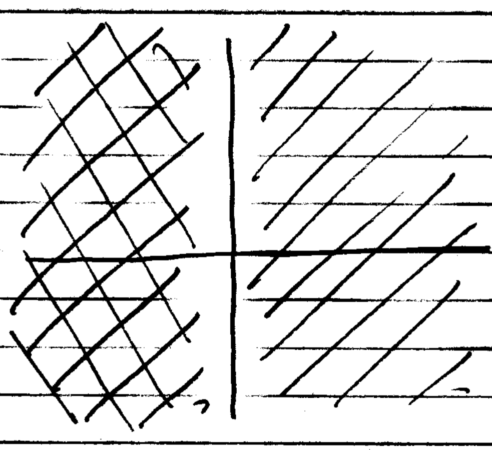
B.E.



Euler



TRAP + IMP. MID



Heun