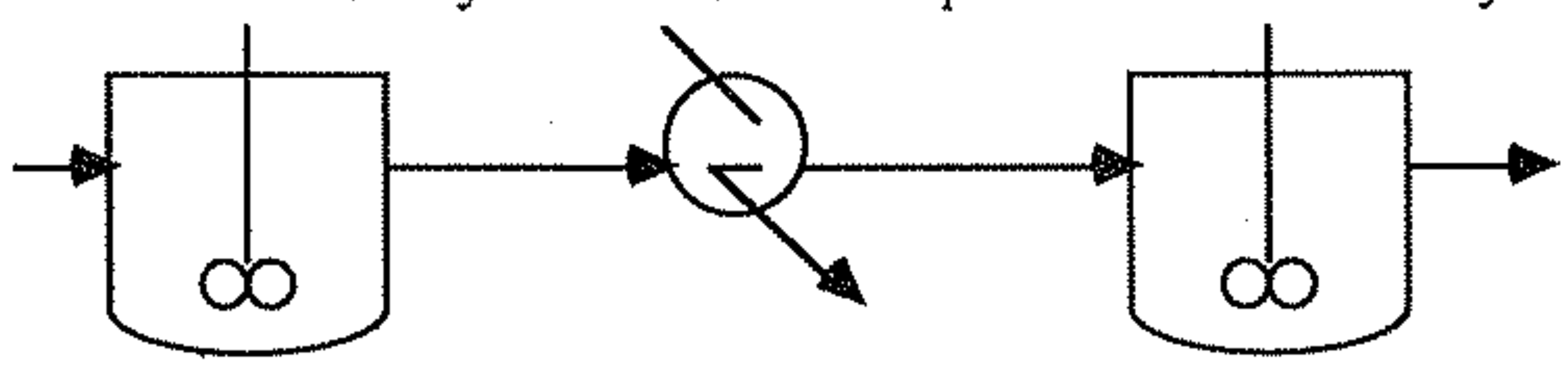
06-606

Assignment 3
Computational Methods

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 ft^3/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.



$V_1 = 500$ ft^3 $\qquad$ $V_2 = 20$ ft^3

$k_1 = 0.05$ min^{-1} $\qquad$ $k_2 = 38$ min^{-1}

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.

$$y_{n+1} = y_n + 1/2\,(k_2 + k_3),$$
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + vh,\, y_n + v\, k_1)$$
$$k_3 = hf(x_n + (1\text{-}v)h,\, y_n + (1\text{-}v)\, k_1)$$

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

$y_1' = -0.1\, y_1 - 49.9\, y_2 \qquad y_1(0) = 3$
$y_2' = -50\, y_2 \qquad y_2(0) = 1.5$
$y_3' = 70\, y_2 - 120\, y_3 \qquad y_3(0) = 3$

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 - Hwk 3

1) second order Gauss formula

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

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

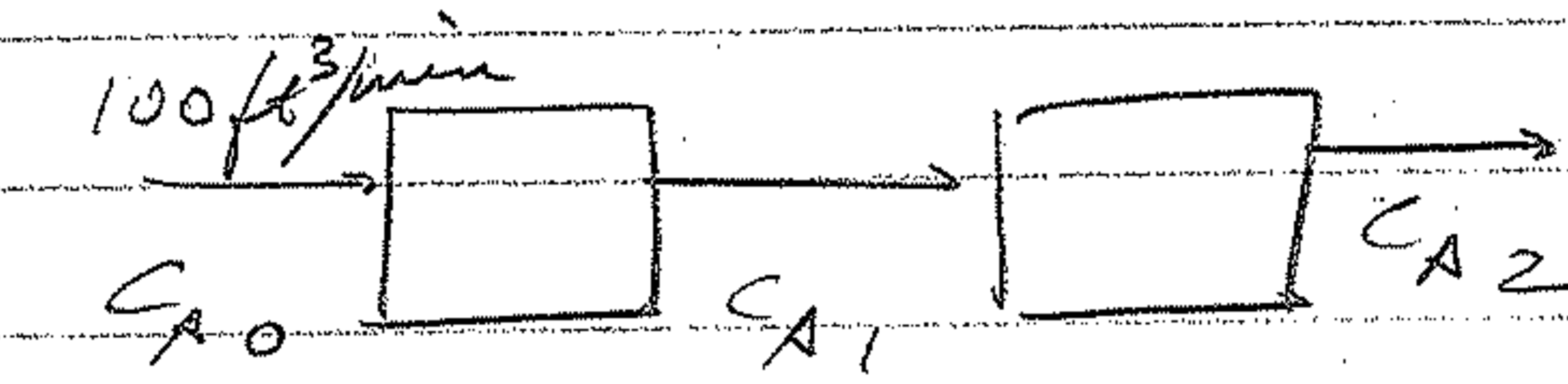
Taylor series

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

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

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.

2) 

$$V_1 \dot{c}_{A1} = F(c_{A0} - c_{A1}) - V_1 k_1 c_{A1}$$

$$V_2 \dot{c}_{A2} = F(c_{A1} - c_{A2}) - V_2 k_2 c_{A2}$$

with $F = 100$

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

leading to:

$$\dot{c}_{A1} = 0.2 c_{A0} - 0.25 c_{A1},\quad c_{A1}(0) = 1.20$$

$$\dot{c}_{A2} = 5 c_{A1} - 43 c_{A2},\quad c_{A2}(0) = 0.1395$$

Analytical solution

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

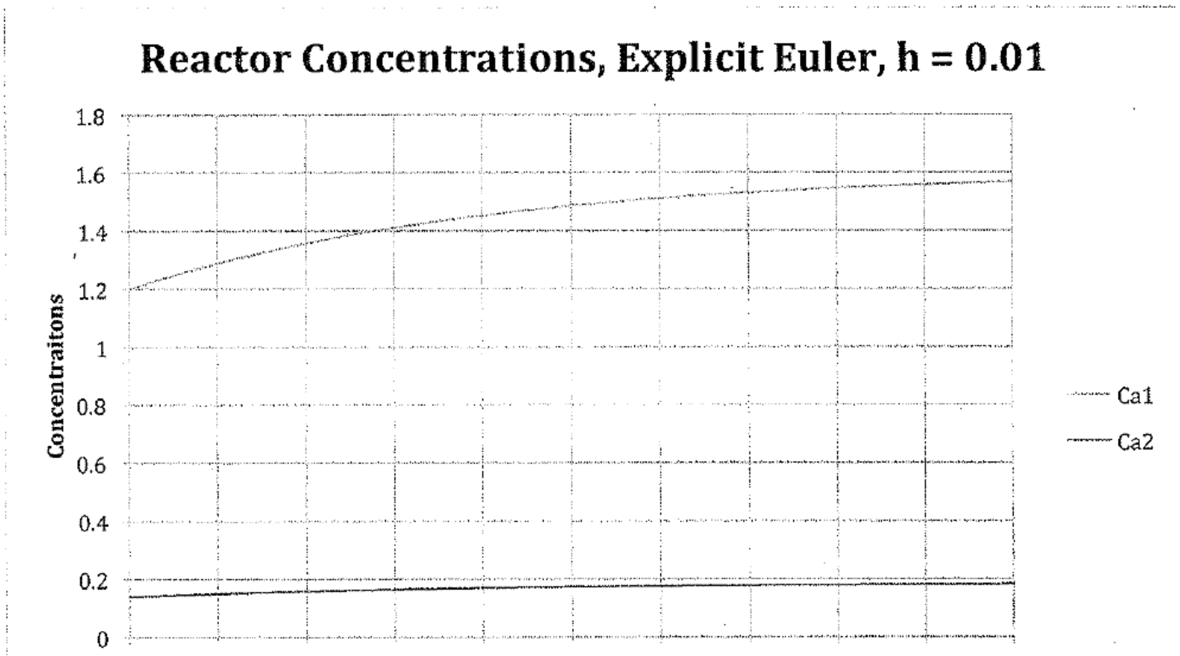
$C_{A1} = 1.6 - 0.4\exp(-0.25t)$

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

Problem is mildly stiff ($S \sim 172$)

for $h=1$, Explicit Euler is unstable

$h = 0.01$, the stable plot is below:



3) Trapezoidal Rule:

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

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

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

Butcher Block

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$

4) R-K method: show order 2

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

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

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

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

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

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

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

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

consistent of order 2

5) $y' = \lambda y \,, \; Re(\lambda) < 0$

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

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

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

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

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

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

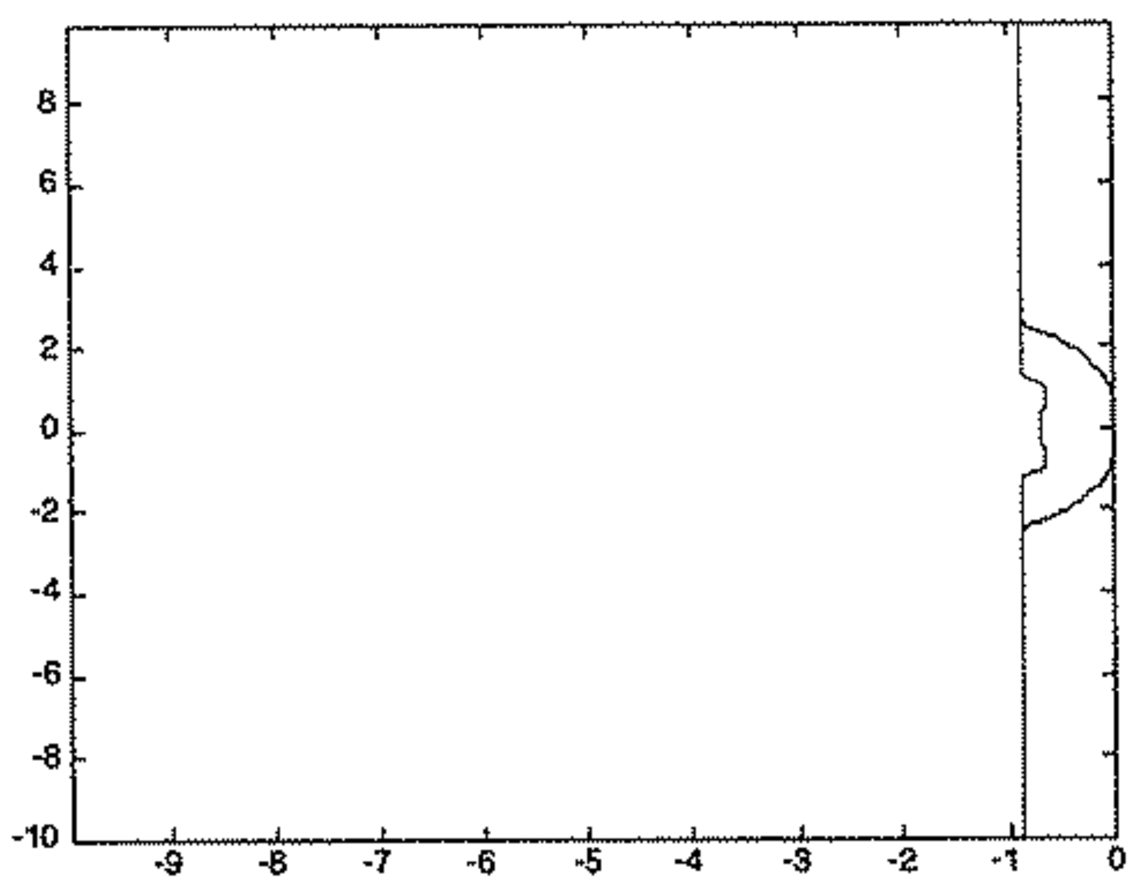
iii) $$y_{n+1} = y_{n-1} + \frac{h}{2}\left(f_n + 3f_{n-1}\right)$$

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

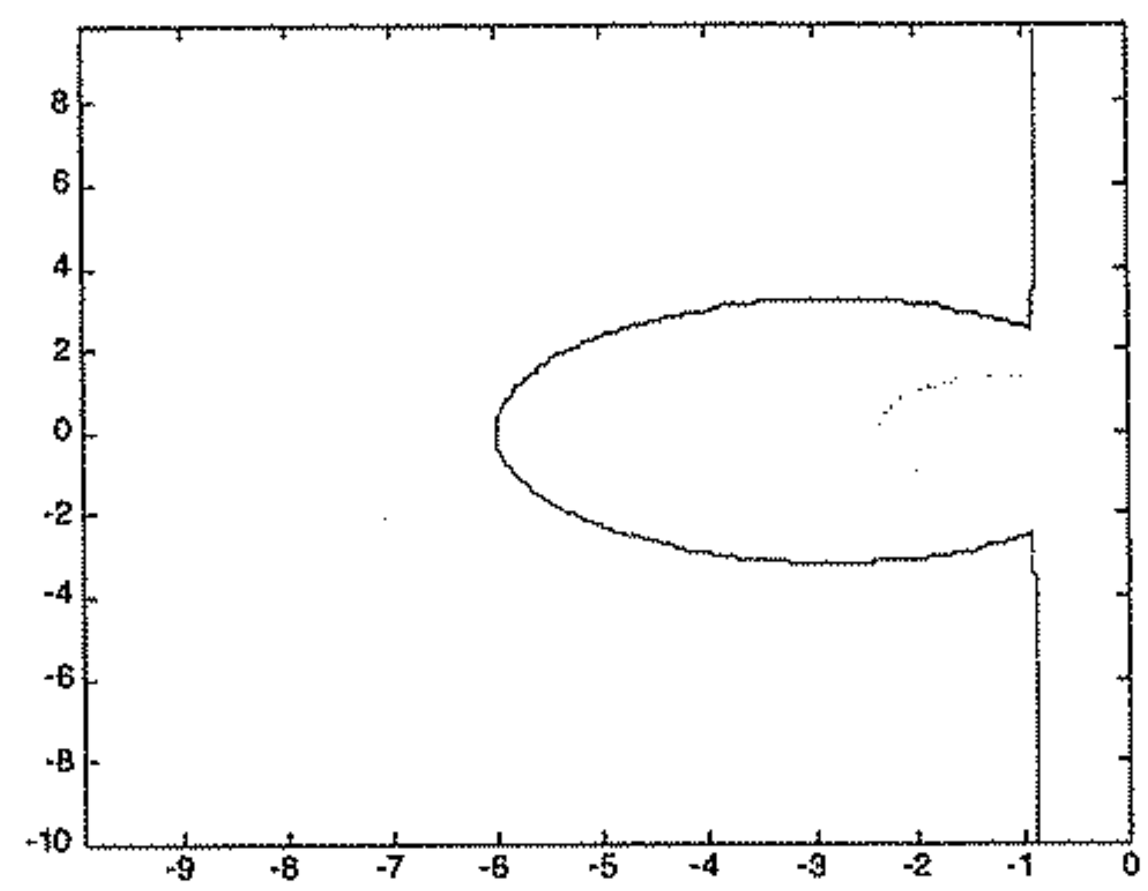
$$\mu = \frac{h\lambda}{4} \pm \left(\left(\frac{h\lambda}{4}\right)^2 + \left(1 + \frac{3h\lambda}{2}\right)\right)^{1/2}$$

(see contour plots)

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



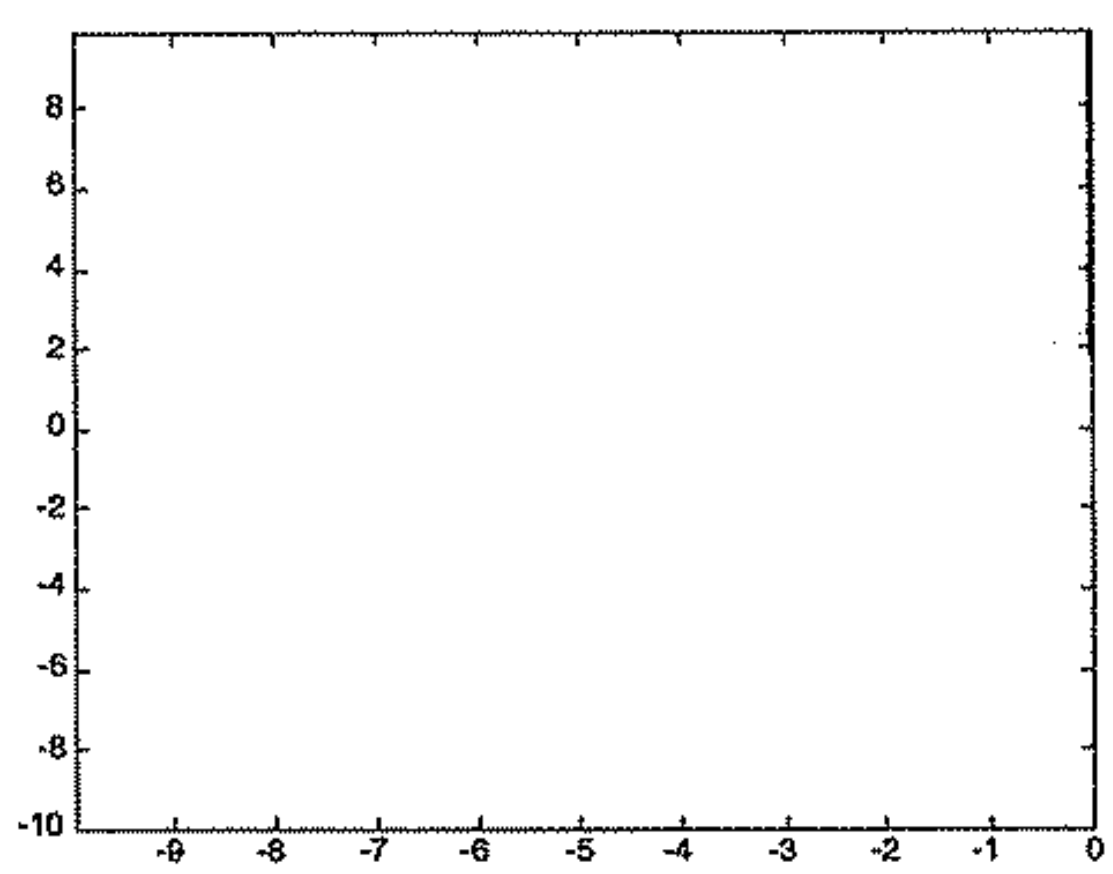
Positive part



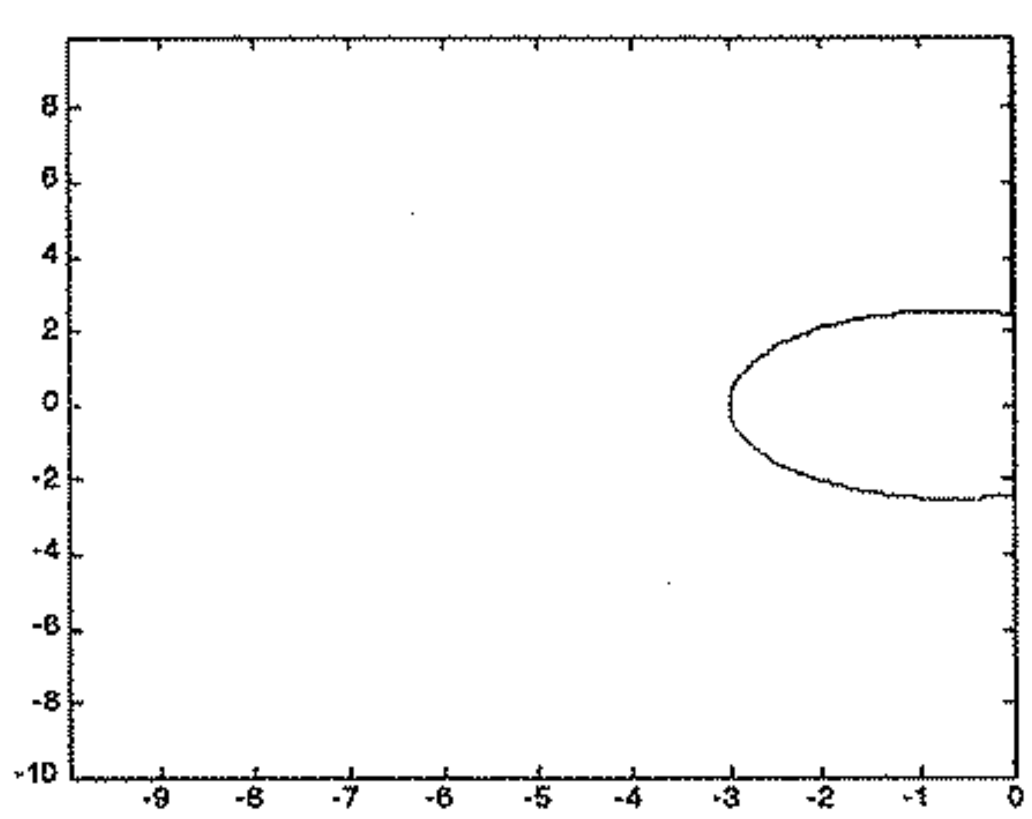
Negative part

The overlap determines the region of absolute stability

1-ii)



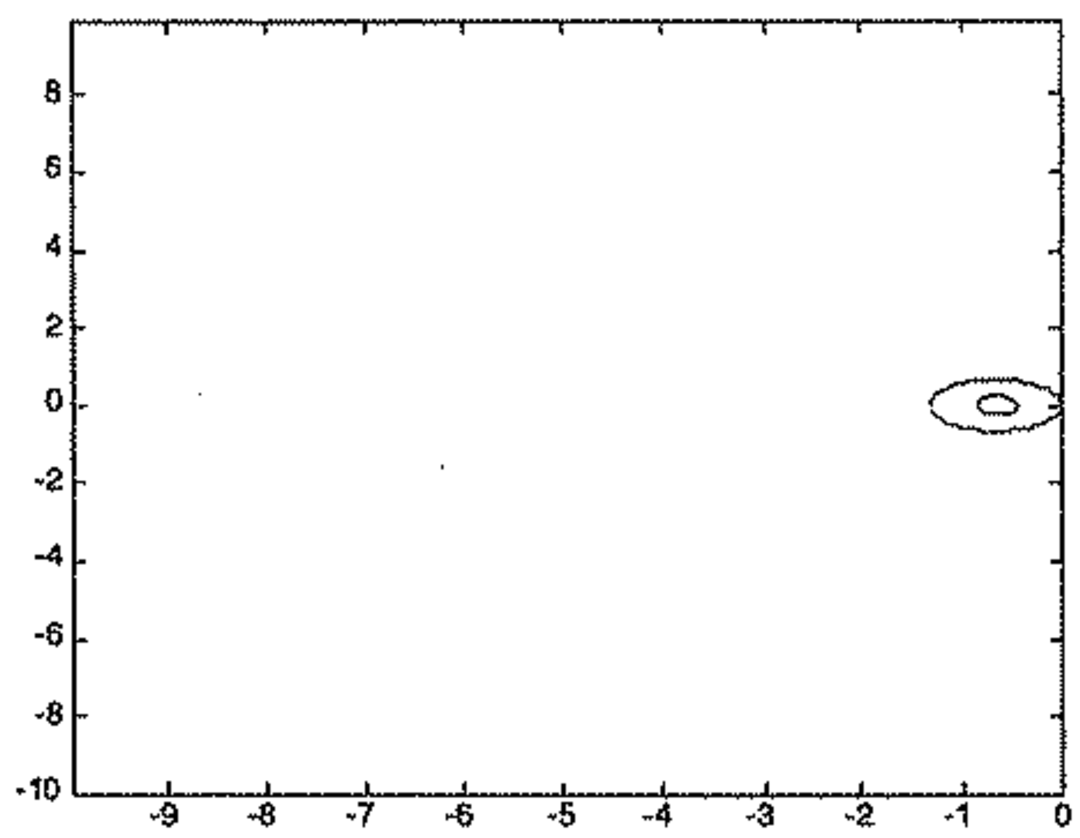
Positive part (Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 0.5 (light) and 1 (dark))



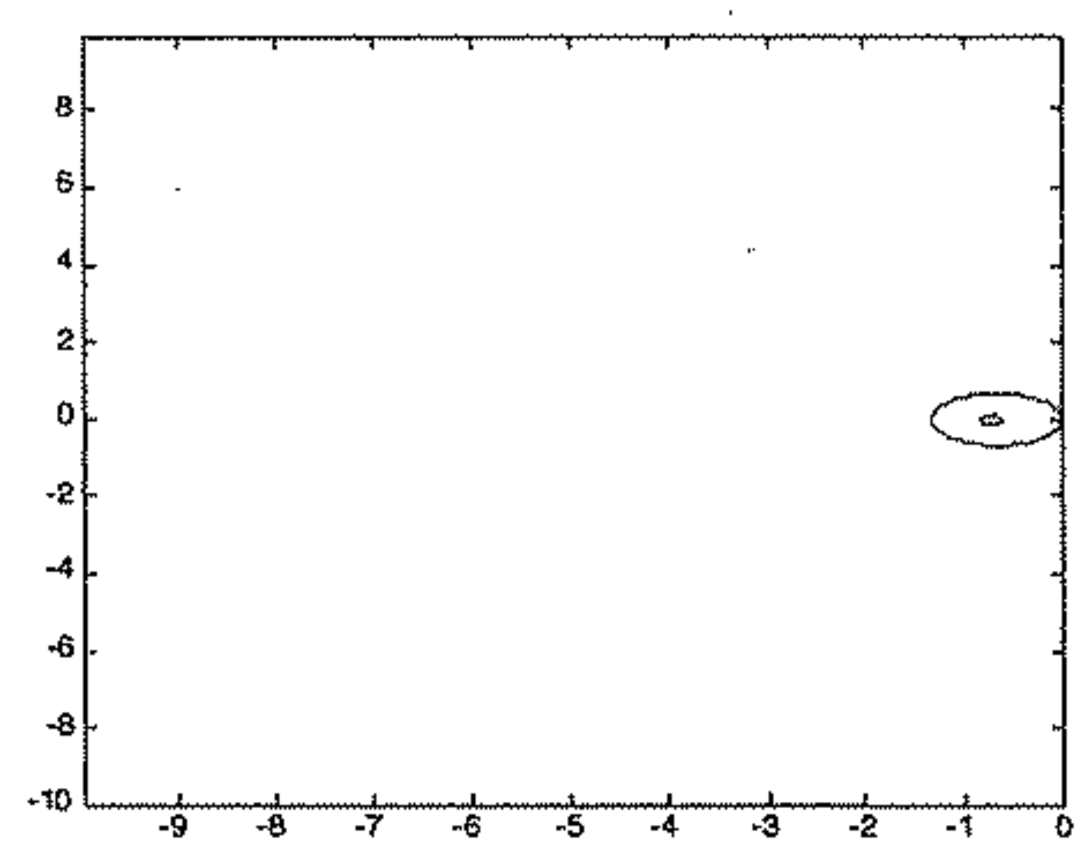
Negative part (Contour plots of $|\mu_+|$ and $|\mu_-|$ for values of 1.0 (light) and 2 (dark))

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

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

$$y_{n+1} = y_n + (B - Ay_n)h$$
$$= (1-Ah)y_n + Bh$$

- consider homogeneous solution

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

$$|\mu| < 1 \Rightarrow -2 < -Ah < 0$$
$$\Rightarrow h \leq 2/A$$

- consider particular solution

$$\mu^P = \mu^P + (B - A\mu^P)h$$
$$\Rightarrow \mu^P = B/A$$

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

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

7) Stiff systems

$$y_1' = -0.1y_1 - 49.9y_2, \quad y_1(0) = 3$$
$$y_2' = -50y_2, \quad y_2(0) = 1.5$$
$$y_3' = 70y_2 - 120y_3, \quad y_3(0) = 3$$

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

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

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

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

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

for stiff system $\dfrac{2.8}{|Re(\lambda)|_{max}} = h_{max} = 0.02$