UNIVERSIDADE DE SÃO PAULO

INSTITUTO DE FÍSICA
CAIXA POSTAL 66318
05315-970 SÃO PAULO - SP
BRASIL

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NONLINEAR DELAY DIFFERENTIAL EQUATIONS: COMPARISON OF INTEGRATION METHODS

C.P. Malta and **M.L.S. Teles**

Instituto de Física, Universidade de São Paulo

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Nonlinear delay differential equations: comparison of integration methods.

C. P. Malta and M. L. S. Teles
Universidade de São Paulo
Instituto de Física
CP 66318, 05315-970 São Paulo, SP, Brazil

Abstract

We compare the performance of the methods of Gear and Runge-Kutta (4th order) for integrating delay differential equations. For the equation considered by us, the Gear method is in general more efficient (convergence is achieved for a step that is greater or equal to the step required by the method of Runge-Kutta). Our results show that the convergence of the solution has to be verified always as a small change of one of the parameters can result in non-convergence for the same step value.

1 Introduction

Delay differential equations (DDE) are used to describe systems involving a time delay, that is, the future evolution depends on the past history of the system. Processes involving time delays are fairly ubiquitous: they are found in physics, biology, medicine, economics, chemistry, engineering, etc. In general, the dynamics of a DDE is more complex than that of its related ordinary differential equation (ODE) , obtained by setting the delay equal to zero. This complexity results from the fact that, due to the delay, the DDE's generate infinite dimensional dynamical systems. DDE's have been studied rather extensively (Bellman and Cooke (1963), Hale (1977), Hale and Verduyn-Lunel (1993), Kuang (1993)) but, in general, only numerical solutions can provide detailed information about the behaviour of the system. Therefore, it is important to compare the performance and the reliability of different methods of numerical integration applied to DDEs. It should be stressed that numerical integration involves discretization, thus making the dimension finite. Even in the case of ODE's, it is necessary to be careful because the discretized equation has more solutions than the continuous equation and, only that solution, that does not change when the step is changed, is solution of both the discretized and the continuous equations. In the present work we make a comparison of the predictor-corrector method of Gear, and the method of Runge-Kutta (Cryer (1972), Kahaner *et al* (1989)). In the section 2 we present the numerical integration methods adapted to delay equations. In the section 3 we compare the results of the various methods and in the section 4 we present the conclusion.

2 The numerical integration methods

We considered the following multi-looped, negative feedback, scalar equation, with delays τ_i:

$$\frac{dP}{dt} = \frac{1}{N}\sum_{i=1}^{N} S_i(P(t-\tau_i)) - P(t), \tag{1}$$

where

$$S_i(X) = \frac{(\theta_i)^{n_i}}{(\theta_i)^{n_i} + (X)^{n_i}}, \quad 0 < \theta_i < 1. \tag{2}$$

The parameters θ_i and n_i govern the threshold and the steepness, respectively, of the sigmoidal function S_i. For solving equation (1) for $t > 0$, it is necessary to give, as initial condition, the function $P(t)$ in the interval $-\max(\tau_i) \leq t \leq 0$. The time is discretized using an integration step h. This step is chosen in such a way that, in units of h, the delays τ_i will be given by integer numbers denoted by d_i. The discretized time will be represented by an integer, and we shall use the following notation:

$$P_k = P(h\,k), \tag{3}$$

and for the sigmoidal function (equation (2))

$$S_k = S(P_k). \tag{4}$$

The initial condition for discretized time is:

$$P_k\,, \quad -\max(d_i) \le k \le 0\,. \tag{5}$$

2.1 The method of Gear

This is a predictor-corrector method but, in the case of equation (1), for which the nonlinearity is restricted to the terms with delay, it is possible to use the corrector formula only, thus making the integration very simple. The three step Gear integrator is given by

$$P_{k+1} = \frac{1}{11}\,(18\,P_k \;-\; 9\,P_{k-1} \;+\; 2\,P_{k-2}\,) \;+\; h\,\frac{6}{11}\,P'_{k+1}\,, \tag{6}$$

where P_j is defined in (3), and the prime indicates the derivative with respect to the argument t. Substituting P'_{k+1} using equation (1), equation (6) becomes:

$$P_{k+1} = \frac{1}{11+6\,h}\,(18\,P_k - 9\,P_{k-1} + 2\,P_{k-2}) + \frac{6\,h}{11+6\,h}\,\frac{1}{N}\sum_{i=1}^{N} S_{k+1-d_i}\,, \tag{7}$$

with S_j given in (4).

2.2 Runge-Kutta 4th order

The 4th order Runge-Kutta method uses the value of the functions in the middle of a step interval, therefore an interpolation is required. The 4th order Runge-Kutta integration formula is given by:

$$\begin{aligned} P_{k+1} &= P_k + \tfrac{h}{6}\,(A_1 + A_2 + A_3 + A_4)\,, \\ A_1 &= \tfrac{1}{N}\textstyle\sum_{i=1}^{N} S_{k-d_i} - P_k\,, \\ A_2 &= \tfrac{1}{N}\textstyle\sum_{i=1}^{N} S_{k-d_i+\frac{1}{2}} - \tfrac{1}{2}A_1 - P_k\,, \\ A_3 &= \tfrac{1}{N}\textstyle\sum_{i=1}^{N} S_{k-d_i+\frac{1}{2}} - \tfrac{1}{2}A_2 - P_k\,, \\ A_4 &= \tfrac{1}{N}\textstyle\sum_{i=1}^{N} S_{k+1-d_i} - A_3 - P_k\,. \end{aligned} \tag{8}$$

We used linear interpolation:

$$P_{j+\frac{1}{2}} = \frac{1}{2}\,(P_{j+1} + P_j)\,. \tag{9}$$

2.3 Comparison of the methods

The equation (1) was studied in Glass and Malta (1990) in order to investigate the existence of aperiodic dynamics as the parameters are varied. The case of aperiodic dynamics is the best one for testing the various methods as, due to the sensitivity to initial conditions, it should be the most difficult case for achieving convergence. Therefore, we have chosen the parameters value for which aperiodic dynamics was found in Glass and Malta (1990):

$$\begin{gathered} N = 3, \\ \theta_1 = 0.4,\ \theta_2 = 0.5,\ \theta_3 = 0.6, \\ \tau_1 = 0.56,\ \tau_2 = 2.01,\ \tau_3 = 0.87, \end{gathered} \tag{10}$$

and $n_1 = n_2 = n_3 = n$ was varied from 25 to 110. As n increases, the system undergoes a period-doubling cascade before an aperiodic solution is obtained. Continuing to increase n, solutions having odd period are obtained.

The periodicity of a solution was checked using the simple test proposed by Rosenblum and Kurths (1995): given a time series of length N, let us move along the time series with a window of length l, and calculate the quantity

$$F(l) = \langle |x_i - x_{i+l}| \rangle\,, \tag{11}$$

for $1 \le l \le l_{\max}$ (the averaging is over i and in order to have sufficient averaging number, $l_{\max} \approx N/5$). The function F has zeros with the same periodicity of the time series.

The calculations were done using Gear and RK, using as initial condition a constant function,

$$P_j = c\;,\; -d_2 \le j \le 0\,. \tag{12}$$

For $c = 0.40$, using $h = 0.01$ and $h = 0.005$, the same solution is obtained for both Gear and RK for $25.00 \le n < 57.90$. The solution is periodic and exhibits a period-doubling cascade up to period 8. For $n = 57.90$, Gear gives a solution of period 16 (in this case we have used $h = 0.005$ and $h = 0.0025$) but RK has not converged: the solutions, for these two step values, differ by a timelag (see figure 1), and the result for $h = 0.0025$ is different from the converged solution obtained using the Gear method (see figure 1). So, RK requires a smaller step for converging at this value of n. For $57.90 < n < 60.00$ both methods have given inconsistent results: the same result was not obtained for the two smaller step values. In the figure 2 we display the graphs of $P(t)$ for $n = 58.50$, $h = 0.005, 0.0025$, using the Gear method. We can see that the two results differ by a timeshift of two peaks. The RK and the Gear results for $h = 0.0025$ exhibit a timelag of six peaks (see the graphs on the bottom of figure 2). This is consistent with aperiodicity that implies sensitivity to initial conditions thus making it difficult to achieve convergence. The function F $(h = 0.005)$ also indicates aperiodicity of solution (or a solution of very long period).

For $n = 60.00$, both methods give a solution of period 5 (see figure 3) that is obtained using $h = 0.01$ (the same result is obtained using $h = 0.005$).

In the interval $60.0 < n \leq 60.45$, we used only the method of Gear. For $60.0 < n \leq 60.41$, convergence was achieved for $h = 0.005$ for several values of n, and the results indicate the existence of a period-doubling sequence of the period 5 solution. For $60.41 < n < 60.45$, both methods do not converge for $h \geq 0.0025$, and the test of Rosenblum and Kurths indicates aperiodicity or very long periods (see figure 4). As F has several minima that get very close to zero, the converged solution will probably have a very long period. For $n = 60.45$, no convergence was obtained but the function F (equation (11)) indicates that there could be a solution of period 25 (see figure 5).

For $n = 60.50$, the Gear and the RK methods converge for $h = 0.005$, and $h = 0.0025$, respectively. We see that the RK results differ by a timeshift of a few peaks, but the result for $h = 0.0025$ is identical to the Gear result for $h = 0.005$. The solution has period 15 (see figure 6), according to the test of Rosenblum and Kurths. For this value of n we have also solved equation (1) for constant initial condition (12) with $c = 0.41$ and $c = 0.39$. The case $c = 0.41$ has not converged for $h \geq 0.0025$ but the test of Rosenblum and Kurths indicates a period 15 solution.

In the interval $60.50 \leq n < 73$, both methods do not converge for the step values above ($h \geq 0.0025$). The test of Rosenblum and Kurths indicates that the solutions are either aperiodic or have very long period. In the figure 7 we display the function F for a few n values in this interval.

Finally, for $73 \leq n \leq 110$ (we did not go beyond this value) both methods give a period 3 solution (see figure 8) that is obtained using $h = 0.01$.

3 Discussion and Conclusion

There exist many analytical methods for studying the properties of systems described by DDE's (the case of stability, for instance). However, mainly in the case of nonlinear systems, very often it is necessary to resort to numerical integration, thus the importance of investigating the suitability of numerical integration methods. There are many investigations aiming at developing robust and general numerical integration methods for DDE's (Paul (1991), Paul and Baker (1991), Baker *et al* (1992)). One problem that may arise is the presence of derivative discontinuities (Wille and Baker (1994)). We have considered only the methods of Gear and RK because they are simple and can be applied to any system that is well behaved, without singularities.

Our results indicate that the Gear method is, in general, more efficient than the RK method for integrating the DDE (1): the Gear code is faster and convergence is achieved for a time step greater than or equal to the time step for which convergence is achieved in the RK method. For the particular case of equation (1) (the nonlinearity is restricted to the term with delay) only the correction formula of Gear is required, thus simplifying the numerical calculation. The RK method of 4th order requires interpolation, while Gear does not.

The two main conclusions to be drawn from our numerical study is that the RK method may require smaller time step for convergence and, most important, the convergence of the solution *must* be checked *always*. It is not possible to make a few tests of time step and then do all the calculations using a single time step. As we have seen, there are values of the

parameters for which $h = 0.01$ is adequate but for other parameter values even $h = 0.0025$ does not give a converged solution. The optimum approach would be to have a variable step size but this is rather nontrivial to implement in the case of DDE's.

We would like to remark that the delays used by us were an integer number of time steps but it would be possible to have delays that are incommensurate with the integration time step. In this case interpolation would be required to calculate the value of the functions in the past.

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Figures and Figures caption

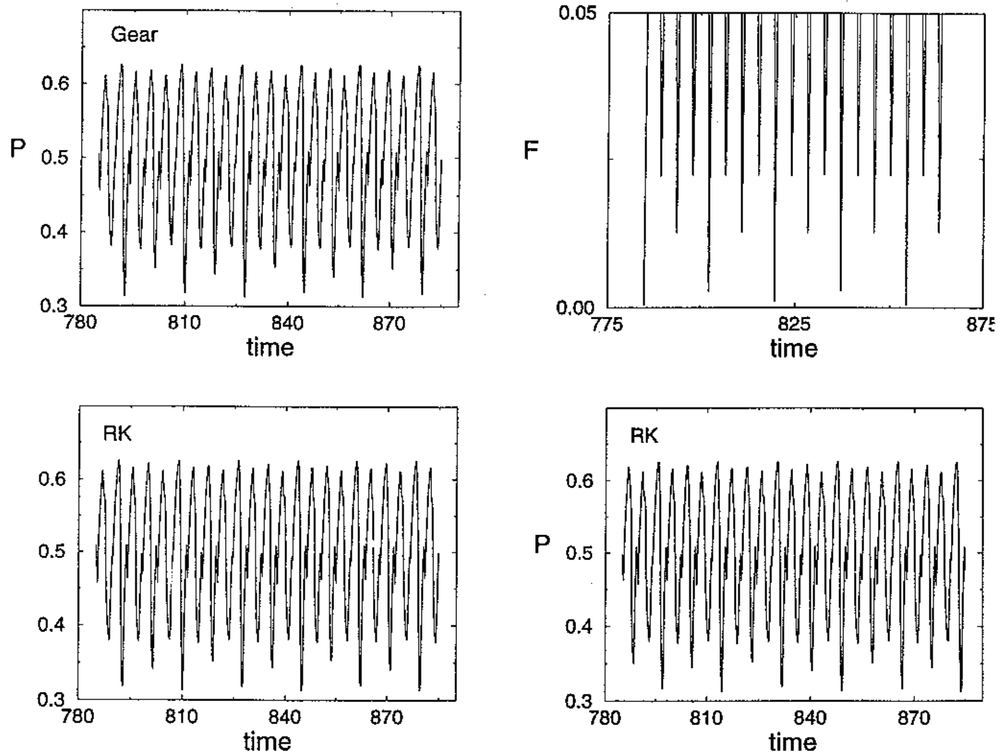

Figure 1: Case $n = 57.90$, with parameter values given in equation (10). On the top we display the solution $P(t)$ obtained using Gear ($h = 0.0025$), and its corresponding function F (see (11)) (we have plotted only part of F in order to make its zeros visible). On the bottom we display the graphs of $P(t)$ (unconverged) obtained using the RK method with $h = 0.005$ (on the left), and $h = 0.0025$ (on the right). We can see that there is a shift of two peaks between the two "solutions".

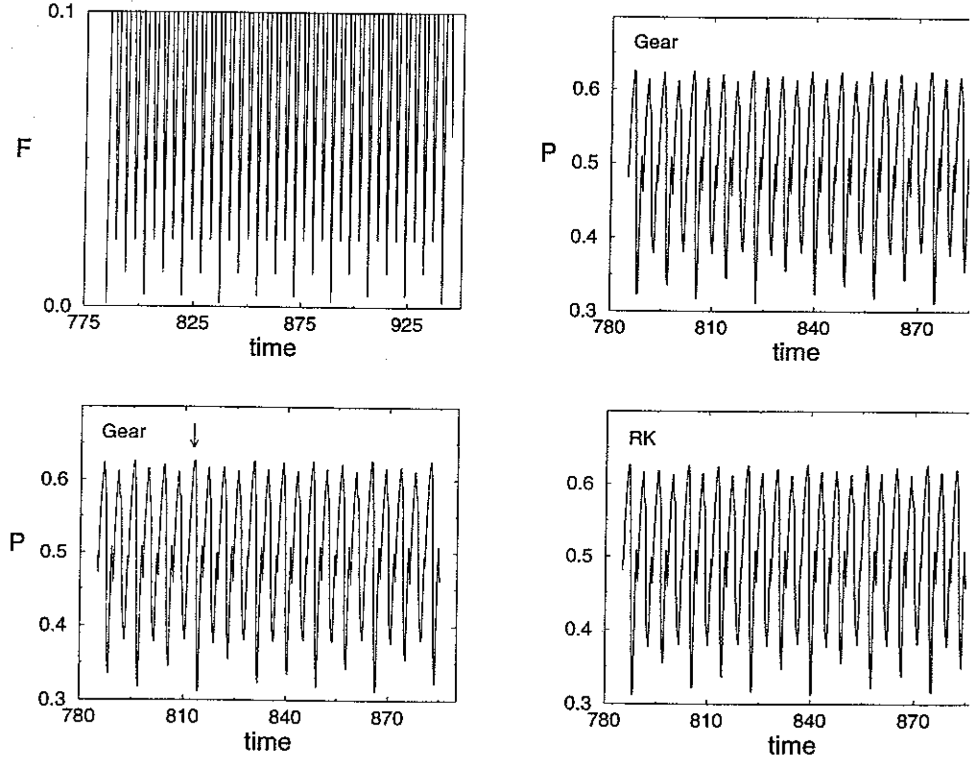

Figure 2: Case $n = 58.50$, with parameter values given in equation (10). On the top we display the result $P(t)$ obtained using Gear ($h = 0.005$), and its corresponding function F (see (11)) (we have plotted only part of F in order to make its zeros visible). On the bottom we display the graphs of $P(t)$ obtained using the methods of Gear and RK with $h = 0.0025$. There is a time shift of six peaks between the two results (indicated by the arrow). The Gear results exhibit a time shift of two peaks.

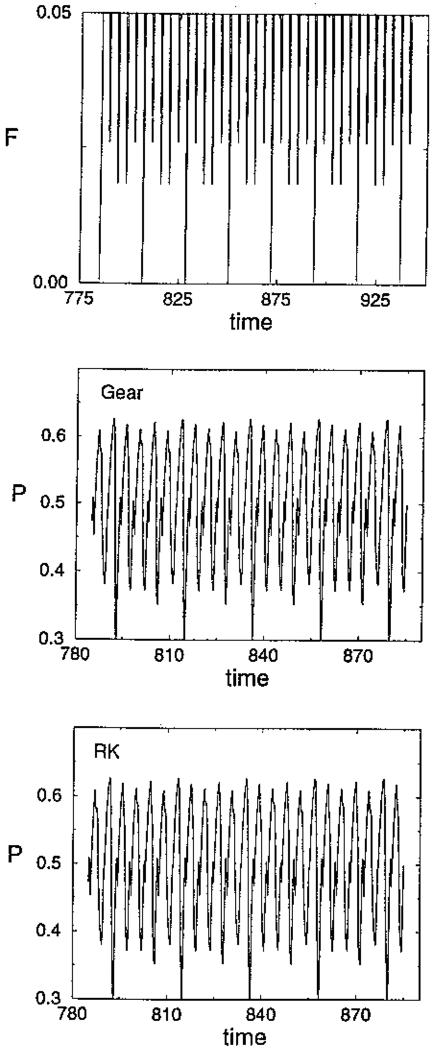

Figure 3: Case $n = 60.0$, with the parameters given in (10). The function F shows that the solutions have period 5. We can see that the solutions $P(t)$ obtained by the two methods are identical. The step size used was $h = 0.005$.

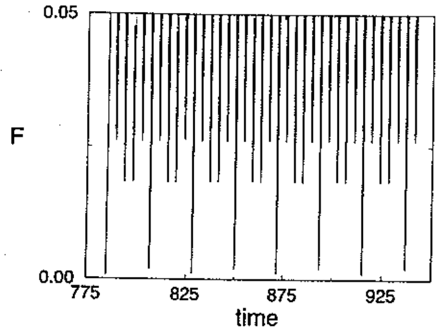

Figure 4: Case $n = 60.43$, with the parameters given in (10). The function F was calculated using the solution by the Gear method. F does not have two zeros in the interval, but as it gets very close to zero many times, we expect that the converged solution will have a long period.

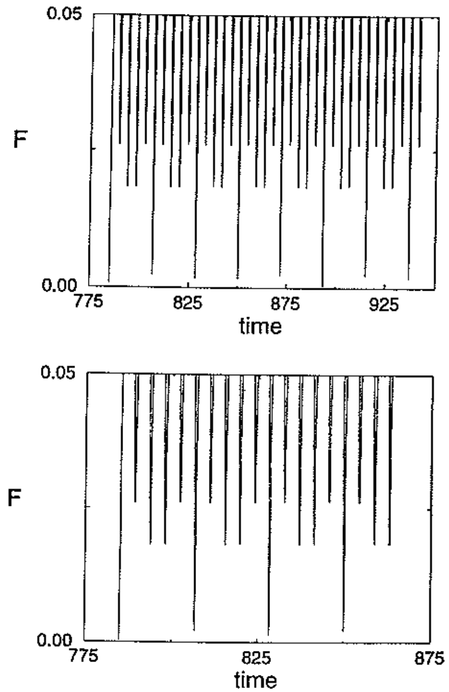

Figure 5: Case $n = 60.45$, with the parameters given in (10). The function F on the top (bottom) corresponds to $h = 0.005$ ($h = 0.0025$). The Gear method was used. The case $h = 0.0025$ shows that the solution does not have period 15.

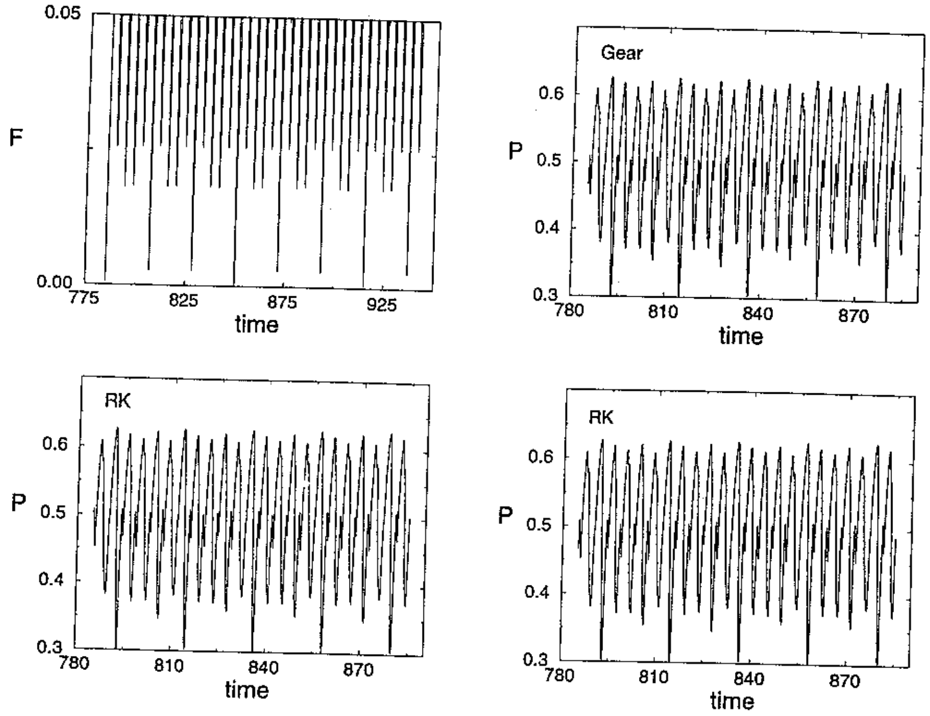

Figure 6: Case $n = 60.5$, with the parameters given in (10). The solution $P(t)$ by the method of Gear was obtained using $h = 0.005$; the results by the method of RK used $h = 0.005$, and $h = 0.0025$, from left to right. The function F was obtained using the Gear solution.

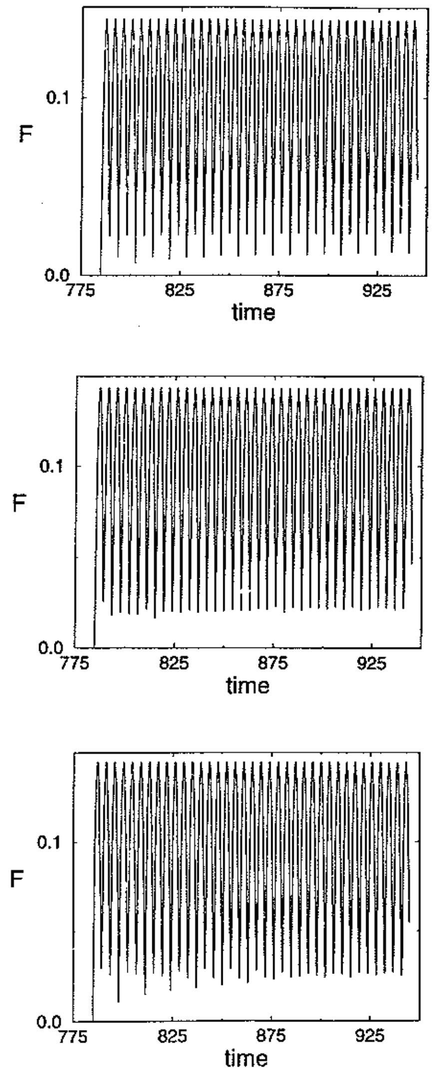

Figure 7: F is displayed for $n = 61, 67, 72$, from top to bottom (Gear method). The solutions have not converged for $h \geq 0.0025$ and F has no zeros, indicating aperiodicity of the corresponding solutions $P(t)$.

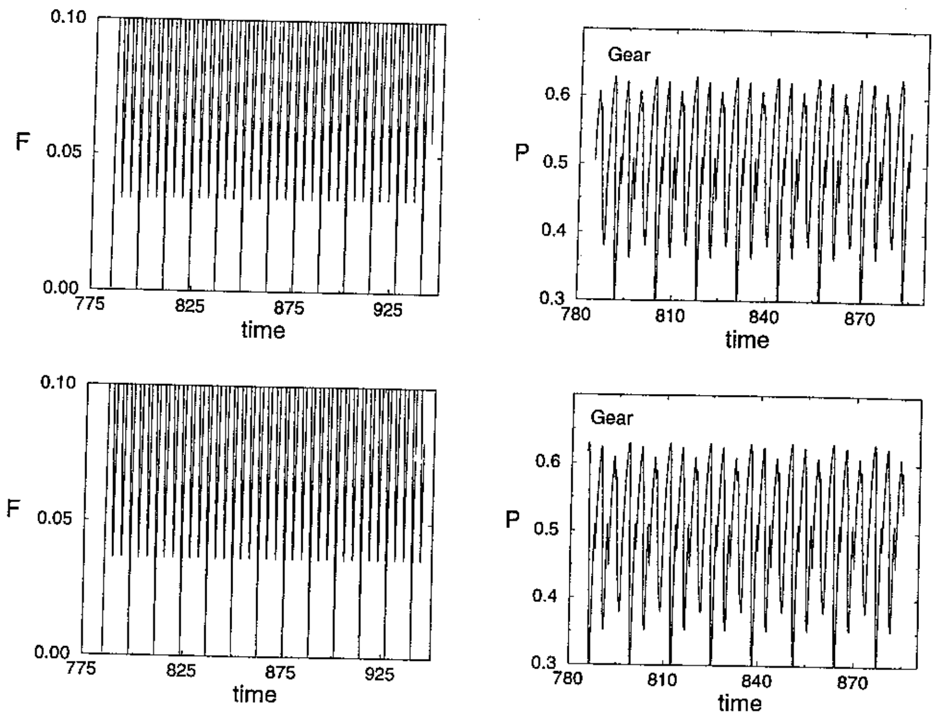

Figure 8: F and $P(t)$ for $n = 73(n = 85)$ are displayed on the top (bottom).