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Numerical simulation of free boundary problems in quadruple precision arithmetic using explicit schemes

Dedicated to the sixtieth birthday of Professor Hideo Kawarada

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1. Introduction

A free boundary problem is a problem whose domain is unknown. We can see many problems in practical phenomena as free boundary problems. They are nonlinear, so numerical simulations are inevitable in analysis. Numerical methods for free boundary problems have been developed and improved, so their numerical simulations are not so difficult recently. However, investigation on reliability of numerical results is not easy. Reliability is usually checked by comparing numerical results obtained in different precision. In the check distinction between round-off error and truncation error is very important. Normal numerical simulations are carried out in double precision arithmetic, so round-off error can be reduced by using quadruple precision arithmetic. In the paper a numerical method which realize numerical simulations of free boundary problems in quadruple precision arithmetic is considered.

In numerical simulations FDM or FEM are very popular as descretization methods. However, changing order is not easy in these methods. From this view point spectral methods are convenient. Numerical methods using spectral collocation methods in space and time were developed to free boundary problems[2-3]. In the methods order can be set easily and arbitrary[3]. However, the methods are implicit in time, so they need adequate iterative methods and they cost much[4]. This means that they are not easily applicable to higher dimensional free boundary problems.

In the paper a numerical method to free boundary problems which is explicit in time and realize numerical simulations in quadruple precision arithmetic is considered.

2. Numerical method

2.1. Higher order explicit scheme

As for accurate simulations of free boundary problems a method which consits of a fixed domain method and spectral collocation methods in space and time was developed. The method realizes arbitrary order in space and time[2-3]. This is advantageous for accuracy. However, it is implicit in time, so it needs adequate iterarive methods and it costs much[4]. This means that it is not easily applicable to higher dimensional free boundary problems. Hence in the paper an explicit method is considered.

Here it should be remarked that many time evolutional free boundary problems have time evolutional equations of motion of the free boudaries like the Stefan condition. This means that it is possible to apply the Runge-Kutta method. As is written in the previous section our purpose is development of numerical methods for the quadruple precision arithmetic. Therefore, usual Runge-Kutta methods are not available. Higher order Runge-Kutta methods are necessary. As for descretization in space spectral collocation methods are used. They are not applicable to free boundary problems directly. So, a fixed domain method using mapping functions is combined.

The concrete procedure of the above method will be shown in its application to test problems.

2.2. Test problem

We cosider the following one-dimensional free boundary problem as a test problem. This problem is related to the free boundary problem describing the pattern formation in diblock copolymer[6]. Here we should remark that our approach is not limited to this problem.

Test Problem(N-N) : Find $s(t)$ and $u(x,t)$ such that

$$\begin{cases} \dfrac{d}{dt}s(t) & = F(s(t),t) \quad t>0 \\ s(0) & = -\dfrac{1}{2} \end{cases}$$

where

$$F(s(t),t) \equiv -u_x^+(s(t),t) \ + \ u_x^-(s(t),t)$$

$$\begin{cases} u_{xx}^+(x,t) & = -2\dfrac{t+\frac{11}{4}}{t+2} & & in\ (-1,s(t))\times t>0 \\ u_{xx}^-(x,t) & = 2\dfrac{t+\frac{3}{4}}{t+2} & & in\ (s(t),1)\times t>0 \\ u_x^+(-1,t) & = u_x^-(1,t)=0 & \textbf{(Neumann-Neumann B.C.)} & for\ t>0 \\ u^+(s(t),t) & = u^-(s(t),t)=0 & & for\ t>0 \end{cases}$$

$$\begin{cases} u^+(x,0) = -\dfrac{11}{8}(x+\dfrac{1}{2})(x+\dfrac{3}{4}) & in\ (-1,s(0)) \\ u^-(x,0) = \dfrac{3}{8}(x+\dfrac{1}{2})(x-\dfrac{5}{2}) & in\ (s(0),1) \end{cases}$$

We also consider two more problems Test Problem(N-D) and Test Problem(D-D) by replacing (Neumann - Neumann B.C.) by the following boundary conditions (Neumann - Dirichlet B.C.) or (Dirichlet - Dirichlet B.C.), respectively.

(Neumann-Dirichlet B.C.):

$$\begin{aligned} u_x^+(-1,t) &= 0 && \textit{for} \quad t>0 \\ u^-(1,t) &= -\frac{(t+\frac{3}{4})(t+3)^2}{(t+2)^3} && \textit{for} \quad t>0 \end{aligned}$$

(Dirichlet-Dirichlet B.C.):

$$\begin{aligned} u^+(-1,t) &= \frac{(t+\frac{11}{4})(t+1)^2}{(t+2)^3} && \textit{for} \quad t>0 \\ u^-(1,t) &= -\frac{(t+\frac{3}{4})(t+3)^2}{(t+2)^2} && \textit{for} \quad t>0 \end{aligned}$$

Exact solutions to these test problems are same and given as follows:

$$\begin{cases} s(t) &= -\dfrac{1}{t+2} & \textit{for} \quad t \geq 0 \\ u^+(x,t) &= -\dfrac{t+\frac{11}{4}}{t+2}(x-s(t))(x+2+s(t)) & \textit{in } [-1,s(t)] \times t \geq 0 \\ u^-(x,t) &= \dfrac{t+\frac{3}{4}}{t+2}(x-s(t))(x-2+s(t)) & \textit{in } [s(t),1] \times t \geq 0 \end{cases}$$

2.3. Fixed domain method

Descretization in space is performed by using spectral collocation methods. Here we should remark that they are applicable only in the interval for one-dimensional problems (or in the rectangular domain for higher dimensional problems). So they are applied after mapping the unknown domain of the problem into the interval $[-1,1]$ [2,5]. Test Problems have two intervals $[-1,s(t)]$ and $[s(t),1]$ separated by the free boundary, so these two intervals are mapped into $[-1,1]$ by different mapping functions. The mapping functions are given as follows:

$$t = \tau \quad \textit{for} \quad \tau \geq 0$$

$$\begin{cases} x^+_{\xi^+\xi^+}(\xi^+,\tau) &= 0 & \textit{in } (-1,1) \times \tau \geq 0 \\ x^+(-1,\tau) &= -1 & \textit{for } \tau \geq 0 \\ x^+(1,\tau) &= s(\tau) & \textit{for } \tau \geq 0 \end{cases}$$

$$\begin{cases} x^-_{\xi^-\xi^-}(\xi^-,\tau) &= 0 & \textit{in } (-1,1) \times \tau \geq 0 \\ x^-(-1,\tau) &= s(\tau) & \textit{for } \tau \geq 0 \\ x^-(1,\tau) &= 1 & \textit{for } \tau \geq 0 \end{cases}$$

Here we should remark that mapping functions on spatial variables are given as solutions of boundary value problems. This method is called numerical grid generation[8]. These boundary value problems are one-dimensional, so we can solve them exactly. However, our purpose is development of methods for higher dimensional free boundary problems. Hence we solve them numerically. Using these mapping functions Test Problem(N-N) is transformed into the following fixed boundary problem.

Test Problem(N-N)′ :

$$\begin{cases} \dfrac{d}{d\tau}s(\tau) & = F(s(\tau),\tau) \\ s(0) & = -\dfrac{1}{2} \end{cases}$$

where

$$F(s(\tau),t) \equiv \frac{1}{x^+_{\xi^+}(1,\tau)}u^+_{\xi^+}(1,\tau) + \frac{1}{x^-_{\xi^-}(-1,\tau)}u^-_{\xi^-}(-1,\tau) \quad \mathit{for}\ \tau > 0$$

$$\begin{cases} \dfrac{1}{(x^+_{\xi^+})^2}u^+_{\xi^+\xi^+} - \dfrac{x^+_{\xi^+\xi^+}}{(x^+_{\xi^+})^3}u^+_{\xi^+} = -2\dfrac{\tau+\frac{11}{4}}{\tau+2} & \mathit{in}\ (-1,1)\times\tau>0 \\ \dfrac{1}{(x^-_{\xi^-})^2}u^-_{\xi^-\xi^-} - \dfrac{x^-_{\xi^-\xi^-}}{(x^-_{\xi^-})^3}u^-_{\xi^-} = 2\dfrac{\tau+\frac{3}{4}}{\tau+2} & \mathit{in}\ (-1,1)\times\tau>0 \\ u^+_{\xi^+}(-1,\tau) = u^-_{\xi^-}(1,\tau) = 0 & \mathit{for}\ \tau>0 \\ u^+(1,\tau) = u^-(-1,\tau) = 0 & \mathit{for}\ \tau>0 \end{cases}$$

$$\begin{cases} u^+(\xi^+,0) = -\dfrac{11}{8}\left(x^+(\xi^+,0)+\dfrac{1}{2}\right)\left(x^+(\xi^+,0)+\dfrac{3}{4}\right) & \mathit{in}\ (-1,s(0)) \\ u^-(\xi^-,0) = \dfrac{3}{8}\left(x^-(\xi^-,0)+\dfrac{1}{2}\right)\left(x^-(\xi^-,0)-\dfrac{5}{2}\right) & \mathit{in}\ (s(0),1) \end{cases}$$

We solve this using spectral collocation methods in space and the higher order Runge-Kutta method in time. Test Problems (N-D) and (D-D) are solved in the same way.

2.4. Higher order Runge-Kutta method

The Runge-Kutta method is very popular in numerical computations of a system of ordinary differential equations. Usually the fourth order formula is used, however it is not adequate here. This is because that our purpose is numerical simulations in quadruple precision arithmetic. So we use higher order Runge-Kutta methods. There are many formulae[7]. Here we adopt formulae with the wide stable region and coefficients given by fractions. The followings are formulae used here.

4th order Runge-Kutta method :

$$\begin{aligned} k_1 &= \Delta t \times F(t_n, y_n) \\ t_i &= \sum_{j=1}^{i-1} B(i,j)k_j \qquad (i = 2,\ldots,4) \end{aligned}$$

$$
\begin{aligned}
k_i &= \Delta t \times F(t_n + a(i)\Delta, y_n + t_i) \quad (i = 2, \ldots, 4) \\
y_{n+1} &= y_n + \sum_{i=1}^{4} C(i) k_i
\end{aligned}
$$

where

$$
\begin{array}{llll}
a(2) = \frac{1}{2} & B(2,1) = \frac{1}{2} & B(4,1) = 0 & C(1) = \frac{1}{6} \\
a(3) = \frac{1}{2} & B(3,1) = 0 & B(4,2) = 0 & C(2) = \frac{1}{3} \\
a(4) = 1 & B(3,2) = \frac{1}{2} & B(4,3) = 1 & C(3) = \frac{1}{3} \\
 & & & C(4) = \frac{1}{6}
\end{array}
$$

6th Runge-Kutta method(Verner formula) :

$$
\begin{aligned}
k_1 &= \Delta t \times F(t_n, y_n) \\
t_i &= \sum_{j=1}^{i-1} B(i,j) k_j \qquad (i = 2, \ldots, 8) \\
k_i &= \Delta t \times F(t_n + a(i)\Delta, y_n + t_i) \quad (i = 2, \ldots, 8) \\
y_{n+1} &= y_n + \sum_{i=1}^{8} C(i) k_i
\end{aligned}
$$

where

$$
\begin{array}{lllll}
a(2) = \frac{1}{18} & B(2,1) = \frac{1}{18} & B(6,1) = -\frac{369}{73} & B(8,1) = \frac{3015}{256} & C(1) = \frac{57}{640} \\
a(3) = \frac{1}{6} & B(3,1) = -\frac{1}{12} & B(6,2) = \frac{72}{73} & B(8,2) = -\frac{9}{4} & C(2) = 0 \\
a(4) = \frac{2}{9} & B(3,2) = \frac{1}{4} & B(6,3) = \frac{5380}{219} & B(8,3) = -\frac{4219}{78} & C(3) = -\frac{16}{65} \\
a(5) = \frac{2}{3} & B(4,1) = -\frac{2}{81} & B(6,4) = -\frac{12285}{584} & B(8,4) = \frac{5985}{128} & C(4) = \frac{1377}{2240} \\
a(6) = 1 & B(4,2) = \frac{4}{27} & B(6,5) = \frac{2695}{1752} & B(8,5) = -\frac{539}{384} & C(5) = \frac{121}{320} \\
a(7) = \frac{8}{9} & B(4,3) = \frac{8}{81} & B(7,1) = -\frac{8716}{891} & B(8,6) = 0 & C(6) = 0 \\
a(8) = 1 & B(5,1) = \frac{40}{33} & B(7,2) = \frac{656}{297} & B(8,7) = \frac{693}{3328} & C(7) = \frac{891}{8320} \\
 & B(5,2) = -\frac{4}{11} & B(7,3) = \frac{39520}{891} & & C(8) = \frac{2}{35} \\
 & B(5,3) = -\frac{56}{11} & B(7,4) = -\frac{416}{11} & & \\
 & B(5,4) = -\frac{54}{11} & B(7,5) = \frac{52}{27} & & \\
 & & B(7,6) = 0 & &
\end{array}
$$

8th order Runge-Kutta method(Verner formula) :

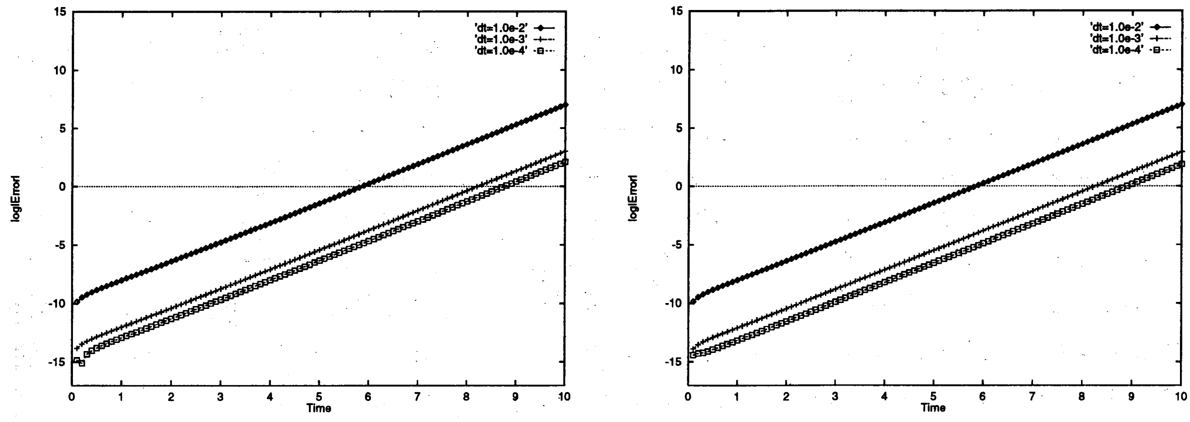
$$
\begin{aligned}
k_1 &= \Delta t \times F(t_n, y_n) \\
t_i &= \sum_{j=1}^{i-1} B(i,j) k_j \qquad (i = 2, \ldots, 13) \\
k_i &= \Delta t \times F(t_n + a(i)\Delta, y_n + t_i) \quad (i = 2, \ldots, 13) \\
y_{n+1} &= y_n + \sum_{i=1}^{13} C(i) k_i
\end{aligned}
$$

where

$a(2) = \frac{1}{4}$	$B(2,1) = \frac{1}{4}$	$B(9,1) = \frac{17176}{25515}$	$B(12,1) = -\frac{27061}{204120}$	$C(1) = \frac{31}{720}$
$a(3) = \frac{1}{12}$	$B(3,1) = \frac{5}{72}$	$B(9,2) = 0$	$B(12,2) = 0$	$C(2) = 0$
$a(4) = \frac{1}{8}$	$B(3,2) = \frac{1}{72}$	$B(9,3) = 0$	$B(12,3) = 0$	$C(3) = 0$
$a(5) = \frac{2}{5}$	$B(4,1) = \frac{1}{32}$	$B(9,4) = -\frac{47104}{25515}$	$B(12,4) = \frac{40448}{280665}$	$C(4) = 0$
$a(6) = \frac{1}{2}$	$B(4,2) = 0$	$B(9,5) = \frac{1325}{504}$	$B(12,5) = -\frac{1353775}{1197504}$	$C(5) = 0$
$a(7) = \frac{6}{7}$	$B(4,3) = \frac{3}{32}$	$B(9,6) = -\frac{41792}{25515}$	$B(12,6) = \frac{17662}{15515}$	$C(6) = \frac{16}{75}$
$a(8) = \frac{1}{7}$	$B(5,1) = \frac{106}{125}$	$B(9,7) = \frac{20237}{145800}$	$B(12,7) = -\frac{71687}{1166400}$	$C(7) = \frac{16807}{79200}$
$a(9) = \frac{2}{3}$	$B(5,2) = 0$	$B(9,8) = \frac{4312}{6075}$	$B(12,8) = \frac{98}{225}$	$C(8) = \frac{16807}{79200}$
$a(10) = \frac{2}{7}$	$B(5,3) = -\frac{408}{125}$	$B(10,1) = -\frac{23834}{180075}$	$B(12,9) = \frac{1}{16}$	$C(9) = \frac{243}{1760}$
$a(11) = 1$	$B(5,4) = \frac{352}{125}$	$B(10,2) = 0$	$B(12,10) = \frac{3773}{11664}$	$C(10) = 0$
$a(12) = \frac{1}{3}$	$B(6,1) = \frac{1}{48}$	$B(10,3) = 0$	$B(12,11) = 0$	$C(11) = 0$
$a(13) = 1$	$B(6,2) = 0$	$B(10,4) = -\frac{77824}{1980825}$	$B(13,1) = \frac{11203}{8680}$	$C(12) = \frac{243}{1760}$
	$B(6,3) = 0$	$B(10,5) = -\frac{636635}{633864}$	$B(13,2) = 0$	$C(13) = \frac{31}{720}$
	$B(6,4) = \frac{8}{33}$	$B(10,6) = \frac{254048}{300125}$	$B(13,3) = 0$	
	$B(6,5) = \frac{125}{528}$	$B(10,7) = -\frac{183}{7000}$	$B(13,4) = -\frac{38144}{11935}$	
	$B(7,1) = -\frac{1263}{2401}$	$B(10,8) = \frac{8}{11}$	$B(13,5) = \frac{2354425}{458304}$	
	$B(7,2) = 0$	$B(10,9) = -\frac{324}{3773}$	$B(13,6) = -\frac{84046}{16275}$	
	$B(7,3) = 0$	$B(11,1) = \frac{12733}{7600}$	$B(13,7) = \frac{673309}{1636800}$	
	$B(7,4) = \frac{39936}{26411}$	$B(11,2) = 0$	$B(13,8) = \frac{4704}{8525}$	
	$B(7,5) = -\frac{64125}{26411}$	$B(11,3) = 0$	$B(13,9) = \frac{9477}{8525}$	
	$B(7,6) = \frac{5520}{2401}$	$B(11,4) = -\frac{20032}{5225}$	$B(13,10) = -\frac{1029}{992}$	
	$B(8,1) = \frac{37}{392}$	$B(11,5) = \frac{456485}{80256}$	$B(13,11) = 0$	
	$B(8,2) = 0$	$B(11,6) = -\frac{42599}{7125}$	$B(13,12) = \frac{729}{341}$	
	$B(8,3) = 0$	$B(11,7) = \frac{339227}{912000}$		
	$B(8,4) = 0$	$B(11,8) = -\frac{1029}{4180}$		
	$B(8,5) = \frac{1625}{9408}$	$B(11,9) = \frac{1701}{1408}$		
	$B(8,6) = -\frac{2}{15}$	$B(11,10) = \frac{5145}{2432}$		
	$B(8,7) = \frac{61}{6720}$			

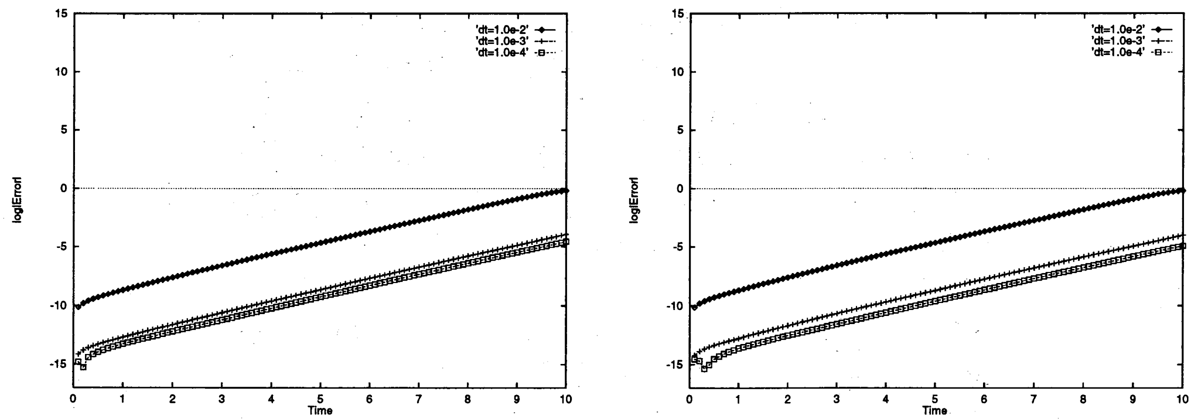
3. Numerical results

Numerical results to Test Problems (N-N),(N-D) and (D-D) are shown here. Gauss-Lobatto collocation points and Chebyshev polynomials are used in the spectral collocation methods[1]. Numerical computations are carried out for several orders in spectral collocation methods and Runge-Kutta methods, in both double and quadruple precision arithmetic. $Error \equiv |s_{exac}(t) - s_{cal}(t)|$ is shown as a function of time t, where $s_{exac}(t)$ is an exact solution and $s_{cal}(t)$ is a computed value. $N+1$ collocation points are used[1]. Numerical computations are carried out on SUN ULTRA.



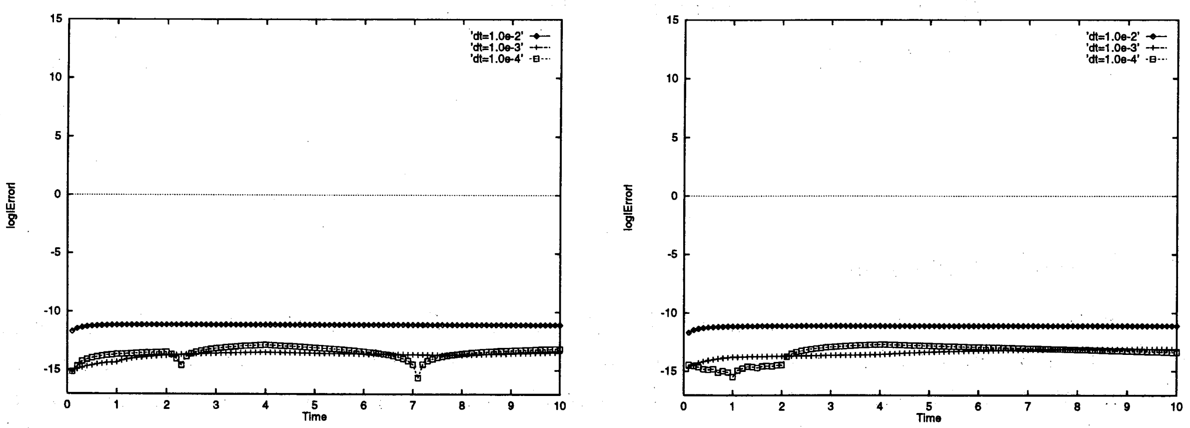
(a) (b)

Figure 1. *Error* for Test Problem(N-N).
Double precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



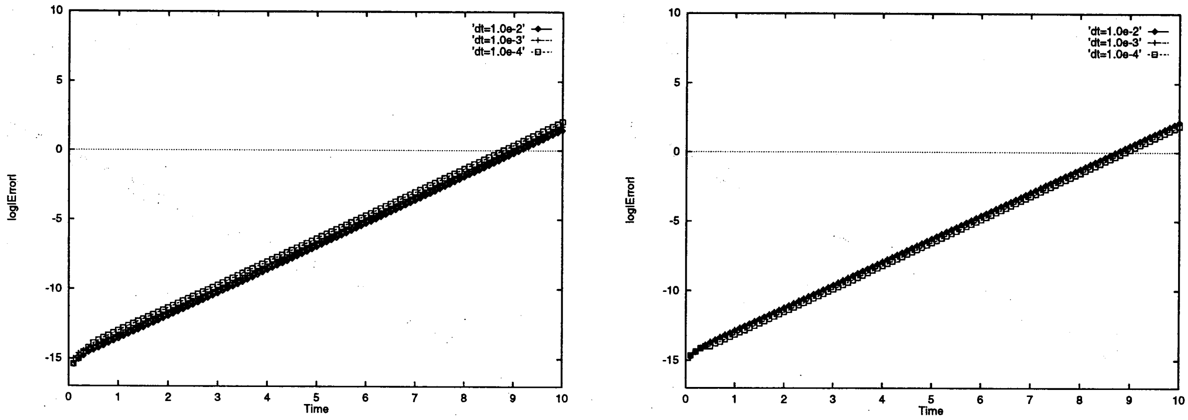
(a) (b)

Figure 2. *Error* for Test Problem(N-D).
Double precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



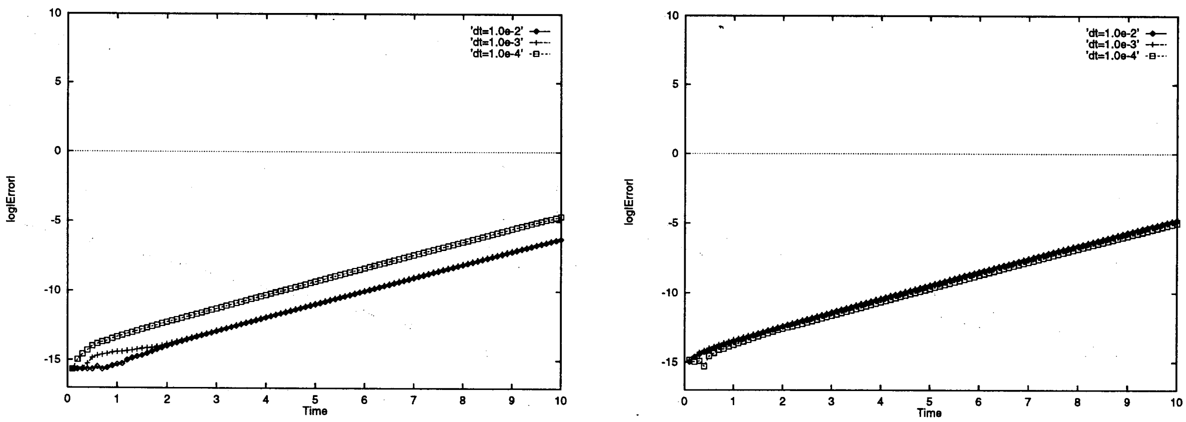
(a) (b)

Figure 3. *Error* for Test Problem(D-D).
Double precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



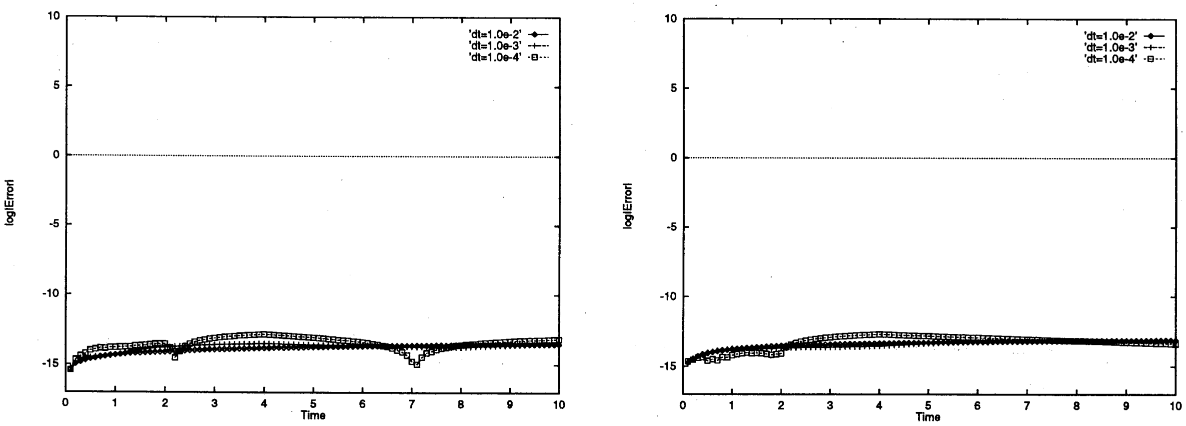
(a) (b)

Figure 4. *Error* for Test Problem(N-N).
Double precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



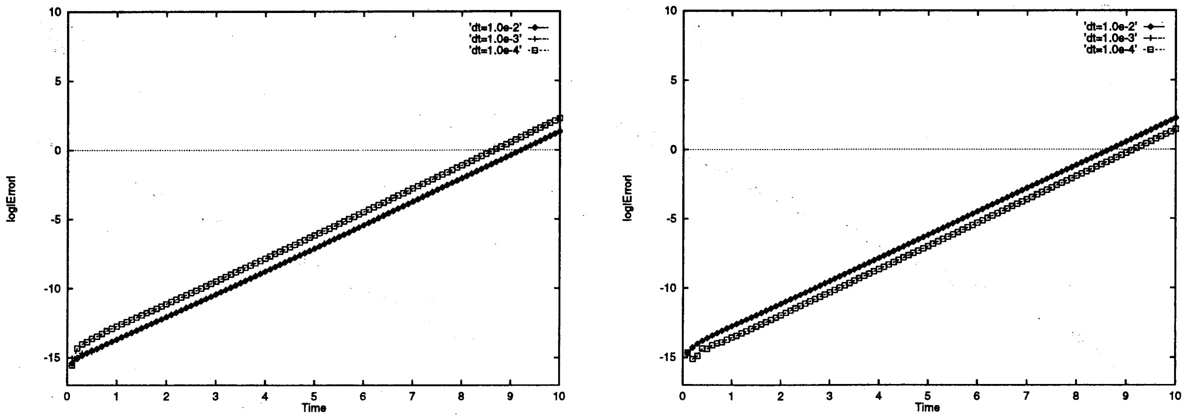
(a) (b)

Figure 5. *Error* for Test Problem(N-D).
Double precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



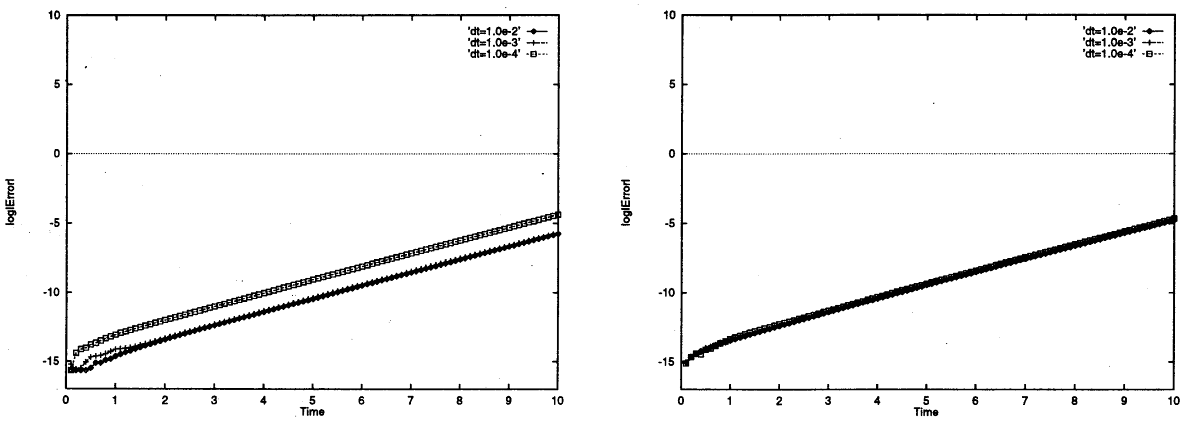
(a) (b)

Figure 6. *Error* for Test Problem(D-D).
Double precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



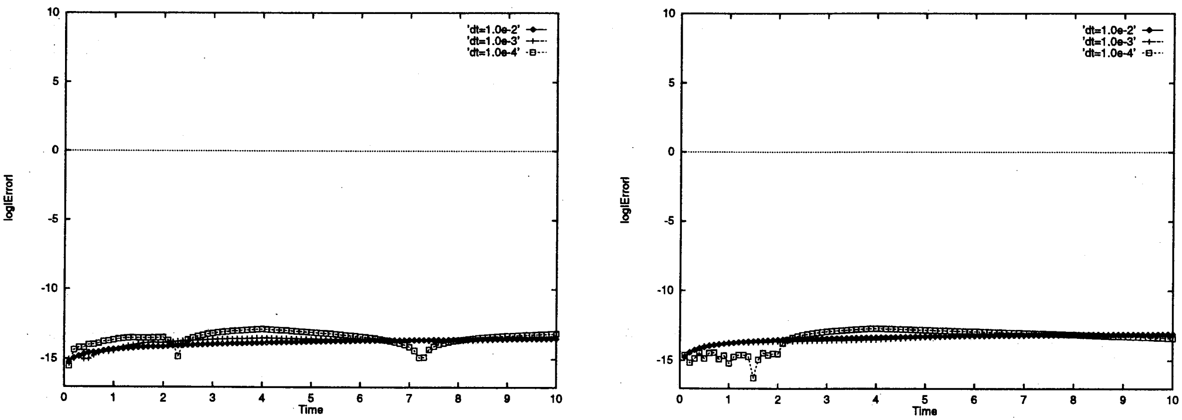
(a) (b)

Figure 7. *Error* for Test Problem(N-N).
Double precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



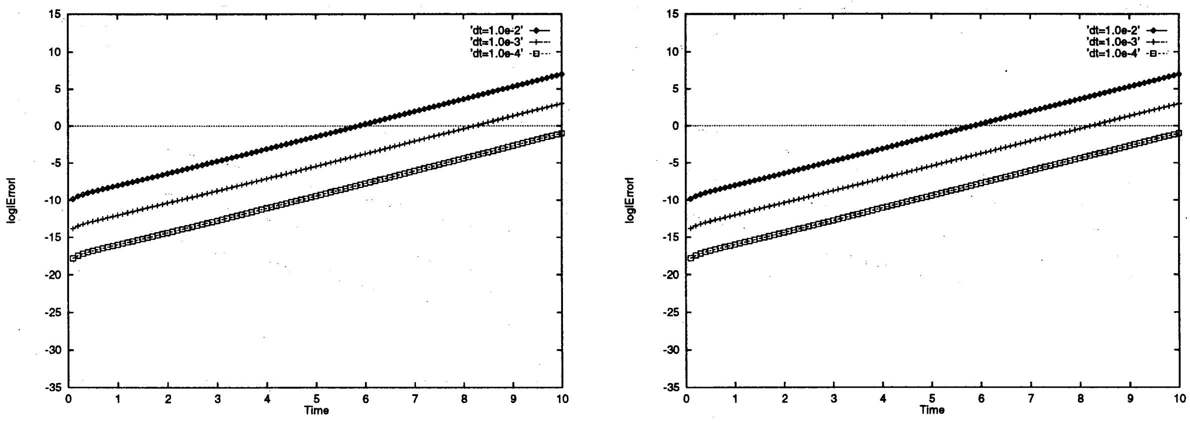
(a) (b)

Figure 8. *Error* for Test Problem(N-D).
Double precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



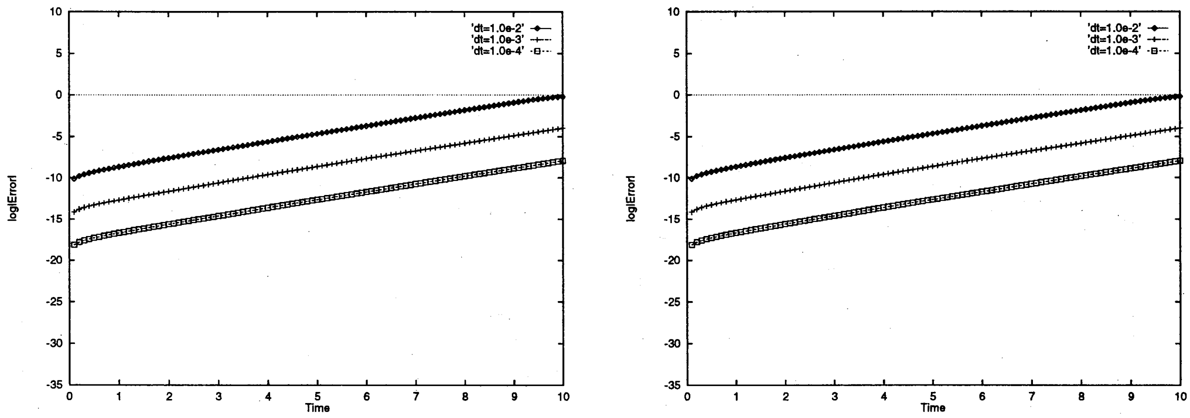
(a) (b)

Figure 9. *Error* for Test Problem(D-D).
Double precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



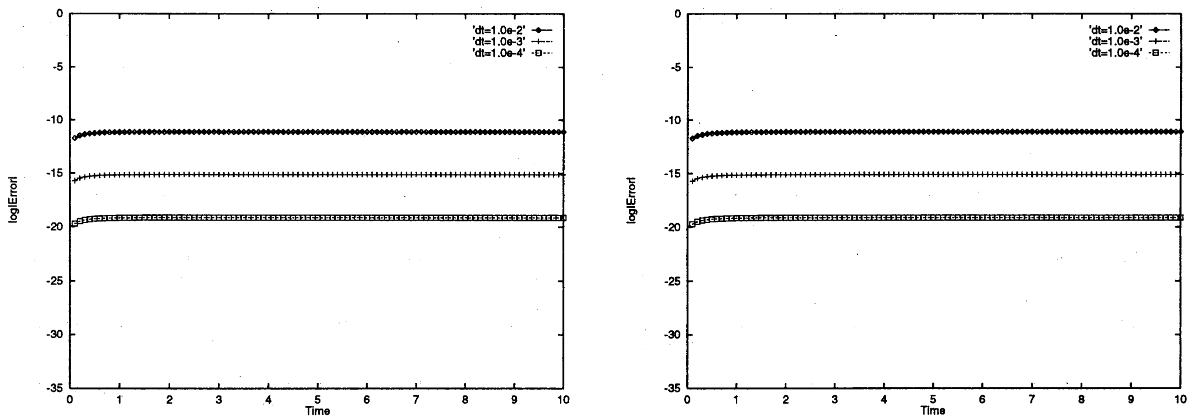
(a) (b)

Figure 10. *Error* for Test Problem(N-N).
Quadruple precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



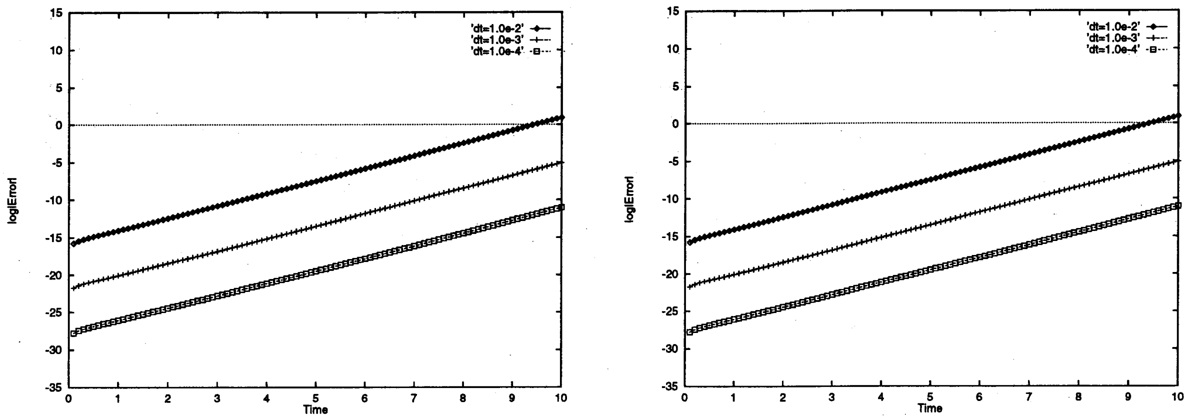
(a) (b)

Figure 11. *Error* for Test Problem(N-D).
Quadruple precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



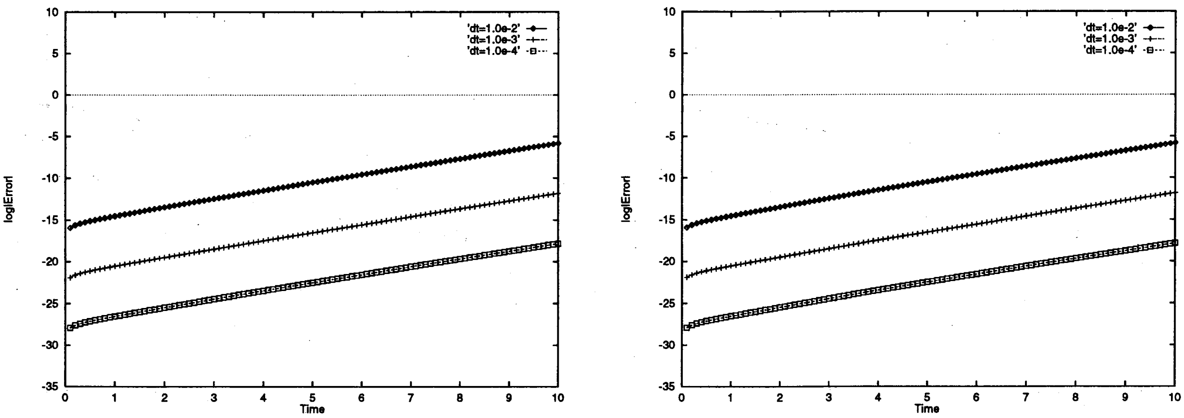
(a) (b)

Figure 12. *Error* for Test Problem(D-D).
Quadruple precision, 4th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



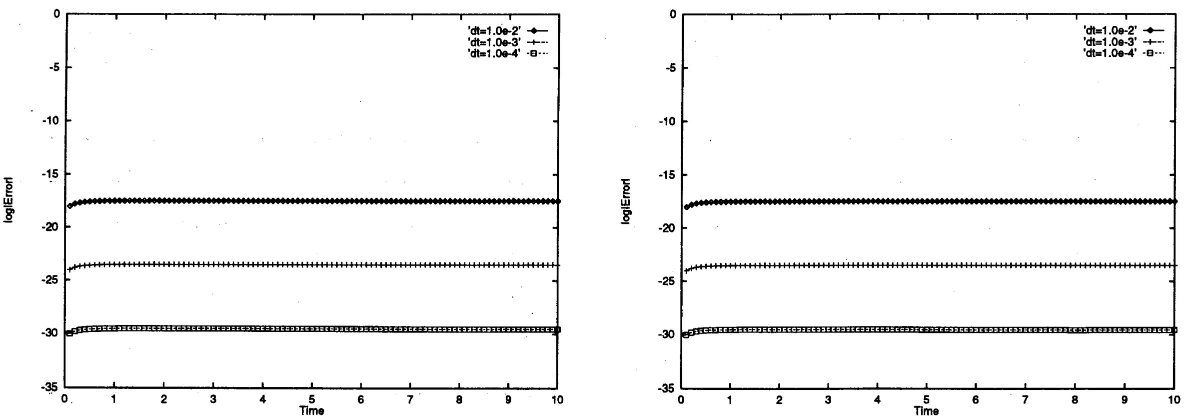
(a) (b)

Figure 13. *Error* for Test Problem(N-N).
Quadruple precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



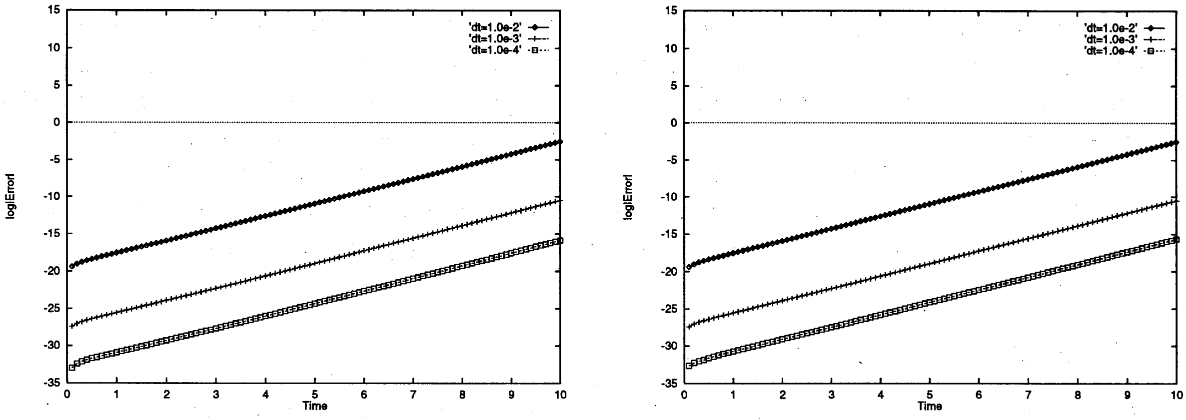
(a) (b)

Figure 14. *Error* for Test Problem(N-D).
Quadruple precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



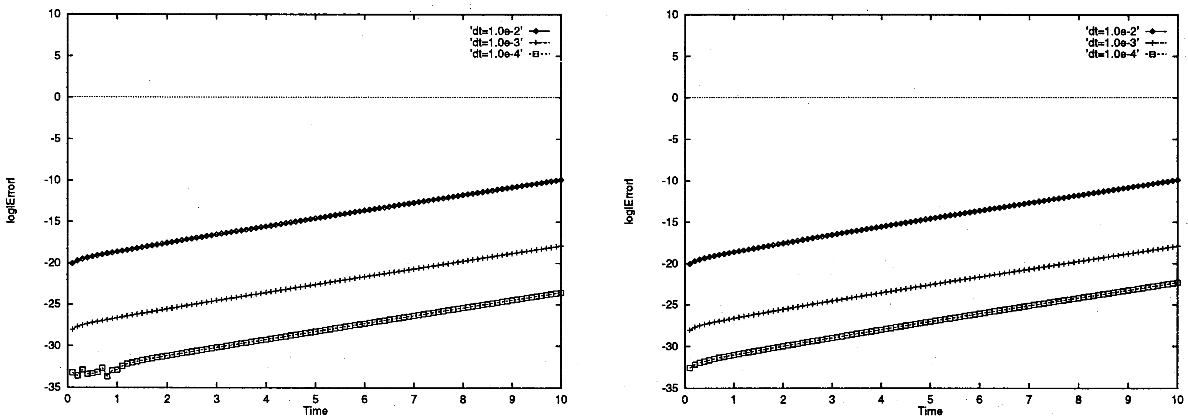
(a) (b)

Figure 15. *Error* for Test Problem(D-D).
Quadruple precision, 6th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



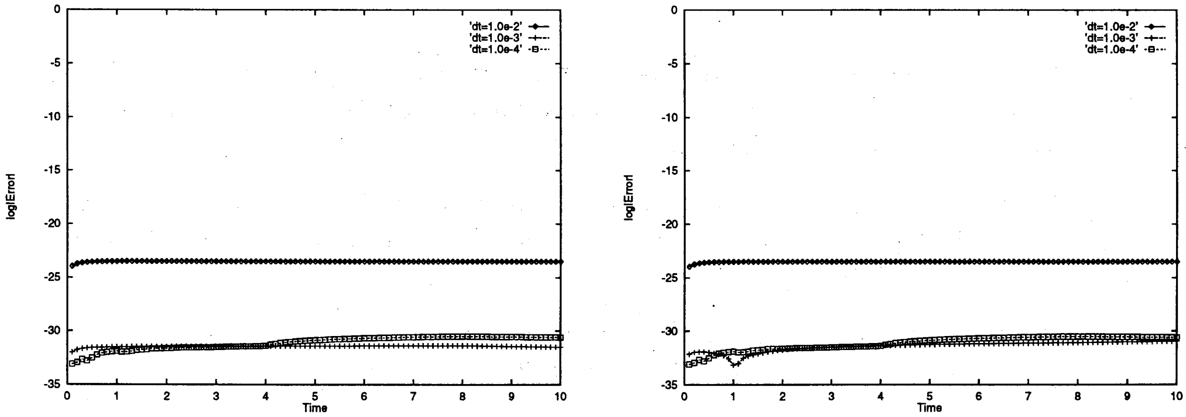
(a) (b)

Figure 16. *Error* for Test Problem(N-N).
Quadruple precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



(a) (b)

Figure 17. *Error* for Test Problem(N-D).
Quadruple precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.



(a) (b)

Figure 18. *Error* for Test Problem(D-D).
Quadruple precision, 8th order Runge-Kutta method, (a) $N = 4$, (b) $N = 6$.

Numerical results in double precision arithmetic are shown in Figures 1-9. They are almost independent of N because spatial order of exact solutions is low. We can see Neumann boundary conditions are delicate in numerical computations. If you do not have any idea in such situations, one answer is to carry out numerical computations in quadruple precision arithmethic.

Numerical results in quadruple precision arithmetic are shown in Figures 10-18. They are almost satisfactory in accuracy. Of course additional considerations are necessary if you need to carry out longer numerical computations for Nuemann boundary conditions.

4. Conclusion

In the paper a numerical method which is explicit and realize numerical simulations of free boundary problems in quadruple precision arithmethic is presented. It consists of a fixed domain method using mapping functions, spectral collocation methods in space and Runge-Kutta methods in time. For evaluation of our method one-dimensional free boundary problems whose exact solutions are known are solved. Numerical results are satisfactory in accuracy. Here we should remark that test problems are one-dimensional, however our method is applicable to higher dimensional free boundary problems.

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