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Stiffly Stable Linear 3-step Methods

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Abstract: The whole class of linear 3-step methods for solving system of ordinary differential equations is shown in a parameter space. Almost all of the existing stiffly stable methods of this class are found. Particular emphasis is given to develop methods with large region of instability in the right half plane which are suitable for stiff systems with the capability of detecting unstable behavior of a problem.

1. Introduction

The numerical solution of ordinary differential equations is a relatively old topic. The typical scientific problems can be solved by using standard methods both easily and cheaply. But there are some kinds of problems which classical methods do not handle very efficiently and reliably. One such problems is *stiff differential equations* with mathematically unstable solutions.

Our study and research is one of the kind of subset of linear multistep methods (LMM) that are better than Backward Differentiation Formulae (BDF) which are widely used in practice for stiff problems. We have restricted the study to 3-step methods only. The ideas, however, can be extended to multistep methods of higher stepnumber

2. What is Stiff Differential Equation?

Consider the example

$$y_1' = -y_1, \qquad y_1(0) = 1$$
$$y_2' = -2000 y_2, \qquad y_2(0) = 1$$

The solution of this system is

$$y_1 = e^{-t}$$
$$y_2 = e^{-2000t}$$

To illustrate the behavior of stiffness let us, for simplicity, use the Euler's Method

$$y_{n+1} = y_n + h\ f(t_n, y_n)$$

to solve this system. To examine absolute stability, we consider in general, the equation $y' = \lambda y$, where λ is a complex number. For this

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

Consequently, Euler's method is absolutely stable in the region

$$|1 + \lambda h| \le 1$$

which is a unit circle in the complex λh-plane centered at (-1 ,0) which is shown in the following figure1.

For our example to achieve stability we then must have

$$|1 - 2000h| \le 1, \quad \text{or,} \ \ 0 < h \le 0.001.$$

This shows that very small stepsizes must be taken to maintain the stability. On the other hand when the transient dies it is not necessary to take h so small for the accuracy of the solution.

λh-plane ($\lambda h = x + iy$)

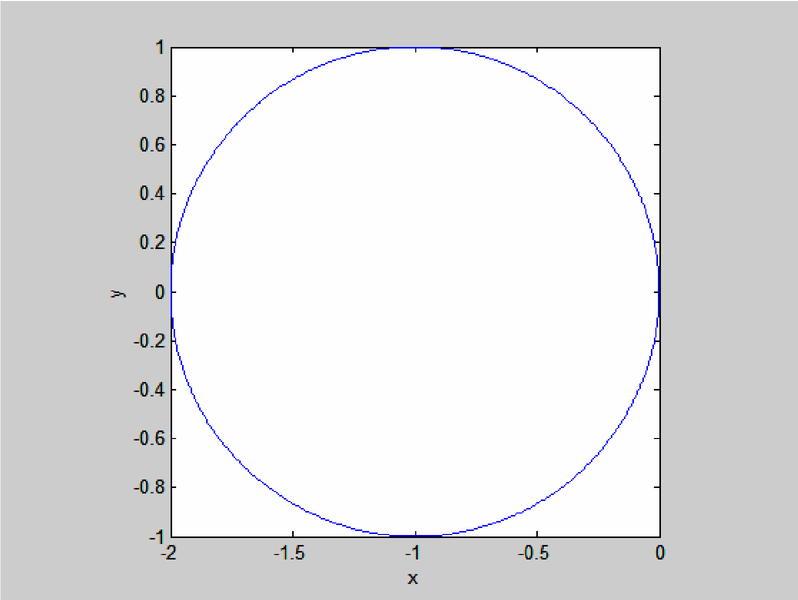

Figure 1

The local truncation error of Euler's method is

$$L[y(t_{n+1}), h] = \frac{1}{2} h^2 y''(t_n) + O(h^3)$$

Thus we have component wise

$$L_1 = \frac{1}{2} h^2 e^{-t}$$

$$L_2 = \frac{1}{2} h^2 (2000)^2 e^{-2000t}$$

For $t > 0.02$ we have $L_1 < h^2 \times 0.49$ and $L_2 < h^2 \times 2 \times 10^{-11}$.

So for $L_1 < 0.005$ we can choose $h = 0.1$ in which case $L_2 < 2 \times 10^{-13}$. But for stability reason we must take $|1 - 2000h| \le 1$, or, $0 < h \le 0.001$. So we see that stability rather than accuracy dictates the step size. This is the phenomenon of stiff differential equations.

3. Danger of too stable methods

The stability region of some methods for the solution of stiff differential equations contain a large portion of right half plane. Backward Euler's method, BDF methods etc. are of this type. These methods when applied to the scalar test problem,

$$y' = \lambda y, \qquad y(0) = 1$$

produce decreasing sequences if $h\lambda$ lies inside the stability region while the exact solution,

$$y(t) = e^{\lambda t} \ ,$$

is decreasing only if $\mathrm{Re}(\lambda) < 0$. Thus the numerical method may in some cases give decreasing solutions when the exact solution is exponentially growing.

4. Linear 3-step Methods

The 3-step LMS method has the form:

$$\sum_{j=0}^{3} \alpha_j y_{n+j} = h \sum_{j=0}^{3} \beta_j f_{n+j} \ , \qquad n = 0, 1, 2, \cdots\cdot$$

where α_j and β_j are real constants, $\alpha_3 \neq 0$. We assume that $\alpha_3 = 1$ and not both α_0 & β_0 are zero. The associated linear difference operator is

$$L[y(t);h] = \sum_{j=0}^{3} [\alpha_j y(t+jh) - h\beta_j y'(t+jh)]$$

Expanding $y(t+jh)$ and $y'(t+jh)$ in Taylor series about t we get

$$L[y(t);h] = C_0 y(t) + C_1 h y^{(1)}(t) + \cdots + C_q h^q y^{(q)}(t) + \cdots$$

where

$$C_0 = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3$$

$$C_1 = \alpha_1 + 2\alpha_2 + 3\alpha_3 - (\beta_0 + \beta_1 + \beta_2 + \beta_3)$$

$$C_q = \frac{1}{q!}(\alpha_1 + 2^q \alpha_2 + 3^q \alpha_3) - \frac{1}{(q-1)!}(\beta_1 + 2^{q-1}\beta_2 + 3^{q-1}\beta_3), \ q = 2,3,\cdots$$

If the order is sought to be p, where $p \geq 1$ then

$$C_0 = C_1 = \cdots\cdot = C_p = 0.$$

For all consistent methods $C_0 = C_1 = 0.$ Thus

$$\alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 = 0$$

$$\alpha_1 + 2\alpha_2 + 3\alpha_3 = \beta_0 + \beta_1 + \beta_2 + \beta_3$$

The corresponding ρ polynomial for all these methods is

$$\rho(\varsigma) = \alpha_3 \varsigma^3 + \alpha_2 \varsigma^2 + \alpha_1 \varsigma + \alpha_0$$

$$= \varsigma^3 + \alpha_2 \varsigma^2 + \alpha_1 \varsigma + \alpha_0 \qquad [\text{since } \alpha_3 = 1]$$

This can be written as

$$\rho(\varsigma) = (\varsigma - 1)[\varsigma^2 + (1+\alpha_2)\varsigma + (1 + \alpha_1 + \alpha_2)]$$

We put

(4.1)
$$1 + \alpha_2 = -a$$
$$1 + \alpha_1 + \alpha_2 = b$$

Then

$$\rho(\varsigma) = (\varsigma - 1)(\varsigma^2 - a\varsigma + b)$$

For the stability requirement (zero-stability), we are interested in those values of a and b for which the quadratic factor

$$\varsigma^2 - a\varsigma + b$$

has roots such that $|\varsigma|<1$, that is, the roots lie inside the unit circle in the complex plane. The easiest way to find this is to find the boundary in the (a,b)-plane where $|\varsigma|=1$ is a root. We see that $\varsigma=-1$ is a root if

(4.2) $$1+a+b=0$$

and $\varsigma=+1$ is a root if

(4.3) $$1-a+b=0.$$

The only other possibility is that a complex conjugate pair on the unit circle occurs. For this $b=1$ and the discriminant must be negative. This occurs when

$$b=1 \quad \text{and} \quad a^2-4<0.$$

This gives the segment

(4.4) $$b=1 \quad \text{and} \quad -2<a<2.$$

The lines (4.2) & (4.3) and the segment (4.43) form a closed region which is a triangle which is shown in Figure 2.

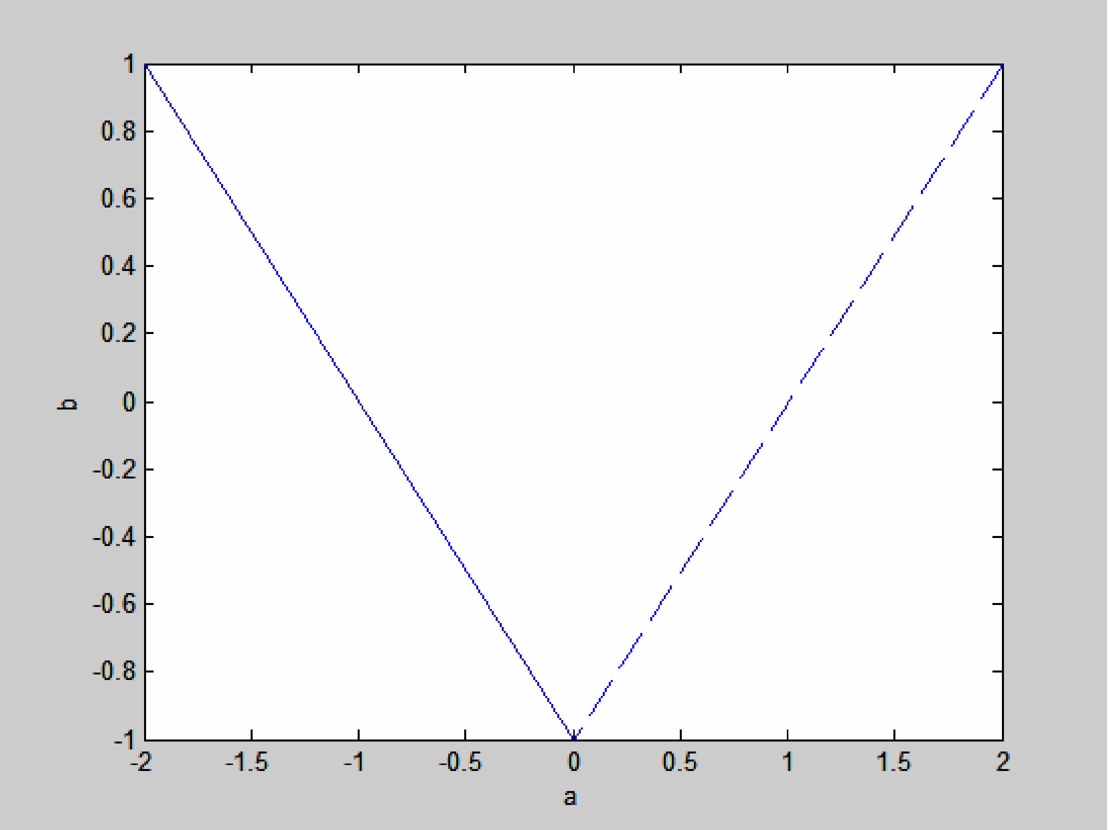

Figure 2

5. The family of 3rd order Linear 3-step Methods

If the order $p=3$, then $C_0=C_1=C_2=C_3=0$. Therefore, we have,

(5.1)
$$\alpha_0+\alpha_1+\alpha_2+\alpha_3=0$$
$$\alpha_1+2\alpha_2+3\alpha_3=\beta_0+\beta_1+\beta_2+\beta_3$$
$$\alpha_1+4\alpha_2+9\alpha_3=2(\beta_1+2\beta_2+3\beta_3)$$
$$\alpha_1+8\alpha_2+27\alpha_3=3(\beta_1+4\beta_2+9\beta_3)$$

and the error constant is given by

(5.2) $$C_4=(\alpha_1+16\alpha_2+81\alpha_3)/24-(\beta_1+8\beta_2+27\beta_3)/6$$

Using (4.1) α_j , $j = 0,1,2,3$ can be written as

$$\alpha_3 = 1$$
$$\alpha_2 = -1 - a \tag{5.3}$$
$$\alpha_1 = a + b$$
$$\alpha_0 = -b$$

While β_j's can be related as

$$\beta_0 + \beta_1 + \beta_2 + \beta_3 = 1 - a + b$$
$$2(\beta_1 + 2\beta_2 + 3\beta_3) = 5 - 3a + b \tag{5.4}$$
$$3(\beta_1 + 4\beta_2 + 9\beta_3) = 19 - 7a + b$$

In these 3 equations there are 4 β's. So to solve β_j in terms of $a, b,$ we introduce another parameter c by putting

$$\beta_3 = c \tag{5.5}$$

So by (5.3) and by solving (5.4) & (5.5) we obtain

$$p = 3$$
$$\alpha_3 = 1$$
$$\alpha_2 = -1 - a$$
$$\alpha_1 = a + b$$
$$\alpha_0 = -b \tag{5.6}$$
$$\beta_3 = c$$
$$\beta_2 = (23 - 5a - b - 36c)/12$$
$$\beta_1 = (-4 - 2a + 2b + 9c)/3$$
$$\beta_0 = (5 + a + 5b - 12c)/12$$

and the error constant (5.2) becomes

$$C_4 = (9 + a + b)/24 - c \tag{5.7}$$

Choosing (a, b) freely from the region shown in Figure 2 and taking c arbitrarily we can obtain all possible zero-stable 3-step linear multistep methods of order 3.

6. Stiffly stable linear 3-step methods

By using Routh-Hurwitz Criterion it can be shown that 3-step methods are stiffly stable if (a, b) lies in the triangular region V bounded by dashed lines in Figure 3 and c satisfies the inequality:

$$0 < (a - b + 11)/24 < c < (a - b + 11)/24 + (1 - b)(1 + 2a + b)/(6(1 - a + b)) . \tag{6.1}$$

Example 1: It is seen that for BDF method $a = 7/11,$ $b = 2/11$ and $c = 6/11$. Clearly (7/11,2/11) lies in V and for this point (6.1) becomes

$$21/44 < 21/44 + 27/44 = 48/44$$

.

$c = 6/11$ clearly satisfies this inequality. Hence 3-step BDF method is stiffly stable. The stability region of this method is the exterior of the simply closed curve shown in Figure 4.

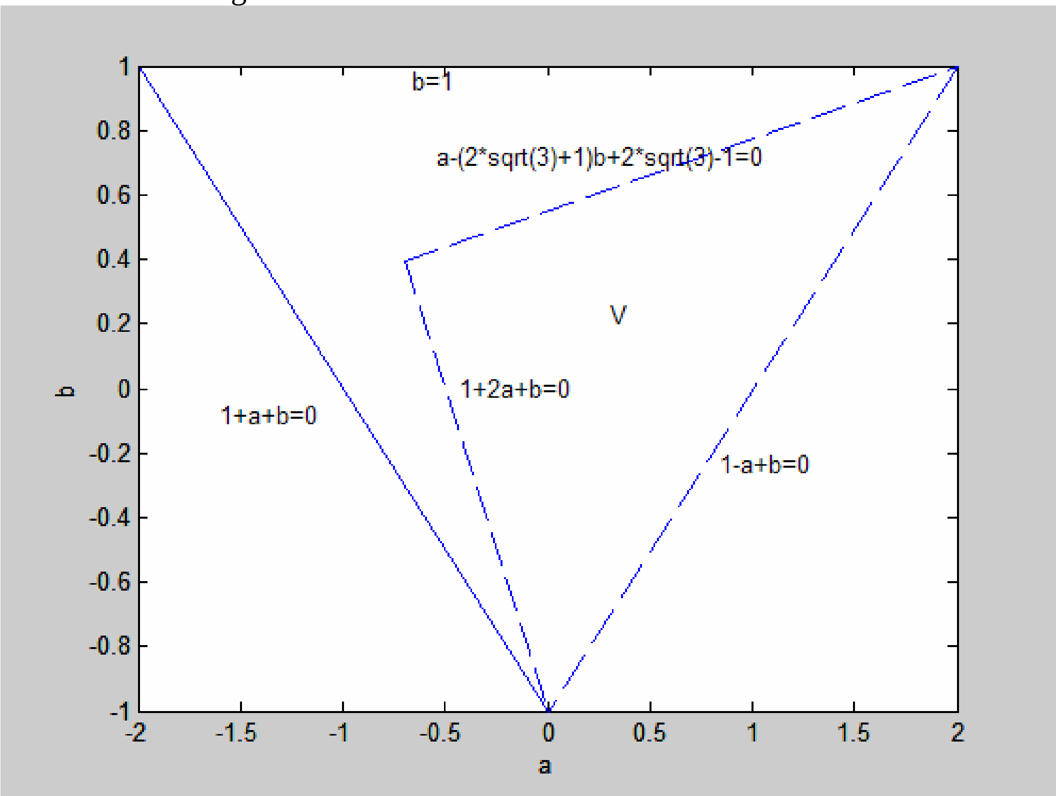

Figure 3

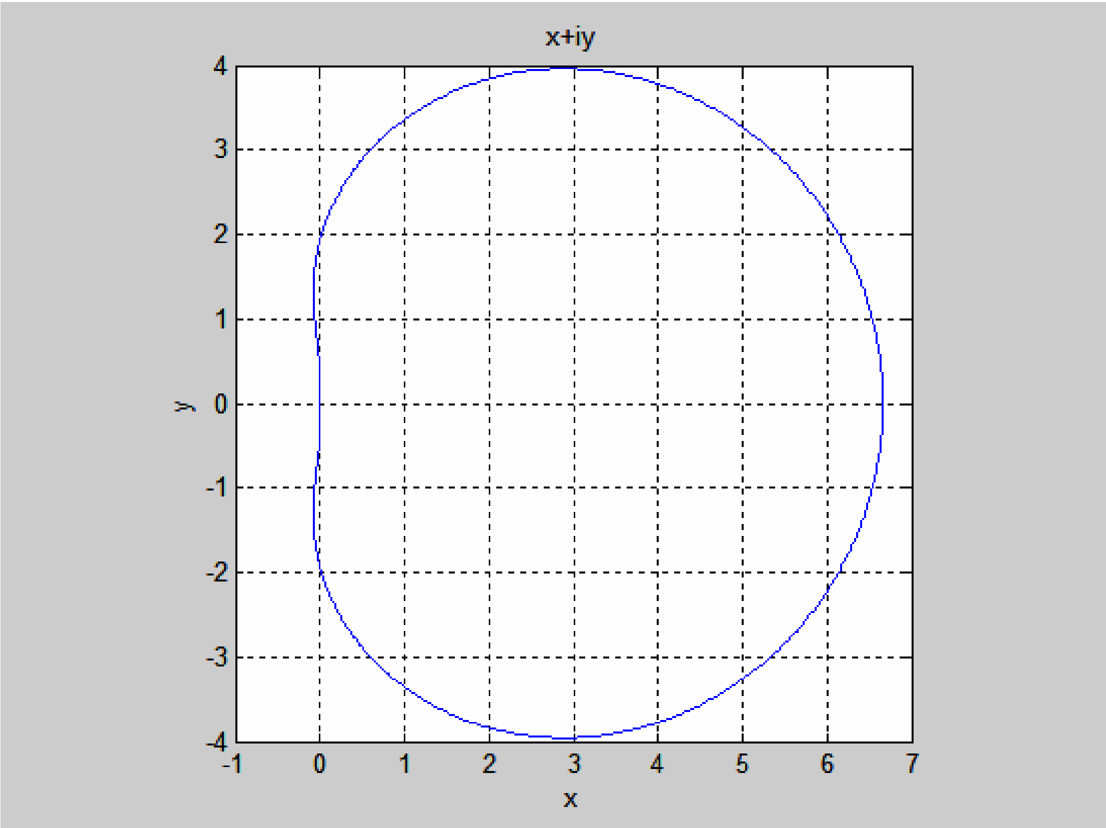

Figure 4

7. Example of danger of too stable methods: Methods like BDF which has small region of instability (see Figure 4) are some times dangerous to some stiff problems. Lindberg (see [1]) described two test problems in which the eigenvalues changes from large negative values to large positive values. We consider one problem here which is:

$$
\begin{aligned}
y_1' &= 10^4 y_1 y_3 + 10^4 y_2 y_4 , & y_1(0) &= 1 \\
y_2' &= -10^4 y_1 y_4 + 10^4 y_2 y_3 , & y_2(0) &= 1 \\
y_3' &= 1 - y_3 , & y_3(0) &= -1 \\
y_4' &= -y_4 - 0.5 y_3 + 0.5 , & y_4(0) &= 0.
\end{aligned}
$$

The exact solution of this problem can be characterized in the following way:

$$
\begin{aligned}
y_3(t) &= 1 - 2e^{-t} \\
y_4(t) &= te^{-t} .
\end{aligned}
$$

If we set $y = [y_1, y_2]^T$, then $y' = A(t)y$ and $y(0) = [1,1]^T$, where

$$
A(t) = 10^4 \begin{bmatrix} 1 - 2e^{-t} & te^{-t} \\ -te^{-t} & 1 - 2e^{-t} \end{bmatrix} .
$$

The eigenvalues of $A(t)$ are

$$
\lambda_{1,2} = 10^4 [(1 - 2e^{-t}) \pm ite^{-t}] .
$$

So initially the eigenvalues are -10^4 and approach to 10^4 as $t \to \infty$. So methods like BDF can not detect the instability of these solutions.

The MATLAB subroutine for stiff problems, namely ODE15S, ODE23S, ODE23T, ODE23TB also could not detect them. With these subroutines the solution of this problem is shown in Figure 5.

But when we use our 3-step method with $a = 1.0, b = 0.1, c = 0.496$ (for example) which has a large instability region (see Figure 6), (with step size $h = 0.1$, for example) the instability of the problem is detected (see Figure 7).

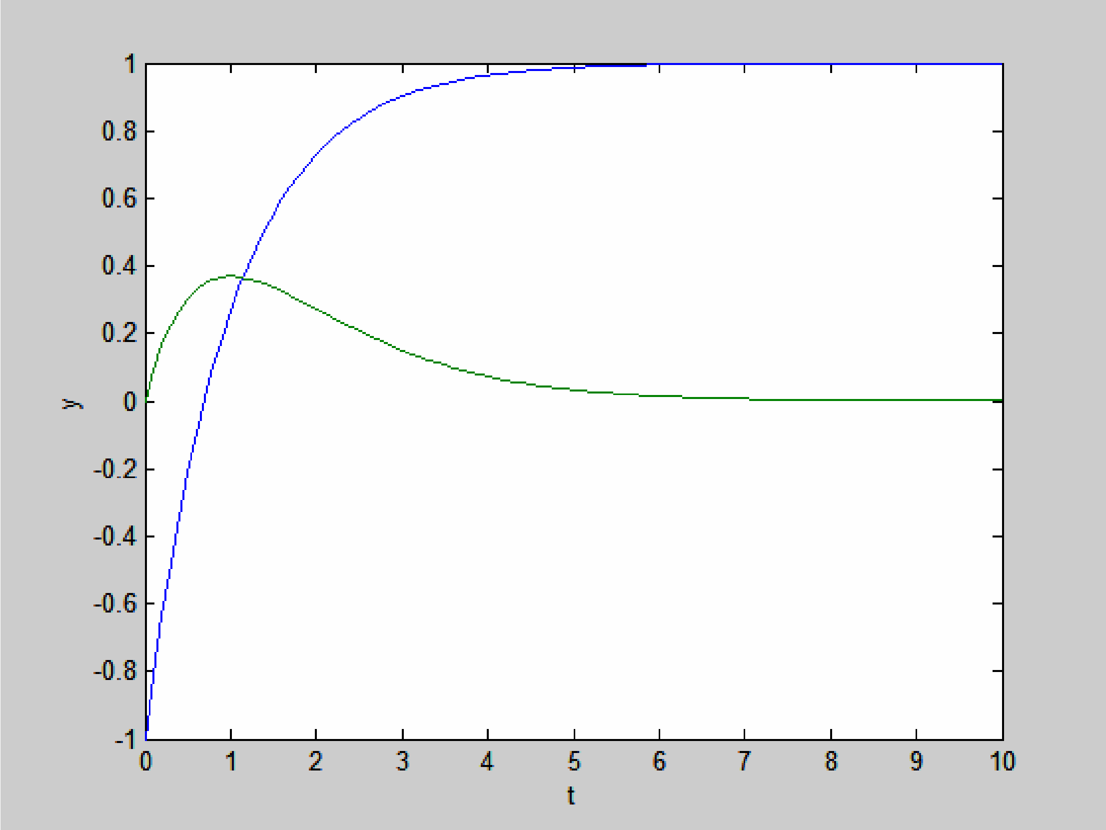

Figure 5

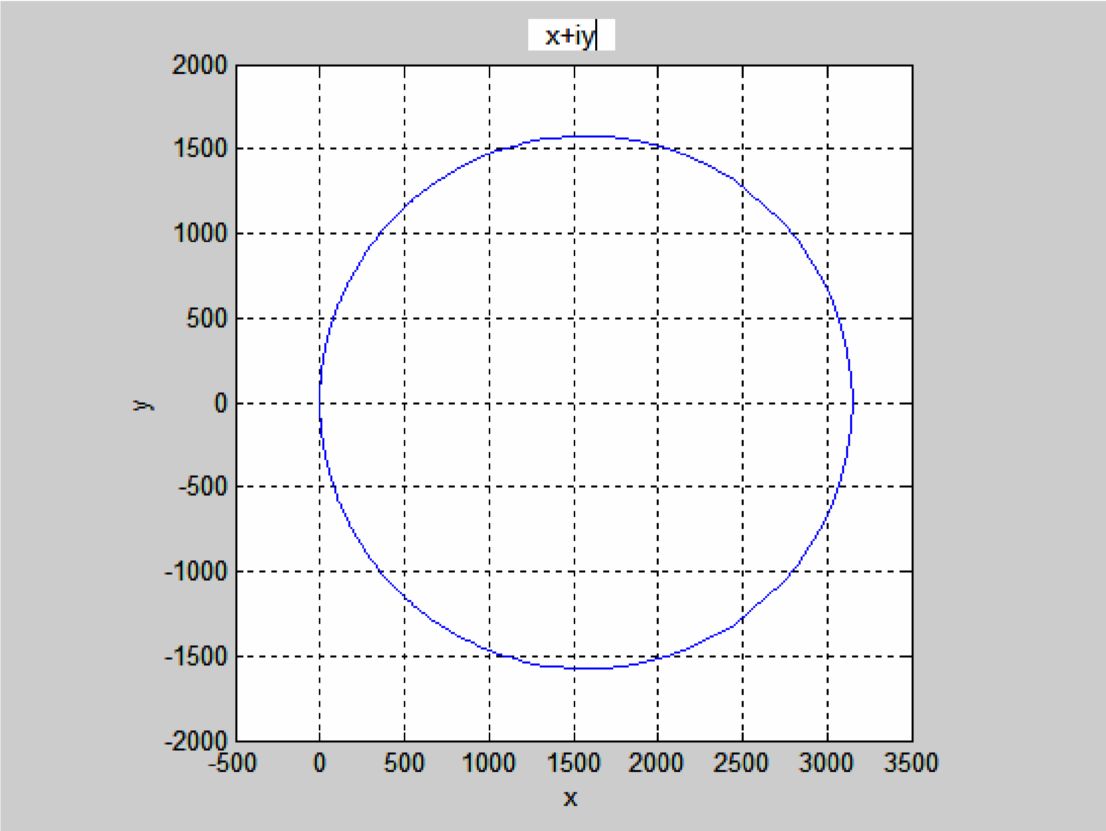

Figure 6

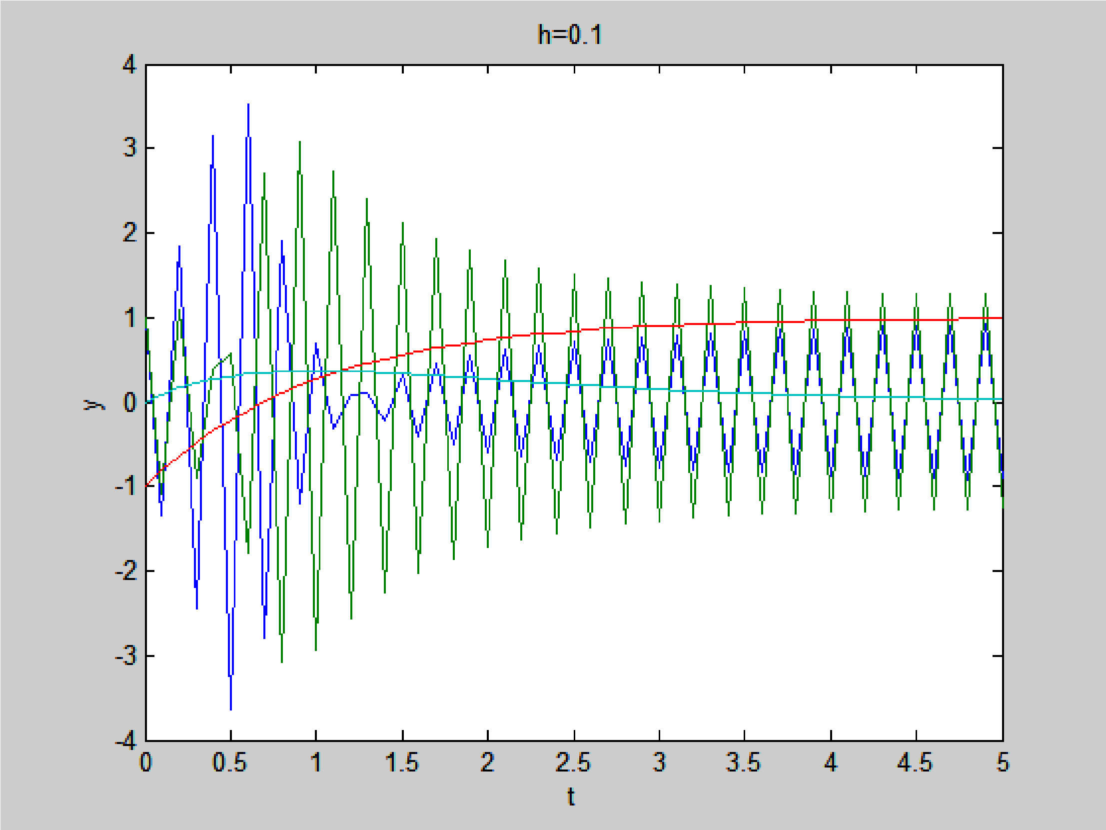

Figure 7

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Reference:

[1]. B. Lindberg, "On a Dangerous Property of Methods for Stiff Differential Equations", BIT, **14** (1974), pp 430-436.