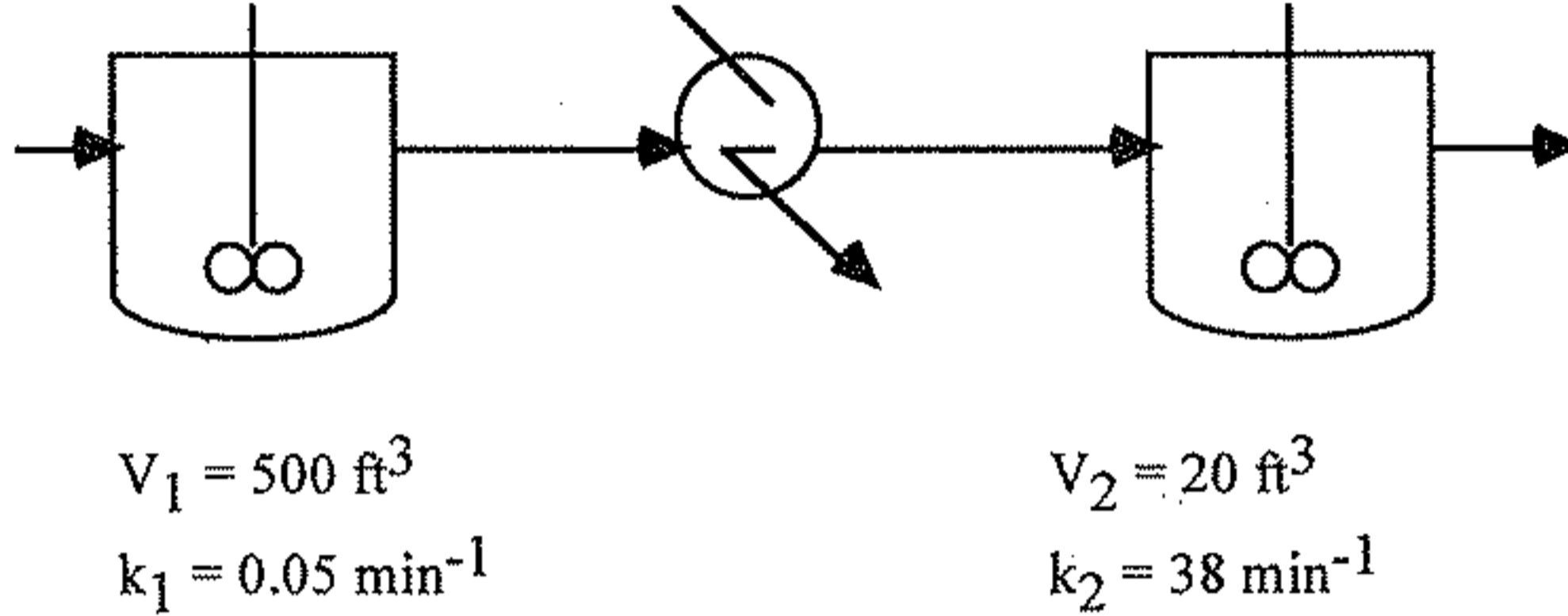


1. Using Taylor series expansion and the chain rule for partial differentiation for $dy/dx = f(x, y)$, derive the implicit 2nd order Gauss formula

$$y_{n+1} = y_n + k_1$$

$$k_1 = h f(x_n + h/2, y_n + k_1/2)$$

2. The reaction $A \rightarrow B$ takes place at steady state in two isothermal CSTR reactors in series as shown below in the figure, with a constant flowrate of $100 \text{ ft}^3/\text{min}$. Obtain the concentrations C_{A1}, C_{A2} as a function of time given that the inlet concentration C_{A0} is perturbed from 1.5 to 2.0 moles/ft^3 . Integrate for the first ten minutes using your favorite method. Plot your results and compare them with the analytical solution.



3. Show that the trapezoidal rule: $y_{n+1} = y_n + h/2 \{f(x_n, y_n) + f(x_{n+1}, y_{n+1})\}$ also corresponds to a 2nd order implicit Runge-Kutta method, and obtain its coefficients in the Butcher block matrix.

4. Show that for any v , the following Runge-Kutta method, is consistent of order 2.

$$y_{n+1} = y_n + 1/2 (k_2 + k_3),$$

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + vh, y_n + v k_1)$$

$$k_3 = hf(x_n + (1-v)h, y_n + (1-v) k_1)$$

5. Investigate the numerical stability of the following methods for $y' = \lambda y, \lambda < 0$

i) $y_{n+1} = y_n + h/12 [5f_{n+1} + 8f_n - f_{n-1}]$ (3rd Order Adams-Moulton Corrector)

ii) $y_{n+1} = y_{n-1} + h/3 [f_{n+1} + 4f_n + f_{n-1}]$ (Milne-Simpson Formula)

iii) $y_{n+1} = y_{n-1} + h/2 [f_n + 3f_{n-1}]$

6. The equation $y' = -Ay + B$ has a general solution $y(x) = c e^{-Ax} + B/A$ where c is an arbitrary constant and thus $y(x) \rightarrow B/A$ as x goes to infinity. If Euler's method is applied to this equation, show that $y_n \rightarrow B/A$ as n goes to infinity only if $h < 2/A$.

7. Consider the system

$$y_1' = -0.1 y_1 - 49.9 y_2 \quad y_1(0) = 3$$

$$y_2' = -50 y_2 \quad y_2(0) = 1.5$$

$$y_3' = 70 y_2 - 120 y_3 \quad y_3(0) = 3$$

- a) Calculate the stiffness ratio and the eigenvalues for this system
 b) Find the analytic solution.
 c) Find the maximum value for which h is stable for a fourth order explicit Runge-Kutta method (see Carnahan and Wilkes for the stability plot.)

Solution - Homework 3

1) second order Runge-Kutta formula

$$y_{i+1} = y_i + k_1$$

$$k_1 = h f(x_i + h/2, y_i + k_1/2)$$

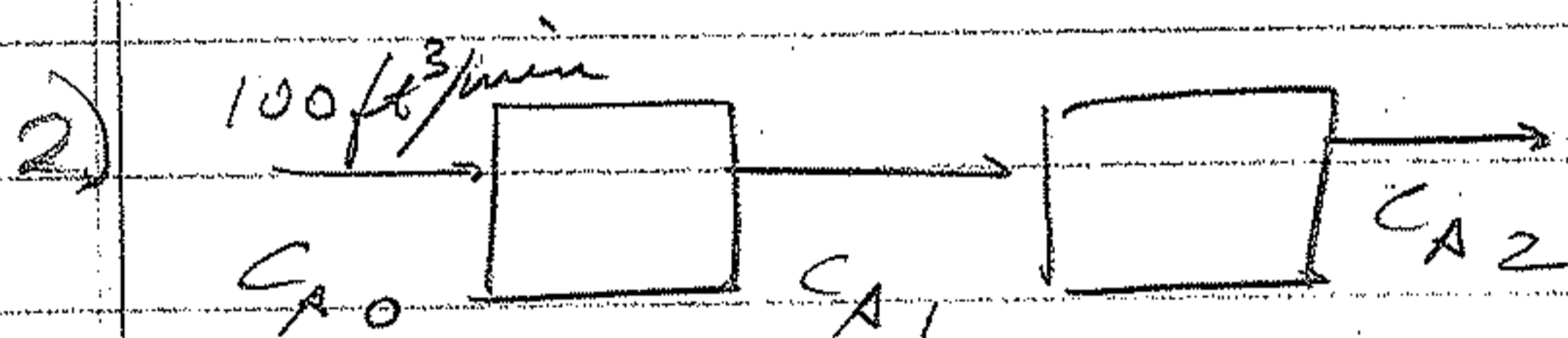
Taylor series

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{h^2}{2} \{ f_x + f_y f \}$$

$$= y_i + h \left\{ f_i + \frac{\partial f}{\partial x} \frac{h}{2} + \frac{\partial f}{\partial y} \frac{k_1}{2} \right\}$$

$$\text{where } k_1 \approx \left(I - h \frac{\partial f}{\partial y} \right)^{-1} h \left(f + \frac{h}{2} \frac{\partial f}{\partial x} \right)$$

all of the coefficients match for h, h^2
Hence the local error is $O(h^3)$ and the method is second order.



$$V_1 \dot{C}_{A1} = F(C_{A0} - C_{A1}) - V_1 k_1 C_{A1}$$

$$V_2 \dot{C}_{A2} = F(C_{A1} - C_{A2}) - V_2 k_2 C_{A2}$$

with $F = 100$

$$V_1 = 500, V_2 = 20, k_1 = 0.05, k_2 = 38, C_{A0}(0) =$$

leading to:

$$\dot{C}_{A1} = 0.2 C_{A0} - 0.25 C_{A1}, C_{A1}(0) = 4.20$$

$$\dot{C}_{A2} = 5 C_{A1} - 43 C_{A2}, C_{A2}(0) = 0.1395$$

Analytical solution

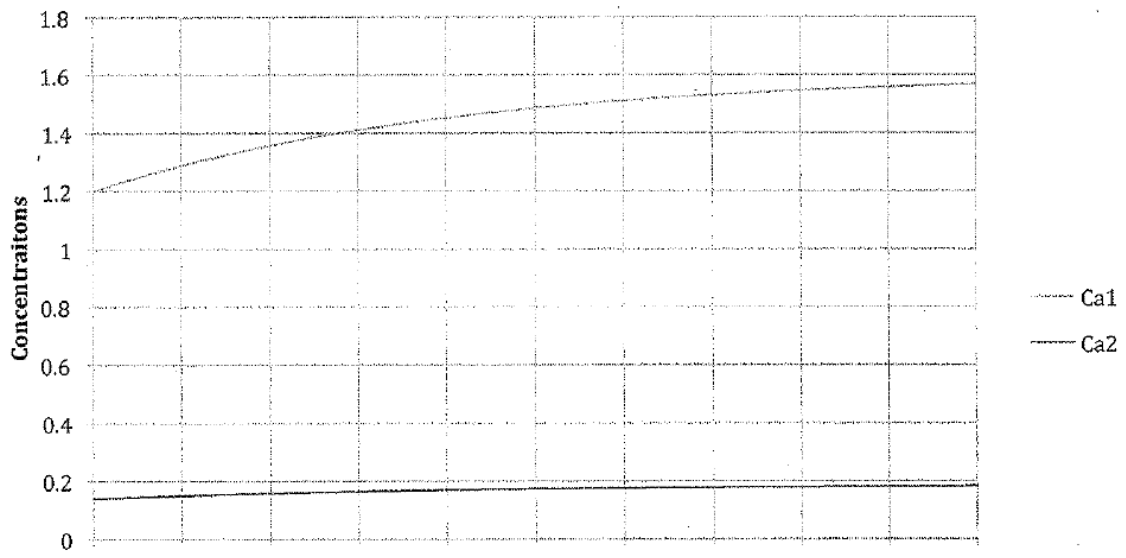
$$C_{A0} = 1.5 - 2.0 \text{ mole/ft}^3 @ t=0$$

$$C_{A1} = 1.6 - 0.4 \exp(-0.25t)$$

$$C_{A2} = 0.186 - 0.04678 \exp(-0.25t) + 2.4 \cdot 10^{-4} \exp(-43t)$$

Problem is mildly stiff ($S \sim 172$)
for $h=1$, Explicit Euler is unstable
 $h=0.01$, the stable plot is below:

Reactor Concentrations, Explicit Euler, $h = 0.01$



3) Trapezoidal Rule:

$$y_{n+1} = y_n + \frac{h}{2} (f(x_n, y_n) + f(x_{n+1}, y_{n+1}))$$

$$k_1 = f(x_n, y_n) h$$

$$k_2 = f(x_{n+1}, y_n + \frac{h}{2}(k_1 + k_2))$$

Butcher's Block

0	0	0
1	1/2	1/2
	1/2	1/2

4) R-K method: show order 2.

$$y_{n+1} = y_n + \frac{1}{2}(k_2 + k_3)$$

$$k_1 = h f(x_n, y_n)$$

$$k_2 = h f(x_n + \sigma h, y_n + \sigma k_1)$$

$$k_3 = h f(x_n + (1-\sigma)h, y_n + (1-\sigma)k_1)$$

$$y_{n+1} = y_n + h f_n + \frac{h^2}{2} \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f \right)$$

$$= y_n + h f_n + \frac{h^2}{2} (\sigma + (1-\sigma)) \frac{\partial f}{\partial x}$$

$$+ \frac{h^2}{2} \left(\sigma \frac{\partial f}{\partial y} k_1 + (1-\sigma) \frac{\partial f}{\partial y} k_1 \right)$$

$$= y_n + h f_n + \frac{h^2}{2} \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f \right) + \dots$$

consistent of order 2

5) $y' = \lambda y, \operatorname{Re}(\lambda) < 0$

i) $y_{n+1} = y_n + \frac{h}{12} (5f_{n+1} + 8f_n - f_{n-1})$

$\mu^{n-1} \left(\left(1 - \frac{5}{12}h\lambda\right)\mu^2 - \left(1 + \frac{2}{3}h\lambda\right)\mu + \frac{h\lambda}{12} \right) = 0$

$\mu = \frac{\left(1 + \frac{2}{3}h\lambda\right) \pm \left(\left(1 + \frac{2}{3}h\lambda\right)^2 - \frac{4}{3}\left(1 - \frac{5}{12}h\lambda\right)\right)^{1/2}}{\left(2 - \frac{5}{6}h\lambda\right)}$

ii) $y_{n+1} = y_{n-1} + \frac{h}{3} [f_{n+1} + 4f_n + f_{n-1}]$

$\mu^{n-1} \left(\left(1 - \frac{h\lambda}{3}\right)\mu^2 - \frac{4h\lambda}{3}\mu - \left(1 + \frac{h\lambda}{3}\right) \right) = 0$

$\mu = \frac{\frac{4h\lambda}{3} \pm \left(\frac{16(h\lambda)^2}{9} + 4\left(1 + \frac{h\lambda}{3}\right)\left(1 - \frac{h\lambda}{3}\right)\right)^{1/2}}{2\left(1 - \frac{h\lambda}{3}\right)}$

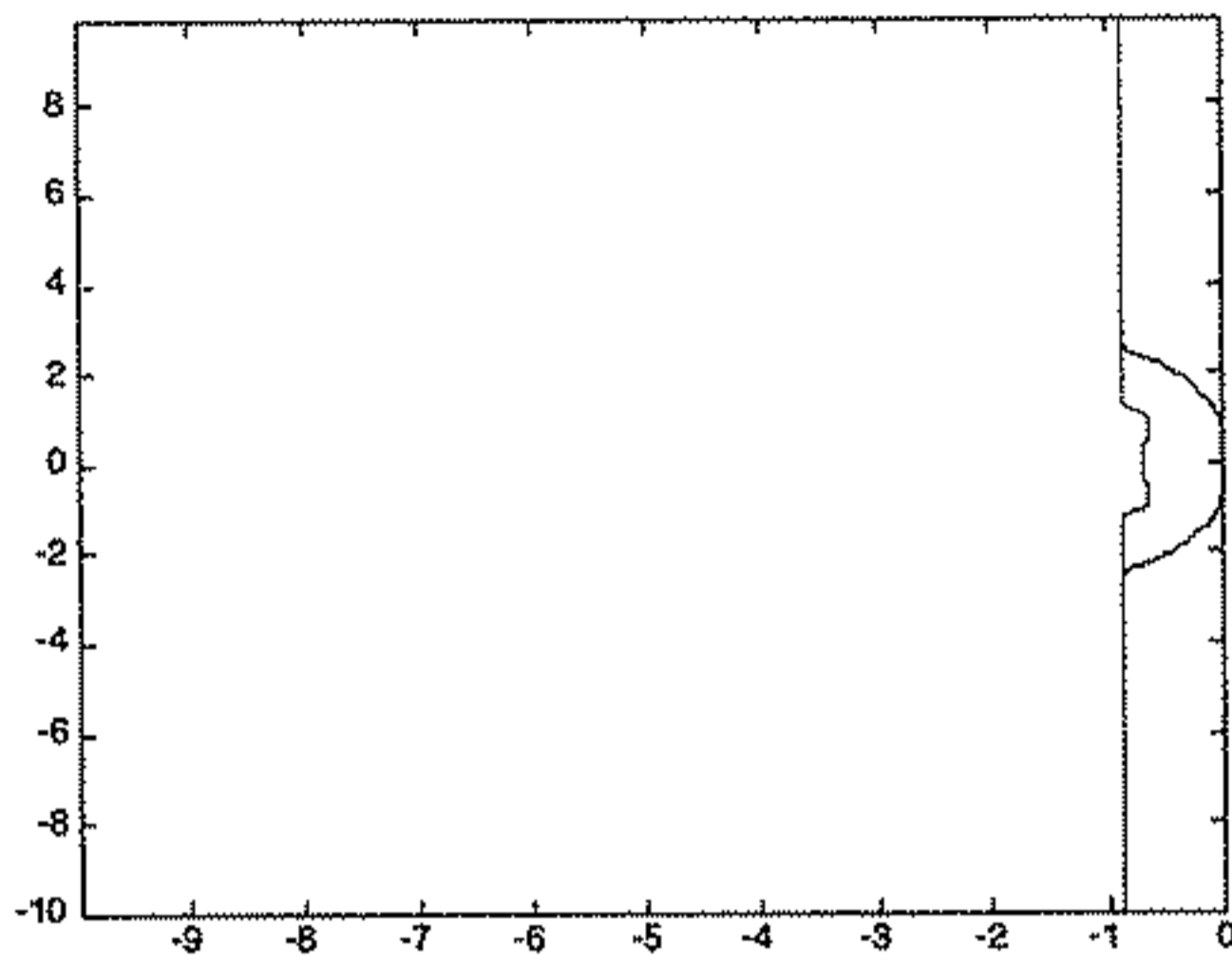
iii) $y_{n+1} = y_{n-1} + \frac{h}{2} (f_n + 3f_{n-1})$

$\mu^{n-1} \left(\mu^2 - \frac{h\lambda}{2}\mu - \left(1 + \frac{3h\lambda}{2}\right) \right) = 0$

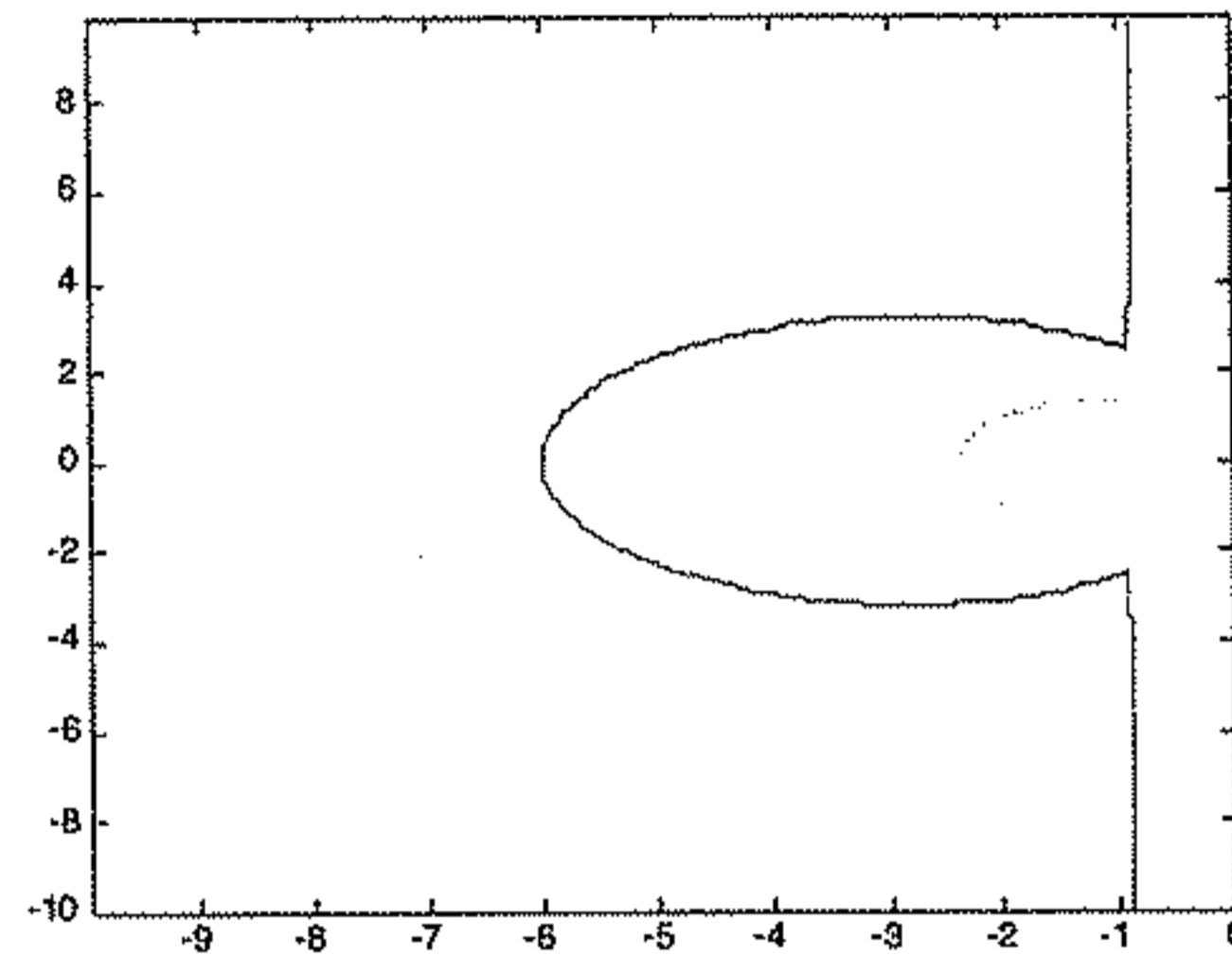
$\mu = \frac{h\lambda}{4} \pm \left(\frac{(h\lambda)^2}{4} + \left(1 + \frac{3h\lambda}{2}\right)\right)^{1/2}$

(see contour plots)

1-i) Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 0.5 (light) and 1 (dark)



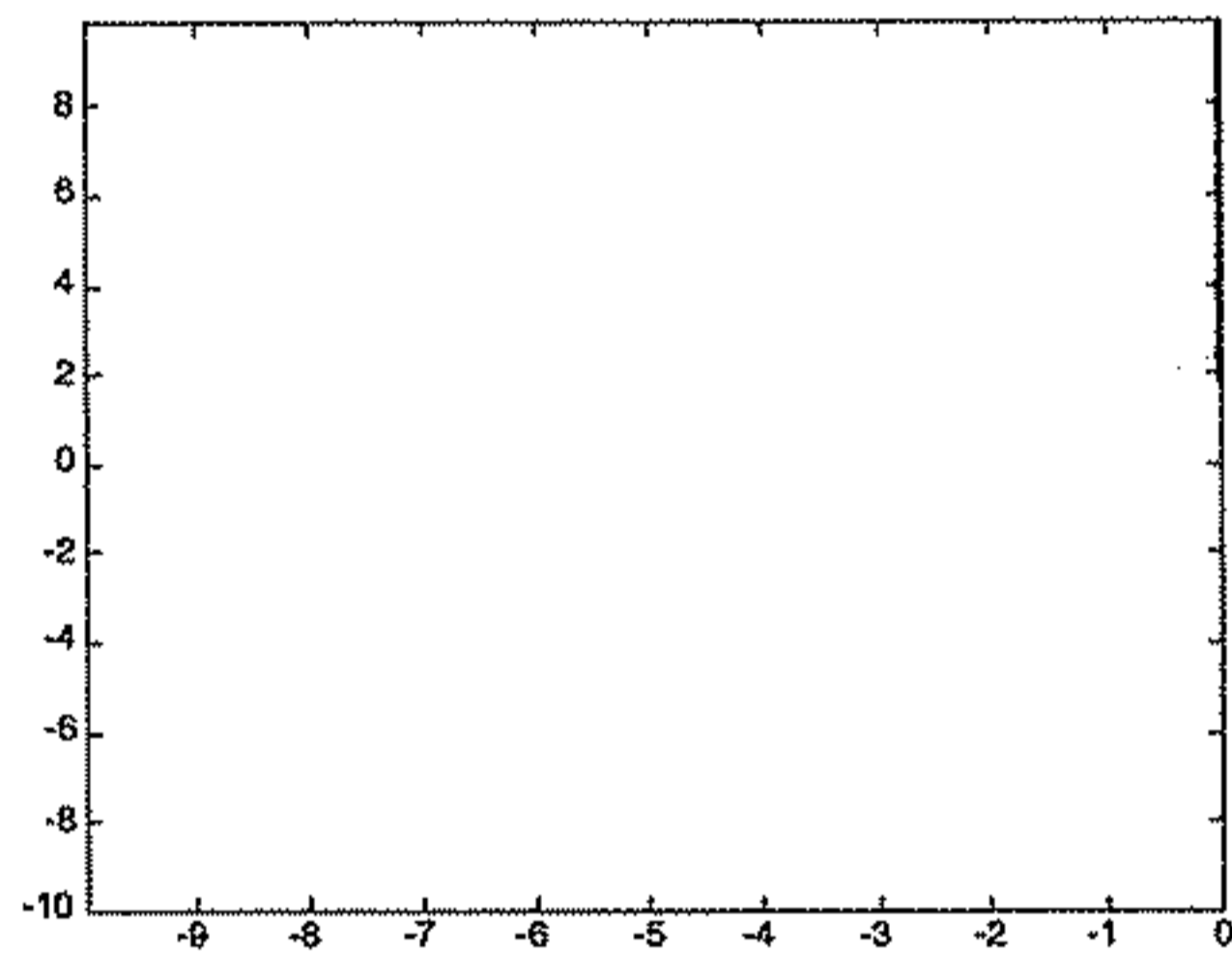
Positive part



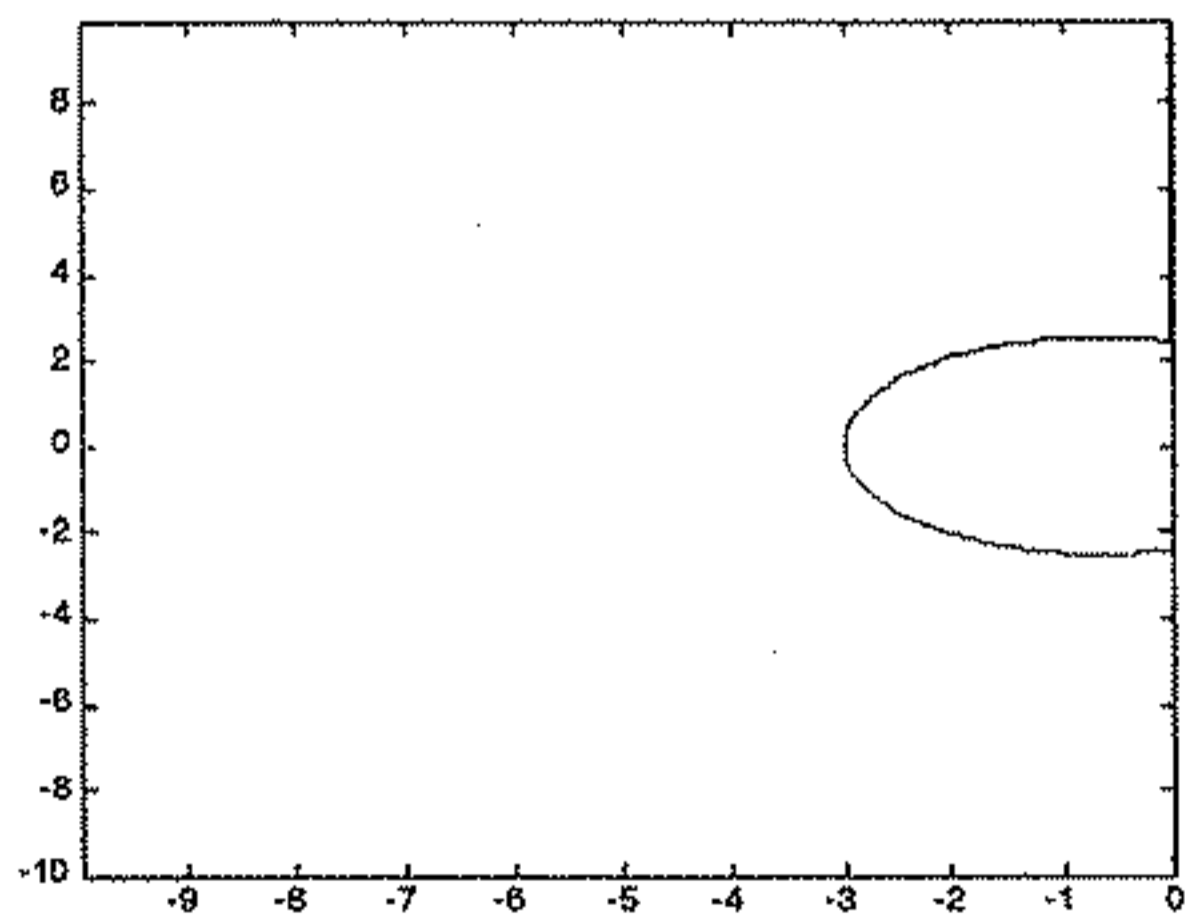
Negative part

The overlap determines the region of absolute stability

1-ii)



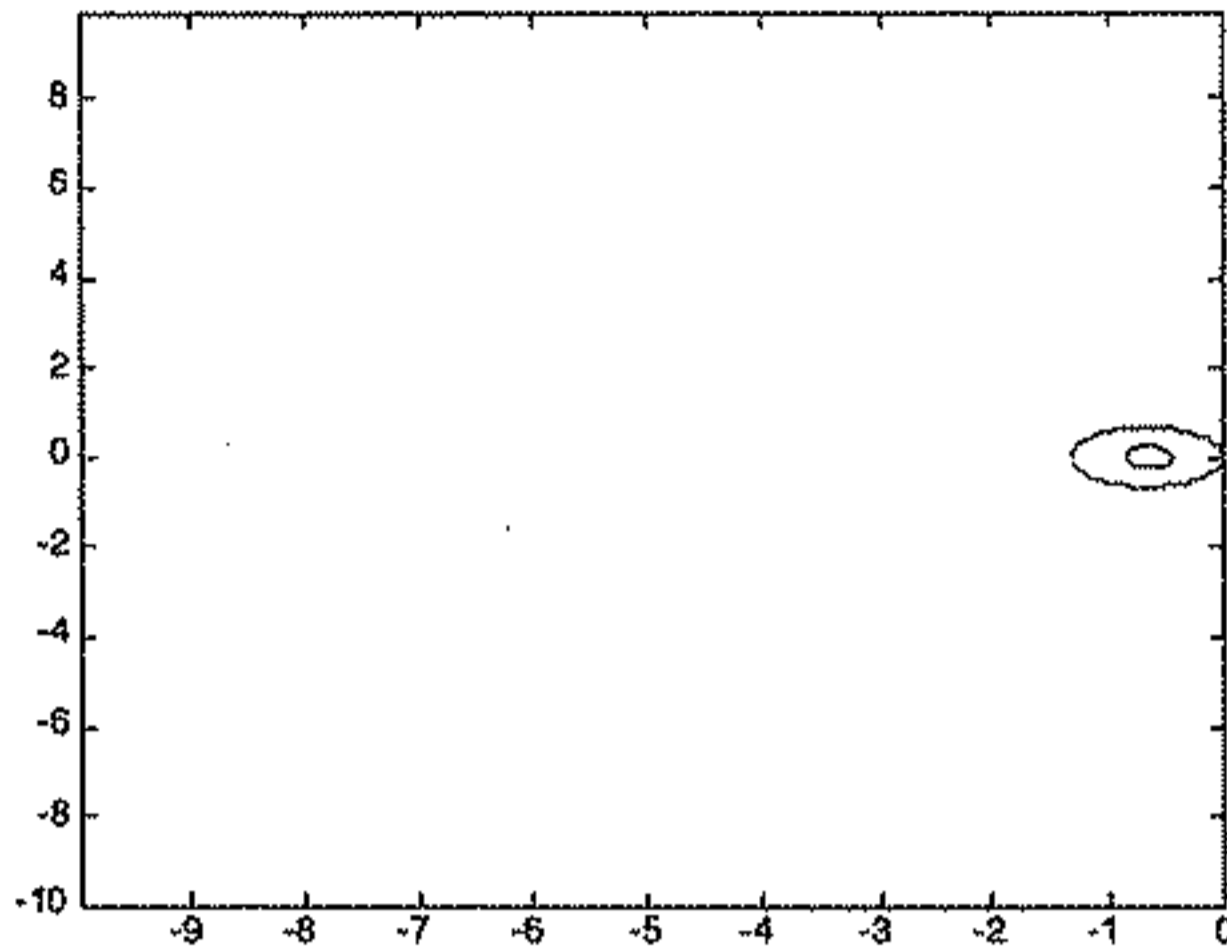
Positive part (Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 0.5 (light) and 1 (dark))



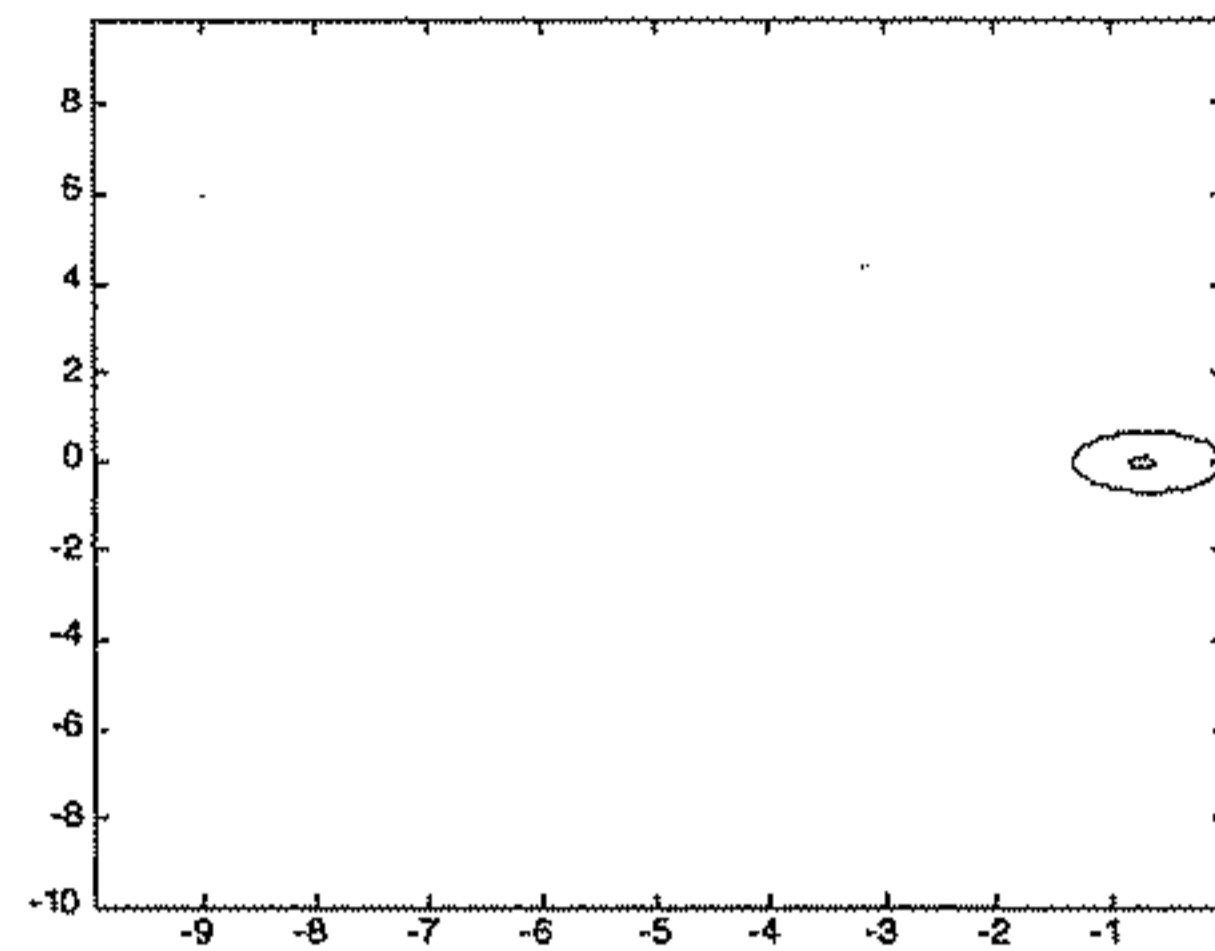
Negative part (Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 1.0 (light) and 2 (dark))

The overlap determines the region of absolute stability. For this problem, there is no such region.

1-iii) Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 0.5 (light) and 1 (dark)



Positive part



Negative part

The overlap determines the region of absolute stability

MATLAB programs

```
1-i
for i = 1:200;
for j = 1:200;
a = -0.05*(i-1)
b = -10 + 0.1*(j-1)
hl = complex(a,b);
mp = ((1+2*hl/3)+((1+2*hl/3)^2 - hl/3*(1-
5*hl/12))^(0.5))/(2-5*hl/6);
mpm(j,i) =
(real(mp)*real(mp)+imag(mp)*imag(mp))^(0.5);
mn = ((1+2*hl/3)-((1+2*hl/3)^2 - hl/3*(1-
5*hl/12))^(0.5))/(2-5*hl/6);
mnm(j,i) =
(real(mn)*real(mn)+imag(mn)*imag(mn))^(0.5);
end;
end;
```

```
i = 1:200;
a = -0.05*(i-1)
j = 1:200;
b = -10 + 0.1*(j-1)
v = [0, 0.5, 1];
contour(a, b, mpm, v);
*****
```

```
1-ii
for i = 1:200;
for j = 1:200;
a = -0.05*(i-1)
b = -10 + 0.1*(j-1)
hl = complex(a,b);
mp = ((4*hl/3)+((4*hl/3)^2 + 4*(1+hl/3)*(1-
hl/3))^(0.5))/(2-2*hl/3);
mpm(j,i) =
(real(mp)*real(mp)+imag(mp)*imag(mp))^(0.5);
```

```
mn = ((4*hl/3)-((4*hl/3)^2 + 4*(1+hl/3)*(1-
hl/3))^(0.5))/(2-2*hl/3);
mnm(j,i) =
(real(mn)*real(mn)+imag(mn)*imag(mn))^(0.5);
end;
end;
```

```
i = 1:200;
a = -0.05*(i-1)
j = 1:200;
b = -10 + 0.1*(j-1)
v = [0, 0.5, 1];
contour(a, b, mpm, v);
*****
```

```
1-iii
for i = 1:200;
for j = 1:200;
a = -0.05*(i-1)
b = -10 + 0.1*(j-1)
hl = complex(a,b)
mp = (hl/4)+((hl/4)^2 +(1+3*hl/2))^(0.5);
mpm(j,i) =
(real(mp)*real(mp)+imag(mp)*imag(mp))^(0.5);
mn = (hl/4)-((hl/4)^2 +(1+3*hl/2))^(0.5);
mnm(j,i) =
(real(mn)*real(mn)+imag(mn)*imag(mn))^(0.5);
end;
end;
```

```
i = 1:200;
a = -0.05*(i-1)
j = 1:200;
b = -10 + 0.1*(j-1)
v = [0, 0.5, 1];
```

6. Alternate stability analysis - Euler's method

$$y' = -Ay + B, \quad y(x) = Ce^{-Ax} + B/A$$

$$\begin{aligned} y_{n+1} &= y_n + (B - Ay_n)h \\ &= (1 - Ah)y_n + Bh \end{aligned}$$

- consider homogeneous solution

$$y_n = C\mu^n \Rightarrow \mu = (1 - Ah), \quad 0$$

$$\begin{aligned} |\mu| < 1 &\Rightarrow -2 < -Ah < 0 \\ &\Rightarrow h < 2/A \end{aligned}$$

- consider particular solution

$$\begin{aligned} \mu^P &= \mu^P + (B - A\mu^P)h \\ &\Rightarrow \mu^P = B/A \end{aligned}$$

$$y_n = C\mu^n + \mu^P = C(1 - Ah)^n + B/A.$$

so for $|1 - Ah| < 1$, y_n is bounded.

7) stiff systems

$$\begin{aligned} y_1' &= -0.1y_1 - 49.9y_2, \quad y_1(0) = 3 \\ y_2' &= -50y_2, \quad y_2(0) = 1.5 \\ y_3' &= 70y_2 - 120y_3, \quad y_3(0) = 3 \end{aligned}$$

a) Eigenvalues

$$\det \begin{bmatrix} -(0.1 + \lambda) & -49.9 & 0 \\ 0 & -(50 + \lambda) & 0 \\ 0 & 70 & -(120 + \lambda) \end{bmatrix} = 0$$

$$\lambda = -0.1, -50, -120, \quad S = 1200.$$

b) Analytical solution

$$y_1(t) = 1.5 \exp(-0.1t) + 1.5 \exp(-50t)$$

$$y_2(t) = 1.5 \exp(-50t)$$

$$y_3(t) = 4.5 \exp(-50t) + 1.5 \exp(-120t)$$

c) From Carnahan & Wilkes, stability limit is $|\operatorname{Re}(\lambda)| < 2.8$

for stiff systems $\frac{2.8}{|\operatorname{Re}(\lambda)|_{\max}} = h_{\max} = 0.025$