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VARIATIONAL METHOD  
IN WAVE PROPAGATION PROBLEMS

by

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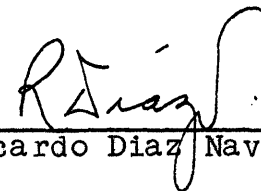
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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science in Geophysics.

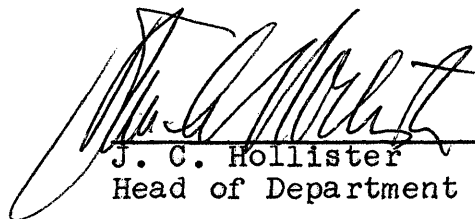
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ACKNOWLEDGEMENTS

I wish to express my sincere appreciation to Dr. Alfred H. Balch, who suggested the subject of this thesis to me and who was a valuable guide throughout this study.

I am also grateful to the other members of my committee: Dr. Frank A. Hadsell and Dr. Ray Mueller, who offered valuable criticism.

I wish to thank El Instituto Mexicano del Petroleo for the financial support provided me in the course of my graduate work at The Colorado School of Mines.

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ABSTRACT

A numerical formulation, based on the calculus of variations and the principle of least action, is proposed for the solution of one-dimensional wave propagation problems. This method is compared with the finite differences methods.

The method consists in fitting a polynomial of second degree between each grid point and minimizing the action integral with respect to the coefficients of the polynomial at each time step.

The computer time involved in the calculations was approximately the same for both methods, although the spacial sample interval could be made about four times larger for the variational method than it was for the finite difference method.

## INTRODUCTION

Variational principles have played an important role in the development of many branches of physics, as in mechanics. It is well known that the problems of particle dynamics can be expressed in a variational form based on the principle of least action as well by Newton's equations of motion. Although there is a correspondence between the two approaches, the physical insight into more complicated systems can often be acquired more easily with the use of the variational approach than with Newton's equations of motion. The variational methods are also useful in determining approximate solutions. These advantages have motivated me to compare the variational methods with the standard finite differences techniques in the solution of one-dimensional wave-propagation problems.

The purpose of this thesis is to show explicitly all the steps of the new proposed variational method in problems in which the solution is known.

The thesis is divided into three parts. In the first part the mathematics of the calculus of variations is developed; in the second part, we deduce the algorithm of the proposed method; and in the third part, we solve problems of wave propagation numerically with different types of boundary conditions.

## THE CALCULUS OF VARIATIONS

### Variational Problems in One Independent Variable

The basic problem of the calculus of variations is to find a function  $y(x)$  for which some given line integral that depends upon this function is an extremum. We begin this chapter with the standard demonstration of how a simple variational problem leads to the Euler-Lagrange equation. This differential equation is equivalent to Newton's equations of motion.

To give a formal definition to our problem, consider the integral

$$I = \int_{x_1}^{x_2} F [ x, y(x), dy/dx ] dx \quad (1)$$

We put the problem in a form in which we can use the differential calculus in obtaining a stationary value for the integral (1) by means of a new parameter  $\alpha$  such that

$$y(x, \alpha) = y(x, 0) + \alpha \eta(x) \quad (2)$$

Note that  $\alpha=0$  corresponds to the stationary value.

We simplify the problem by imposing the condition:

$$\eta(x_1) = \eta(x_2) = 0 \quad (3)$$

Using the parametric representation as in (2), we obtain:

$$I(\alpha) = \int_{x_1}^{x_2} F[x, \gamma(x, \alpha), d\gamma(x, \alpha)/dx] dx \quad (4)$$

If  $I(\alpha)$  is to be stationary, then we must have

$$\left( \partial I / \partial \alpha \right)_{\alpha=0} = 0 \quad (5)$$

Now, substituting (2) into eq. (4), we obtain

$$I(\alpha) = \int_{x_1}^{x_2} F[x, \gamma + \alpha \eta, \gamma' + \alpha \eta'] dx \quad (6)$$

Expanding  $I(\alpha)$  in the Taylor series about  $\alpha=0$  and keeping only the linear term since  $\alpha$  is small, we have

$$I(\alpha) = I(0) + \alpha \left( \partial I / \partial \alpha \right)_{\alpha=0} \quad (7)$$

By the usual methods of differentiating under the integral sign, one finds that

$$I(\alpha) = I(0) + \alpha \int_{x_1}^{x_2} \left( \frac{\partial F}{\partial y} \eta + \frac{\partial F}{\partial y'} \eta' \right) dx \quad (8)$$

For  $I(\alpha)$  to coincide with  $I(0)$ , we require that

$$\int_{x_1}^{x_2} \left( \frac{\partial F}{\partial y} \eta + \frac{\partial F}{\partial y'} \eta' \right) dx = 0 \quad (9)$$

Now, we integrate the second term in eq. (9) by parts,

$$\eta \frac{\partial F}{\partial y'} + \int_{x_1}^{x_2} \left( \frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'} \right) \eta dx = 0 \quad (10)$$

The integrated part vanishes because  $\eta$  vanishes at the end points  $x_1$  and  $x_2$ . Therefore, if the integral is to vanish for arbitrary  $\eta(x)$ , we require that

$$\frac{\partial F}{\partial y} - \frac{d}{dx} \frac{\partial F}{\partial y'} = 0 \quad (11)$$

This differential equation is known as the Euler-Lagrange equation. Its solution represent a curve for which the variation of an integral of the form given in eq. (1) vanishes.

The fundamental problem of the calculus of variations, as we have shown, can be easily generalized for the case in

which the function  $F$  depends on many independent variables  $y_i(x)$  and their derivatives  $y_i'(x)$ ,  $i = 1, 2, \dots, N$ .

We wish to minimize the integral

$$I = \int_1^2 \left( F(y_1(x), y_2(x), \dots, y_1'(x), y_2'(x), \dots, x) \right) dx \quad (12)$$

subject to a fixed-ends boundary conditions.

As in the case of one independent variable, we consider the integral  $I$  as a function of the parameter  $\alpha$ , which labels all the possible curves  $y_i(x, \alpha)$ . Thus we may introduce  $\alpha$  by setting

$$\begin{aligned} y_1(x, \alpha) &= y_1(x, 0) + \alpha \eta_1(x) \\ y_2(x, \alpha) &= y_2(x, 0) + \alpha \eta_2(x) \\ &\cdot \quad \quad \cdot \quad \quad \cdot \\ y_N(x, \alpha) &= y_N(x, 0) + \alpha \eta_N(x) \end{aligned} \quad (13)$$

where  $y_1(x, 0)$ ,  $y_2(x, 0)$ , etc., are the solutions of the extremem problem and  $\eta_i$ ,  $i = 1, 2, \dots, N$ , are a completely arbitrary functions of  $x$ , except that they vanish at the end points.

Proceeding as before, we obtain the condition analogous to eq. (9)

$$\int_1^2 \sum_i \left( \frac{\partial F}{\partial y_i} \eta_i + \frac{\partial F}{\partial y_i'} \eta_i' \right) dx = 0 \quad (14)$$

Again, we integrate the integral involved in the second term of eq. (14) by parts, and obtain the result

$$\int_1^2 \frac{\partial F}{\partial y_i'} \eta_i' dx = \frac{\partial F}{\partial y_i'} \eta_i \Big|_1^2 - \int_1^2 \eta_i \frac{d}{dx} \left( \frac{\partial F}{\partial y_i'} \right) dx$$

where the first term vanishes, since we have a variation with fixed end points. Thus eq. (14) becomes

$$\int_1^2 \sum_i \left( \frac{\partial F}{\partial y_i} - \frac{d}{dx} \left( \frac{\partial F}{\partial y_i'} \right) \right) \eta_i dx = 0 \quad (15)$$

Therefore, if the integrand vanishes for arbitrary  $\eta$ , we must require that

$$\frac{\partial F}{\partial y_i} - \frac{d}{dx} \frac{\partial F}{\partial y_i'} = 0 \quad (16)$$

The result given in eq. (16) states that for the case at hand we just write an Euler-Lagrange equation for each variable.

We will see in the next section that, by suitable transformations, it is possible to derive Newton's equations of motion for conservative systems from the Euler-Lagrange equations.

### The Principle of Least Action

The Newtonian laws of motion provide a mathematical structure which describes the motion of interacting particles. Although the formulation of Newton is most commonly studied

in elementary physics, there is a second and alternate method of expressing the behavior of a mechanical system. This alternate mathematical description is called the principle of least action.

The instantaneous configuration of a system is prescribed by the values of  $n$  generalized coordinates  $q_1, q_2, \dots, q_n$ , and corresponds to a particular point in an  $n$ -dimensional  $q$ -space. This  $n$ -dimensional space is therefore, known as the configuration space. As time goes on, the state of the system changes, and the system point moves in the configuration space tracing out a curve and describing the motion of the system.

We denote by  $C_1$  the configuration of a mechanical system, i.e., the aggregate of the positions of the individual particles at an instant  $t_1$ . Similarly,  $C_2$  denotes the configuration at a latter time  $t_2$ . We call the configuration path or orbit of the system the curve joining  $C_1$  and  $C_2$  in the configuration space. The actual or dynamic orbit depends upon the constraints on the system and the forces which influence the motion. We also restrict the possible orbits between the two configurations to those which fulfill the condition that the total energy along the varied paths is the same as along the actual path.

The principle of least action states that a mechanical system with a kinetic energy  $T$  and a potential energy  $V$  behaves within a time interval  $t_1 \leq t \leq t_2$ , for a given initial

and end positions, so that

$$A = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t) dt \quad (17)$$

assumes a stationary value.

The integral  $A$  is known as the action integral, and the integrand  $L$  is called the Lagrangian of the system and it is defined as

$$L = T - V \quad (18)$$

We note that the action integral has the form stipulated in eq. (12), and so we make the transformations

$$x \rightarrow t, \quad y_i \rightarrow q_i$$

$$F(y_i, y_i', x) \rightarrow L(q_i, \dot{q}_i, t)$$

The Euler-Lagrange equations become the Lagrange equations of motion

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \quad (19)$$

The Lagrange equations of motion are in turn equivalent to Newton's, as indicated by the following example. Consider a particle of mass  $m$  moving in a potential field  $V(x_1, x_2, x_3)$ .

The kinetic energy of the particle is

$$T = \left( m/2 \right) \left( \dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2 \right)$$

and the action integral is

$$A = \int_{t_1}^{t_2} dt \left[ \frac{m}{2} \left( \dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2 \right) - V(x_1, x_2, x_3) \right]$$

Applying the eq. (19) to the integrand, one finds that

$$m \frac{d^2 x_i}{dt^2} = - \frac{\partial V}{\partial x_i} \quad i = 1, 2, 3$$

This equation is clearly the Newtonian equation of motion describing the trajectory of the particle in a force field.

### Variational Problems in Two Independent Variables

We consider the double integral

$$I = \iint_D F(x, y, w, w_x, w_y) dx dy \quad (20)$$

where  $w_x = \partial w / \partial x$ ,  $w_y = \partial w / \partial y$

The integration of eq. (20) is carried out over a given domain D in the x-y plane. The function F is twice differentiable with respect to the indicated arguments. We proceed to derive the partial differential equation which must be satisfied in order that the integral I be stationary with respect to a continuously differentiable functions  $w(x, y)$  which assume prescribed values on the boundary curve

C of the domain D.

We label, as before, all the possible trajectories by the parameter  $\alpha$

$$w(x, y, \alpha) = w(x, y) + \alpha \eta(x, y) \quad (21)$$

where  $w(x, y)$  is assumed to be the stationary function and is a completely arbitrary function, except that it is required to vanish on C.

Using the parametric representation mentioned above, we write the the eq. (20) as

$$I(\alpha) = \iint_D F(x, y, w + \alpha \eta, w_x + \alpha \eta_x, w_y + \alpha \eta_y) dx dy \quad (22)$$

Expanding  $I(\alpha)$  in the Taylor series about  $\alpha = 0$  and keeping only the linear term, since  $\alpha$  is small, we obtain

$$I(\alpha) = I(0) + \alpha \iint_D \left( \frac{\partial F}{\partial w} \eta + \frac{\partial F}{\partial w_x} \eta_x + \frac{\partial F}{\partial w_y} \eta_y \right) dx dy \quad (23)$$

If the integral I is to be stationary, then we must have

$$\left( \frac{\partial I}{\partial \alpha} \right)_{\alpha=0} = 0$$

Consequently, we require that

$$\iint_D \left( \frac{\partial F}{\partial w} \eta + \frac{\partial F}{\partial w_x} \eta_x + \frac{\partial F}{\partial w_y} \eta_y \right) dx dy = 0 \quad (24)$$

Now, applying Green's theorem to the last two terms in eq. (24) and using  $\frac{\partial}{\partial x} \left( \eta \frac{\partial F}{\partial w_x} \right) = \eta_x \frac{\partial F}{\partial w_x} + \eta \frac{\partial^2 F}{\partial x \partial w_x}$  and  $\frac{\partial}{\partial y} \left( \eta \frac{\partial F}{\partial w_y} \right) = \eta_y \frac{\partial F}{\partial w_y} + \eta \frac{\partial^2 F}{\partial y \partial w_y}$ , we obtain

$$\iint_D \eta \left[ \frac{\partial F}{\partial w} - \frac{\partial}{\partial x} \frac{\partial F}{\partial w_x} - \frac{\partial}{\partial y} \left( \frac{\partial F}{\partial w_y} \right) \right] dx dy + \int_C \eta \left[ \frac{\partial F}{\partial w_x} \frac{dx}{ds} + \frac{\partial F}{\partial w_y} \frac{dy}{ds} \right] ds = 0 \quad (25)$$

The second integral vanishes since  $\eta(x,y) = 0$  on  $C$ .

Therefore, we obtain

$$\iint_D \eta \left[ \frac{\partial F}{\partial w} - \frac{\partial}{\partial x} \left( \frac{\partial F}{\partial w_x} \right) - \frac{\partial}{\partial y} \left( \frac{\partial F}{\partial w_y} \right) \right] dx dy = 0$$

If the integrand is to vanish for arbitrary  $\eta(x)$ , the function  $F(x,y)$  must satisfy

$$\frac{\partial F}{\partial w} - \frac{\partial}{\partial x} \frac{\partial F}{\partial w_x} - \frac{\partial}{\partial y} \frac{\partial F}{\partial w_y} = 0 \quad (26)$$

This is the Euler-Lagrange equation in two independent variables.

## THE VIBRATING STRING PROBLEM

### The Derivation of the Differential Equation

The problem chosen here as the basis of comparison of the various methods is the problem of the vibrations of a stretched string between two fixed points. This special boundary condition will be included in a general computer program which can handle all the different types of boundary conditions. We have chosen this particular problem since the kinetic and potential energy can be easily evaluated, and therefore, the elastic parameters can be identified for any one dimensional wave propagation problem.

Let us consider, then, an elastic string, stretched under a tension  $\tau$  between two points on the x-axis (Fig. 1). In formulating the problem we assume that

- a) The mass of the string is uniformly distributed.
- b) The motion takes place entirely in one plane, and in this plane each particle moves at right angles to the equilibrium position of the string.
- c) The deflection of the string during the motion is so small that the resulting change in length has no effect on the tension  $\tau$ .
- d) The string is perfectly flexible, i.e., it can transmit force only in the direction of its length.
- e) The amplitude of the vibration is very small.
- f) There is no frictional damping, so we deal with a conservative system.

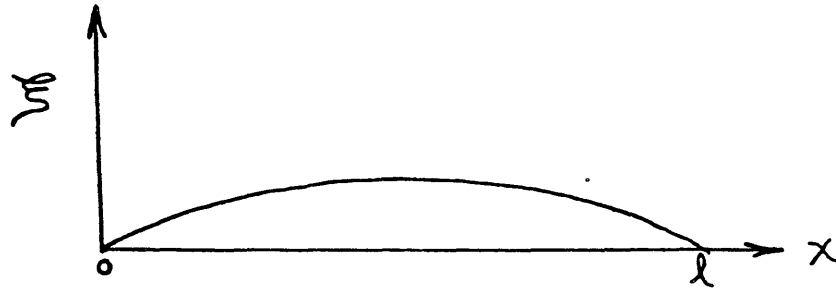


Figure 1. A typical configuration of the string

The transverse displacement of the string is denoted by the function  $\xi(x,t)$ , which describes the shape of the string during the course of the vibration. The fact that the ends are fixed, we have the condition  $\xi(0,t) = \xi(l,t) = 0$  for all times.

If  $\rho$  represents the constant mass/length of the string, the kinetic energy  $dT$  of an element  $dx$  will be

$$dT = \frac{1}{2} \rho \left( \frac{\partial \xi}{\partial t} \right)^2 dx \quad (27)$$

and, therefore, for the entire string

$$T = \frac{1}{2} \rho \int_0^l \left( \frac{\partial \xi}{\partial t} \right)^2 dx \quad (28)$$

The potential energy is given by the product of the total external force and the increase of length. We will consider the tension  $\tau$  which is exerted upon the ends as the only external force. Hence we obtain

$$V = \tau \left[ \int_0^l ds - l \right] \quad (29)$$

If we expand  $ds/dx$  according to the binomial theorem and neglect terms of second and higher order, we obtain

$$\frac{ds}{dx} = \left( 1 + \left( \frac{\partial \xi}{\partial x} \right)^2 \right)^{1/2} \approx 1 + \frac{1}{2} \left( \frac{\partial \xi}{\partial x} \right)^2$$

Therefore, eq. (29) becomes

$$V = \frac{1}{2} \tau \int_0^l \left( \frac{\partial \xi}{\partial x} \right)^2 dx \quad (30)$$

In order to find the motion of the string in a certain time interval  $t_1 \leq t \leq t_2$ , we have to find, according to the principle of least action, the stationary value of the integral

$$A = \frac{1}{2} \int_{t_1}^{t_2} \int_0^l \left[ \rho \left( \frac{\partial \xi}{\partial t} \right)^2 - \tau \left( \frac{\partial \xi}{\partial x} \right)^2 \right] dx dt \quad (31)$$

Consequently, the function which describes the actual motion of the string is one that gives the action integral an extremum with respect to the function  $\xi(x, t)$ , which describes the actual configuration at  $t = t_1$  and  $t = t_2$  and vanishes, for all  $t$  at  $x = 0$  and  $x = l$ . The times  $t_1$  and  $t_2$  are completely arbitrary.

If we make the transformations in eq. (20)

$$y \rightarrow t, \quad w \rightarrow \xi, \quad F \rightarrow L = \frac{1}{2} \left[ \rho \left( \frac{\partial \xi}{\partial t} \right)^2 - \tau \left( \frac{\partial \xi}{\partial x} \right)^2 \right]$$

then the eq. (26) becomes

$$\tau \frac{\partial^2 \xi}{\partial x^2} = \rho \frac{\partial^2 \xi}{\partial t^2} \quad (32)$$

This partial differential equation describes the actual motion of the vibrating string.

### Finite Differences Approximation

Our approach is to digitize the function  $\xi(x,t) \rightarrow \xi(n\Delta x, m\Delta t)$  and consider the configurations of the string\* at three consecutive times, i.e.,  $t = 0, \Delta t, 2\Delta t$ . According to the principle of least action, we keep the configurations at the first and third times fixed and proceed to evaluate the position of the string at the second configuration that makes the action integral stationary. This gives us a relationship among the three configurations (Fig. 2).

The motion of the string is described by a second order partial differential equation given in (32). In order to solve this equation we must supply, besides the boundary conditions, the configurations of the string at the first two time steps. Since the three configurations are related to each other, we can express the third configuration in terms of the first and second ones. In general, the computation

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(\*) The use of the string as illustration is purely a matter of convenience, and any quantity satisfying the wave equation possesses the properties developed for the string.

algorithm will be as follows: given the configurations at  $(m-1)\Delta t$  and  $m\Delta t$ , we evaluate the configuration at  $(m+1)\Delta t$ , for  $m=1,2,3,\dots,M$ . In reference to figure 2, the system starts off with the displacements known at the  $X^{ed}$  intersections and the algorithm will find the displacements at the other intersections.

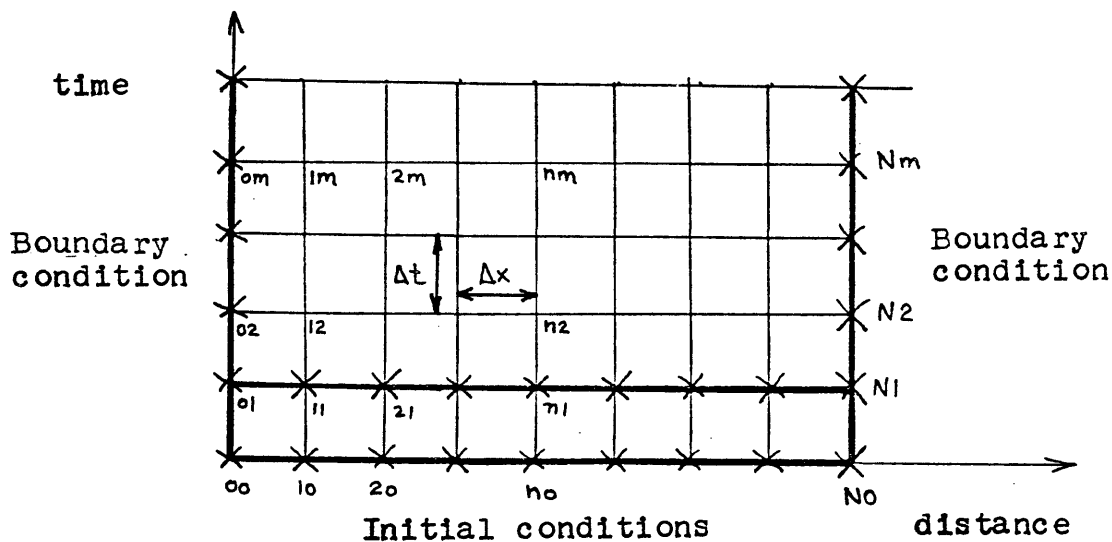


Figure 2.- The finite differences scheme.

The next stage is to approximate integrations by sums.

The action integral becomes:

$$\begin{aligned}
 A = & \frac{\rho}{2} \sum_{n=1}^N \left[ \left( \frac{\xi_{n1} - \xi_{n0}}{\Delta t} \right)^2 + \left( \frac{\xi_{n2} - \xi_{n1}}{\Delta t} \right)^2 \right] \Delta x \Delta t + \\
 & - \frac{\tau}{2} \sum_{n=1}^N \left[ \left( \frac{\xi_{n0} - \xi_{n-1,0}}{\Delta x} \right)^2 + \left( \frac{\xi_{n1} - \xi_{n-1,1}}{\Delta x} \right)^2 + \left( \frac{\xi_{n2} - \xi_{n-1,2}}{\Delta x} \right)^2 \right] \Delta x \Delta t
 \end{aligned}
 \tag{33}$$

The action integral is stationary between  $0 \leq t \leq 2 \Delta t$   
if

$$\frac{\partial A}{\partial \xi_{n1}} = 0 \quad \text{for } n = 1, 2, \dots, N - 1$$

Used with (33), this gives us  $n$  as a free index and

$$\rho \frac{\Delta x}{\Delta t} \left( \xi_{n1} - \xi_{n0} - \xi_{n2} + \xi_{n1} \right) - \tau \frac{\Delta t}{\Delta x} \left( \xi_{n1} - \xi_{n-1,1} - \xi_{n+1,1} + \xi_{n1} \right) = 0$$

$$\begin{aligned} \text{Define } \frac{\Delta x}{\Delta t} &= \lambda \\ \frac{\tau}{\rho} &= v^2 \end{aligned} \quad (34)$$

When it is solved for  $\xi_{n2}$ , the last equation becomes

$$\xi_{n2} = -\xi_{n0} + (2 - 2v^2/\lambda^2) \xi_{n1} + v^2/\lambda^2 (\xi_{n-1,1} + \xi_{n+1,1}) \quad (35)$$

$$n = 1, 2, \dots, N - 1$$

In general, the action integral between  
 $(m-1)\Delta t \leq t \leq (m+1)\Delta t$  is stationary if

$$\begin{aligned} \frac{\partial A}{\partial \xi_{nm}} &= 0 & n &= 1, 2, \dots, N - 1 \\ & & m &= 1, 2, \dots, M \end{aligned}$$

which yields the result

$$\xi_{n,m+1} = -\xi_{n,m-1} + 2(1 - v^2/\lambda^2) \xi_{nm} + v^2/\lambda^2 (\xi_{n-1,m} + \xi_{n+1,m}) \quad (36)$$

This result is the same as that which we would obtain if we applied finite-differences methods directly in the partial differential equation given by eq. (32).

### Proposed Method Using the Calculus of Variations

We propose to fit a quadratic  $ax^2 + bx + c$  to each grid point. It is hoped that we may thus obtain the same accuracy in the solutions in less computer time since larger sample intervals should be acceptable. We plan to investigate how large the sampling interval can be made, while still obtaining accurate solutions.

We digitize the time variable, leaving the space variable continuous, i.e.,

$$\xi(x, t) \longrightarrow \xi(x, m \Delta t)$$

Consider the interval  $0 \leq x \leq 1$ , and subdivide it into  $N$  subintervals  $0 = x_0 < x_1 < x_2 \cdots < x_N = 1$

Let  $\eta_n(x, m \Delta t)$  be the quadratic approximation to the function  $\xi(x, m \Delta t)$  in the subinterval  $x_{n-1} < x < x_n$  so that  $\eta_n(x, m \Delta t) = \xi(x, m \Delta t)$  for  $x = x_{n-1}$  and  $x = x_n$

Thus, the function  $\eta_n(x, m \Delta t)$  can be written as

$$\eta_n(x, m \Delta t) = a_{nm} [x - (n-1)h]^2 + b_{nm} [x - (n-1)h] + c_{nm} \quad (37)$$

where  $h = x_n - x_{n-1}$

We have  $3N$  different coefficients for each  $m$ , but the

conditions of continuity of the function  $\eta_n(x, m\Delta t)$  and its first derivative\* at  $x = nh$ ,  $n = 1, 2, \dots, N - 1$ , along with the boundary conditions at  $x = 0$  and  $x = Nh$ , give  $2N$  equations. Thus we should be able to eliminate  $2N$  coefficients and finish up with only  $N$  coefficients to be determined, using the calculus of variations.

Analogously to the discrete case, we keep the coefficients in the first and third configurations fixed and we minimize the action integral with respect to the coefficients in the second configuration. In this way we obtain a relationship among the three configurations.

For the  $N$ -subinterval case, we have

$$\begin{aligned} \eta_1(x, m\Delta t) &= a_{1m}x^2 + b_{1m}x + c_{1m} \\ \eta_2(x, m\Delta t) &= a_{2m}(x-h)^2 + b_{2m}x + c_{2m} \\ &\vdots \\ \eta_N(x, m\Delta t) &= a_{Nm}[x-(N-1)h]^2 + b_{Nm}[x-(N-1)h] + c_{Nm} \end{aligned} \quad (38)$$

The boundary condition at  $x = 0$  is  $\eta_1(x, m\Delta t)|_{x=0} = \xi_{0m}$ , and gives the result

$$c_{1m} = \xi_{0m} \quad (39)$$

---

(\*) These conditions are equivalent to having continuity of displacements and stresses.

The conditions of continuity of the function  $\eta_n(x, m \Delta t)$  and its first derivative yield the result

$$\begin{aligned} a_{nm} h^2 + b_{nm} h + c_{nm} &= c_{n+1, m} \\ 2 a_{nm} h + b_{nm} &= b_{n+1, m} \end{aligned} \quad (40)$$

The boundary condition at  $x = Nh$  is

$$\eta_N(x, m \Delta t) \Big|_{x=Nh} = \sum N m \quad (41)$$

Now using the equations (39) through (41), we can solve for the  $a_{nm}$ 's and  $c_{nm}$ 's in terms of the  $b_{nm}$ 's. We have a system of  $2N - 1$  equations, since we evaluate the coefficient  $c_{1m}$  explicitly.

For simplicity, we are going to work out the case  $N = 4$ . Later on, we generalize for any number of intervals.

From the equations (39), (40) and (41), we obtain the system of linear equations

$$\begin{array}{cccccc|cccc} h^2 & 0 & 0 & 0 & -1 & 0 & 0 & a_{1m} & -b_1 h - \sum_0 m \\ 2h & 0 & 0 & 0 & 0 & 0 & 0 & a_{2m} & b_{2m} - b_{1m} \\ 0 & h^2 & 0 & 0 & 1 & -1 & 0 & a_{3m} & -b_{2m} h \\ 0 & 2h & 0 & 0 & 0 & 0 & 0 & a_{4m} & b_{3m} - b_{2m} \\ 0 & 0 & h^2 & 0 & 0 & 1 & -1 & c_{2m} & -b_{3m} h \\ 0 & 0 & 2h & 0 & 0 & 0 & 0 & c_{3m} & b_{4m} - b_{3m} \\ 0 & 0 & 0 & h^2 & 0 & 0 & 1 & c_{4m} & -b_{4m} h - \sum_4 m \end{array} \quad (42)$$

From the even-numbered rows, we obtain

$$a_{1m} = (1/2h) (b_{2m} - b_{1m}) \quad (43)$$

$$a_{2m} = (1/2h) (b_{3m} - b_{2m}) \quad (44)$$

$$a_{3m} = (1/2h) (b_{4m} - b_{3m}) \quad (45)$$

The first row reads:

$$h^2 a_{1m} - c_{2m} = -b_{1m} h - \xi_{0m}$$

Substituting the equation (43) into this equation and solving for  $c_{2m}$ , we obtain

$$c_{2m} = \frac{h}{2} (b_{1m} + b_{2m}) + \xi_{0m} \quad (46)$$

The third row reads:

$$h^2 a_{2m} + c_{2m} - c_{3m} = -b_{2m} h$$

Substituting eq. (44) and (46) into this equation and solving for  $c_{3m}$ , we obtain

$$c_{3m} = \frac{h}{2} (b_{1m} + 2b_{2m} + b_{3m}) + \xi_{0m} \quad (47)$$

The fifth row reads:

$$h^2 a_{3m} - c_{3m} - c_{4m} = -b_{3m} h$$

Substituting eq. (45) and (47) into this equation and solving for  $c_{4m}$ , we obtain

$$c_{4m} = \frac{h}{2} (b_{1m} + 2b_{2m} + 2b_{3m} + b_{4m}) + \xi_{0m} \quad (48)$$

Finally, the seventh row reads:

$$h^2 a_{4m} + c_{4m} = -b_{4m} h + \xi_{4m}$$



The following stage is to discretize the time variable, leaving the space variable continuous in the action integral between  $0 \leq t \leq 2 \Delta t$ .

We approximate the velocity  $\frac{\partial \xi}{\partial t}$  of the string between  $t_1 < t < t_2$  as

$$\frac{\partial \xi}{\partial t} \approx \frac{\xi(x, t_2) - \xi(x, t_1)}{t_2 - t_1} \quad (52)$$

Therefore, the action integral (31) for  $t_1 = 0$  and  $t_2 = 2 \Delta t$ , can be written as

$$A = \frac{1}{2} \rho \Delta t \int_0^l \left[ \left( \frac{\xi(x, \Delta t) - \xi(x, 0)}{\Delta t} \right)^2 + \left( \frac{\xi(x, 2\Delta t) - \xi(x, \Delta t)}{\Delta t} \right)^2 \right] dx \quad (53)$$

$$- \frac{1}{2} \tau \Delta t \int_0^l \left[ \left( \frac{\partial \xi(x, 0)}{\partial x} \right)^2 + \left( \frac{\partial \xi(x, \Delta t)}{\partial x} \right)^2 + \left( \frac{\partial \xi(x, 2\Delta t)}{\partial x} \right)^2 \right] dx$$

and it is stationary if  $\frac{\partial A}{\partial b_{n1}} = 0$  for  $n = 1, 2, \dots, N$

Thus we obtain

$$\frac{\partial A}{\partial b_{n1}} = \frac{\rho}{\Delta t} \int_0^l \left[ -\xi(x, 0) + 2\xi(x, \Delta t) - \xi(x, 2\Delta t) \right] \frac{\partial \xi(x, \Delta t)}{\partial b_{n1}} dx$$

$$- \tau \Delta t \int_0^l \frac{\partial \xi(x, \Delta t)}{\partial x} \frac{\partial^2 \xi(x, \Delta t)}{\partial x \partial b_{n1}} dx = 0 \quad (54)$$

Set

$$I_n = \int_0^l \left[ -\xi(x, 0) + 2\xi(x, \Delta t) - \xi(x, 2\Delta t) \right] \frac{\partial \xi(x, \Delta t)}{\partial b_{n1}} dx \quad (55)$$

$$J_n = \int_0^l \frac{\partial \xi(x, \Delta t)}{\partial x} \frac{\partial^2 \xi(x, \Delta t)}{\partial x \partial b_{n1}} dx \quad (56)$$

The two last integrals  $I_n$  and  $J_n$ ,  $n = 1, 2, \dots, N$ , are evaluated in the appendix.

Therefore, in terms of the integrals (55) and (56), the equation (54) takes the form:

$$\frac{\partial A}{\partial b_{n1}} = \frac{\int}{\Delta t} I_n - \tau \Delta t J_n \quad (57)$$

$$n = 1, 2, \dots, N$$

Now, using the equations (A-11) and (A-28) of the appendix, we write the last equation as

$$\begin{aligned} & \frac{\int}{\Delta t} \left[ \frac{h^3}{120} R_{nk} (-b_{k0} + 2b_{k1} - b_{k2}) + \right. \\ & \left. \frac{h^2}{60} (-\xi_{00} + 2\xi_{01} - \xi_{02}) S_n + \frac{h^2}{60} (-\xi_{N0} + 2\xi_{N1} - \xi_{N2}) V_n \right] \\ & = \frac{\tau}{\int} \Delta t \left[ \frac{h}{6} U_{nk} b_{k1} + \frac{\xi_{01} - \xi_{N1}}{6} T_n \right] \end{aligned}$$

After using the definitions given in eq. (34) with  $h = \Delta x$  and simplifying the last equation, we obtain

$$\begin{aligned} & \frac{R_{nk}}{20} (-b_{k0} + 2b_{k1} - b_{k2}) + \frac{S_n}{10h} (-\xi_{00} + 2\xi_{01} - \xi_{02}) \quad (58) \\ & + \frac{V_n}{10h} (-\xi_{N0} + 2\xi_{N1} - \xi_{N2}) = \frac{v^2}{x^2} \left( U_{nk} b_{k1} + \frac{\xi_{01} - \xi_{N1}}{h} \right) T_n \end{aligned}$$

If  $(R)^{-1}$  is the inverse matrix of  $(R)$ , by multiplying by  $(R)^{-1}$  the equation (58) we obtain

$$\frac{1}{20} (-b_{k0} + 2b_{k1} - b_{k2}) + \frac{1}{10h} (-\xi_{00} + 2\xi_{01} - \xi_{02}) R_{kn}^{-1} S_n$$

$$+ \frac{1}{10h} (-\xi_{N0} + 2\xi_{N1} - \xi_{N2}) R_{kn}^{-1} V_n = \frac{v^2}{\lambda^2} \left( R_{kn}^{-1} U_{nl} b_{li} + \frac{\xi_{01} - \xi_{N1}}{h} R_{kn}^{-1} T_n \right)$$

Define the matrix  $D_{kn}$  by

$$D_{kn} = R_{kl}^{-1} U_{ln} \quad (60)$$

and the vectors  $P_k$ ,  $Q_k$  and  $X_k$  by

$$P_k = R_{kl}^{-1} S_l$$

$$Q_k = R_{kl}^{-1} T_l \quad (61)$$

$$X_k = R_{kl}^{-1} V_l$$

where one sums on the repeated index.

The quantities given in (60) and (61) will be stored in the computer since we are going to need them to evaluate the coefficients  $b_{nm}$  at every time step.

Thus we can write the matrix equation (59) as

$$\frac{-b_{k0} + 2b_{k1} - b_{k2}}{20} + \frac{-\xi_{00} + 2\xi_{01} - \xi_{02}}{10h} P_k + \frac{-\xi_{N0} + 2\xi_{N1} - \xi_{N2}}{10h} X_k$$

$$= \frac{v^2}{\lambda^2} \left[ D_{kl} b_{li} + \frac{Q_k}{h} \xi_{01} - \frac{Q_k}{h} \xi_{N1} \right]$$

The process starts off with the configurations at times 0 and  $\Delta t$ ; thus we solve the last equation for  $b_{k2}$ :

$$b_{k2} = -b_{k0} + \left( 2 - \frac{20v^2}{\lambda^2} D_{kl} \right) b_{l1} + \frac{20v^2}{h\lambda^2} Q_k (\xi_{N1} - \xi_{01})$$

$$+ \frac{2}{h} (-\xi_{00} + 2\xi_{01} - \xi_{02}) P_k + \frac{2}{h} (-\xi_{N0} + 2\xi_{N1} - \xi_{N2}) X_k$$

$$k = 1, 2, \dots, N \quad (63)$$

Therefore the computational algorithm is

$$b_{k,m+1} = -b_{k,m-1} + \left( 2 - \frac{20v^2}{\lambda^2} D_{kl} \right) b_{lm} +$$

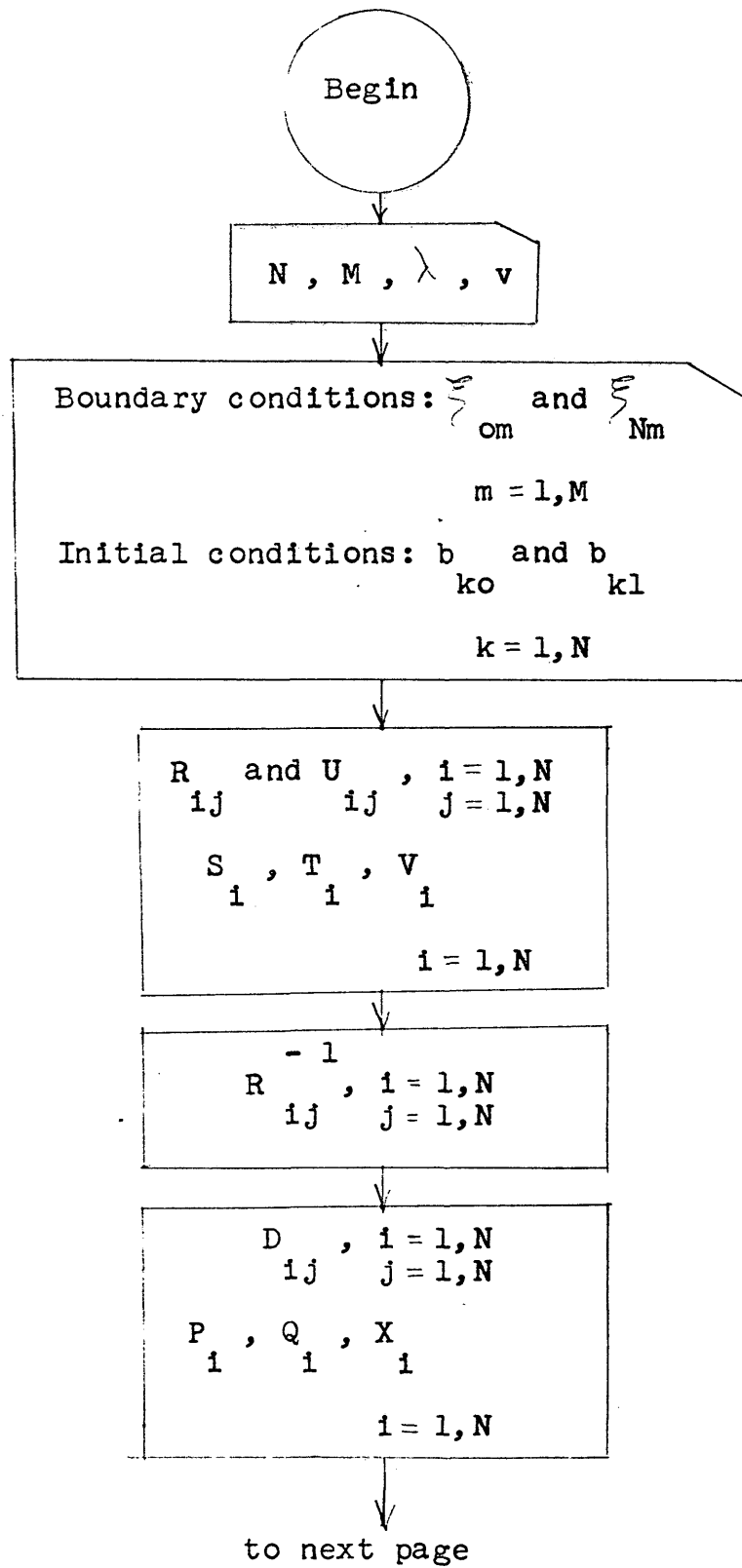
$$+ \frac{20v^2}{h\lambda^2} Q_k (\xi_{Nm} - \xi_{0m}) + \frac{2}{h} (-\xi_{0,m-1} + 2\xi_{0m} - \xi_{0,m+1}) P_k$$

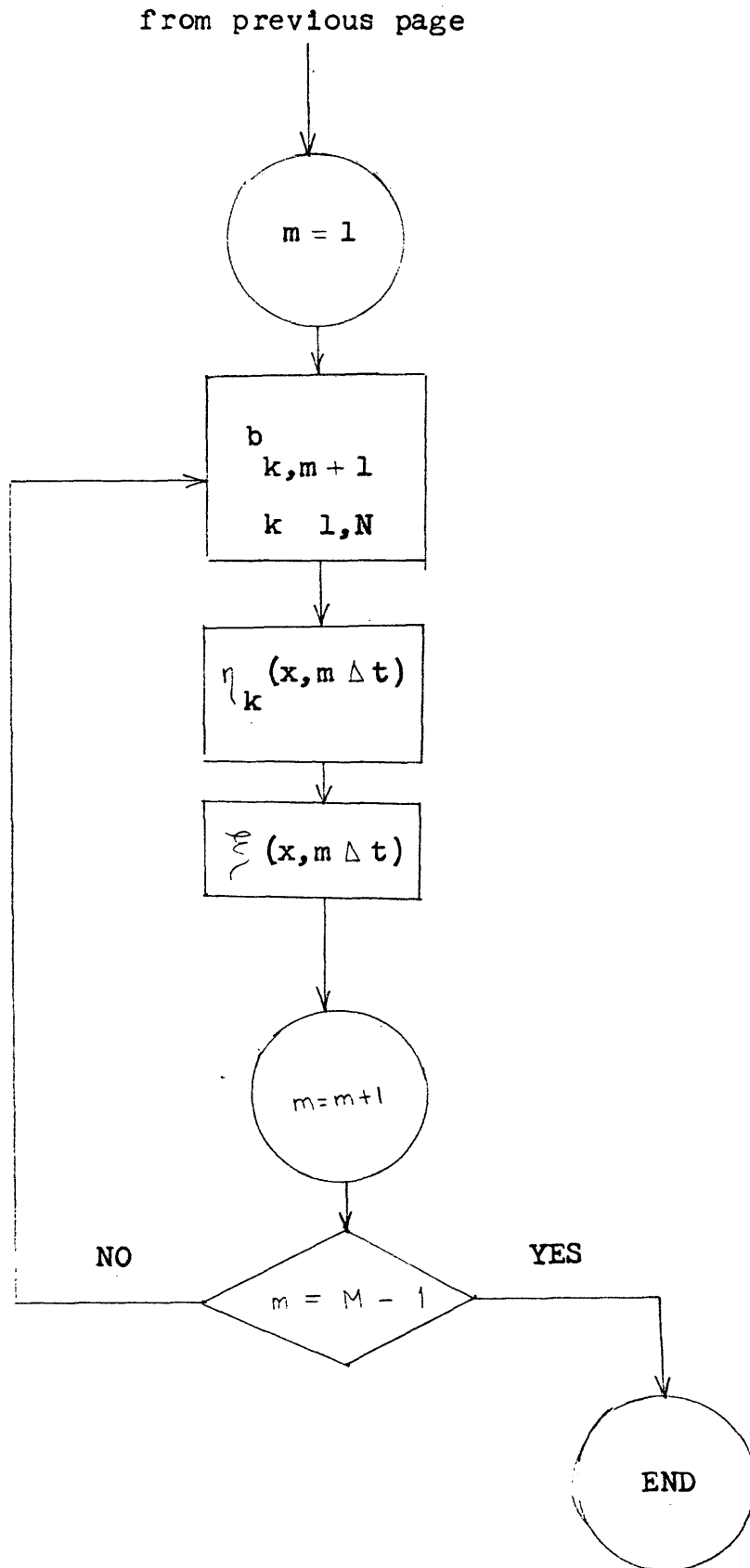
$$+ \frac{2}{h} (-\xi_{N,m-1} + 2\xi_{N,m} - \xi_{N,m+1}) X_k$$

$$k = 1, 2, \dots, N \quad (64)$$

$$m = 1, 2, \dots, M$$

which is illustrated in the following flow chart





## FORTRAN Implementation

## List of Principal Variables

Program symbol	Definition	
M	Total number of time steps.	
N	Number of intervals in the string	
v	Wave propagation velocity	
$\lambda$	<u>grid spacing in the x-direction</u> grid spacing in the t-direction	
R	Matrix with elements given by eq. (A-13) through (A-17)	
S	Vector with elements given by eq. (A-18)	
V	Vector with elements given by eq. (A-19)	
U	Matrix with elements given by eq. (A-29)	
T	Vector with elements given by eq. (A-30)	
R <sup>-1</sup>	Inverse matrix of R	
D	Matrix with elements given by eq. (60)	
P <sub>1</sub> Q <sub>1</sub> X <sub>1</sub>	} Vectors with elements defined by eq. (61)	
$\xi$		Transverse displacement of the string.
$\eta$		Quadratic approximation to $\xi$ .

### APPLICATIONS

We consider here two examples in the comparison of the solutions obtained with the use of our computational algorithm vs. the finite differences methods. In the first example, we illustrate a problem with a fixed boundary conditions at both ends; and in the second example we illustrate a problem with a free end at  $x=0$  and a fixed end at  $x=1$ .

#### First Example: Vibrating string with fixed boundary conditions

One of the first problems to be attacked through the use of the partial differential equations was that of the vibrations of a stretched flexible string. Today, it is still an excellent example of a fixed boundary conditions problem.

##### a) Finite differences method.

The solution of the problem is as follows: starting off with the first and second configurations, we evaluate, using eq. (36), the  $m$ th configuration for  $m = 3, 4, \dots, M$ .

The following data were used:

DELTA X= 0.01 m

DELTA T= 0.002 sec

LENGTH OF THE STRING = 1 m.

WAVE PROPAGATION VELOCITY 4 m/sec

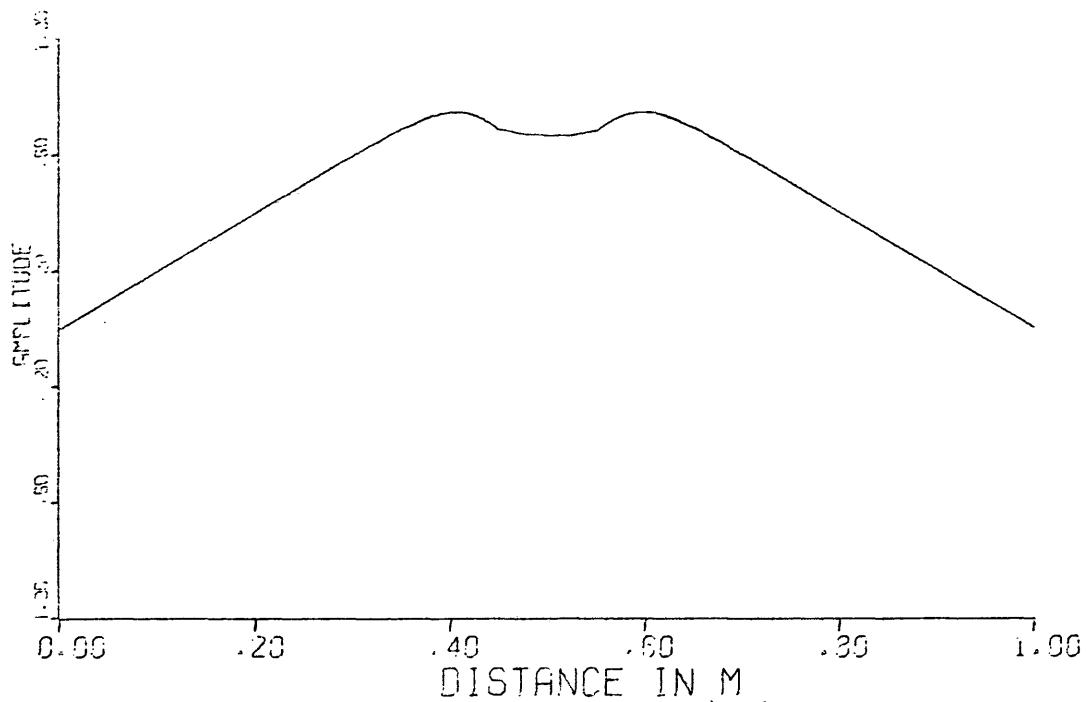
FIRST CONFIGURATION

$$\begin{aligned} \overset{\sim}{u}_{k_0} &= 2k \Delta x & 0 \leq k \leq 50 \\ \overset{\sim}{v}_{k_0} &= -2k \Delta x + 2 & 50 \leq k \leq 100 \end{aligned}$$

SECOND CONFIGURATION

The second configuration is calculated so that the initial velocity of the string is zero.

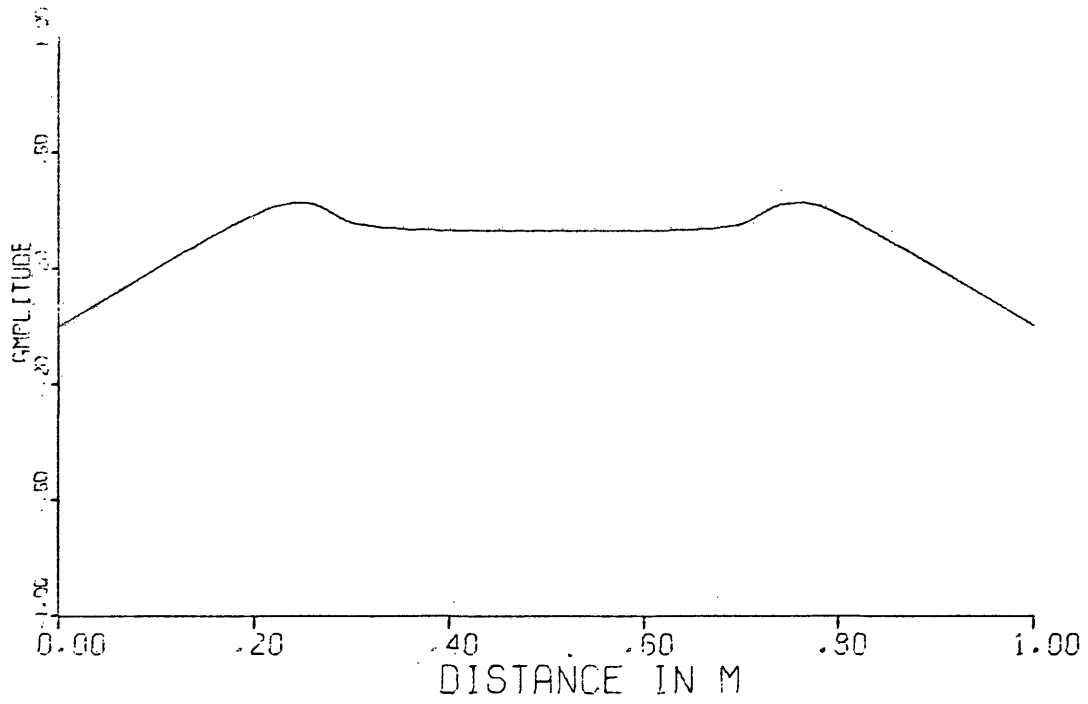
We show in the next five pages the configuration of the string at time step  $0.020 k \Delta t$ ,  $k = 0, 1, 2, \dots, 9$ .



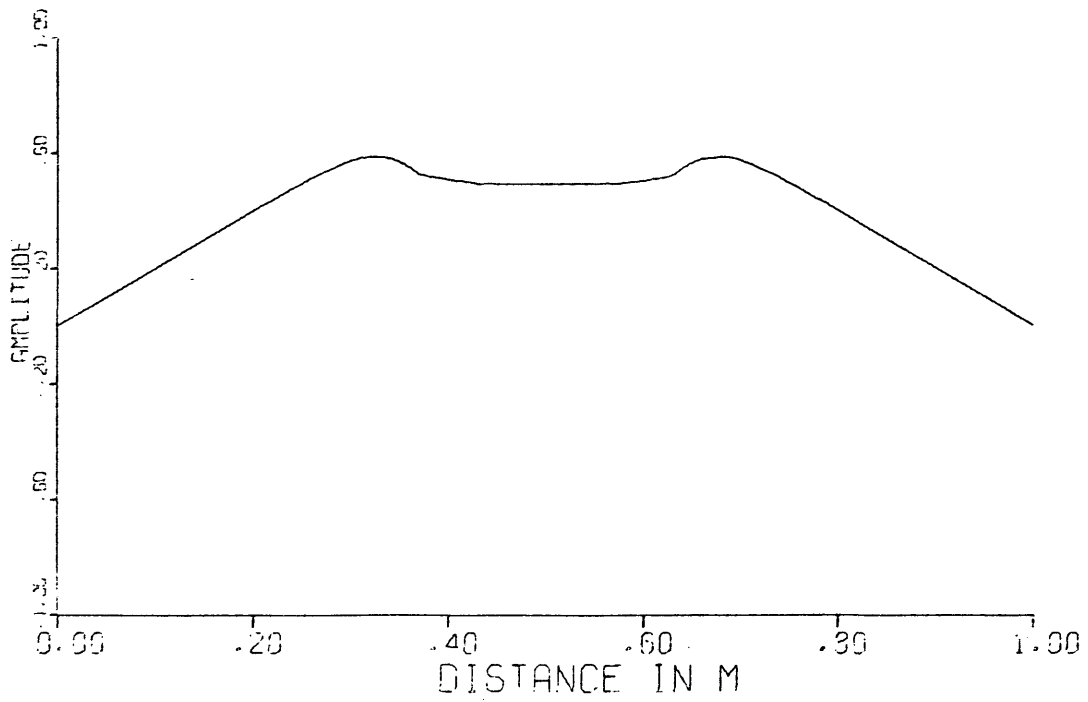
Configuration at  $T = 0.020$  sec



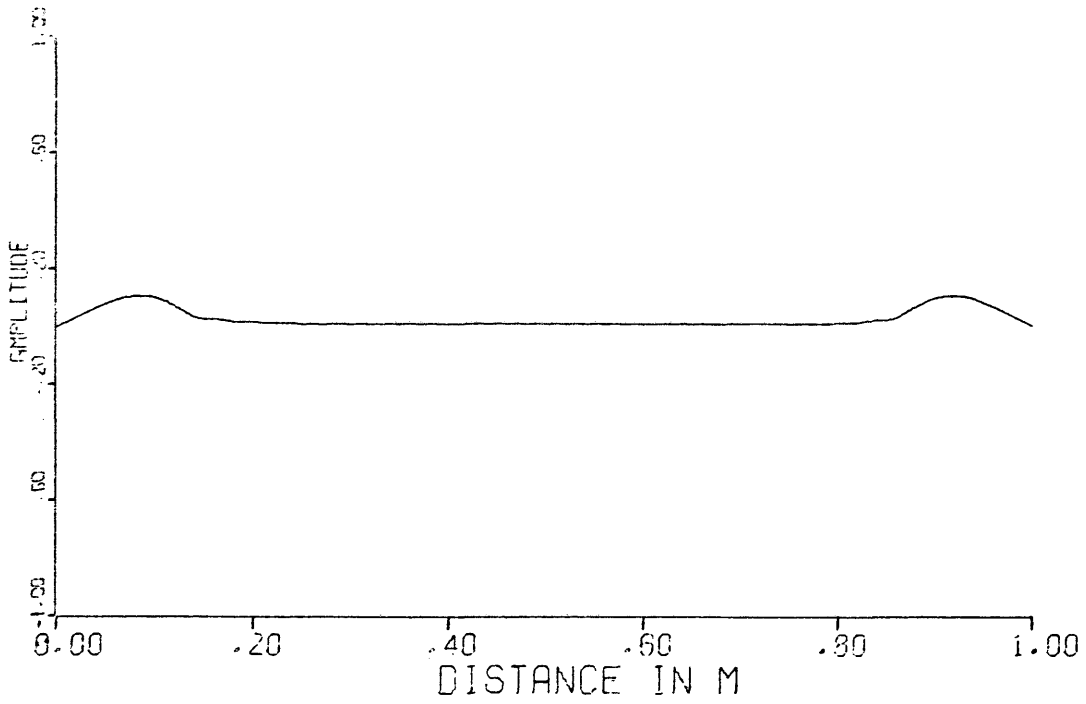
Configuration at  $T = 0.000$  sec



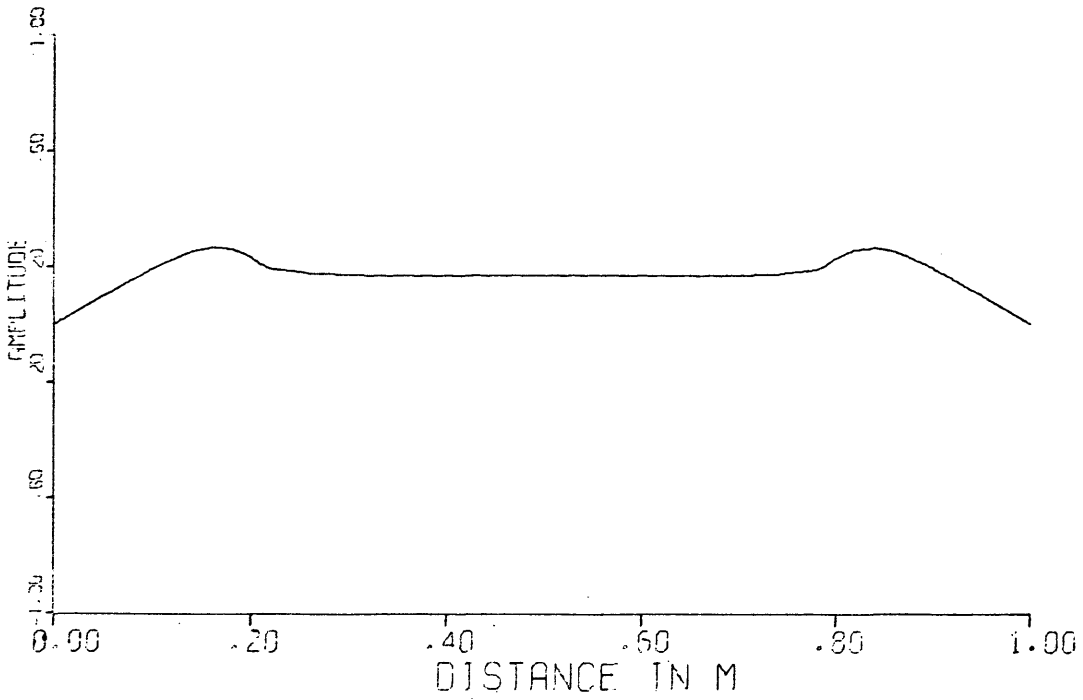
Configuration at  $T = 0.060$  sec



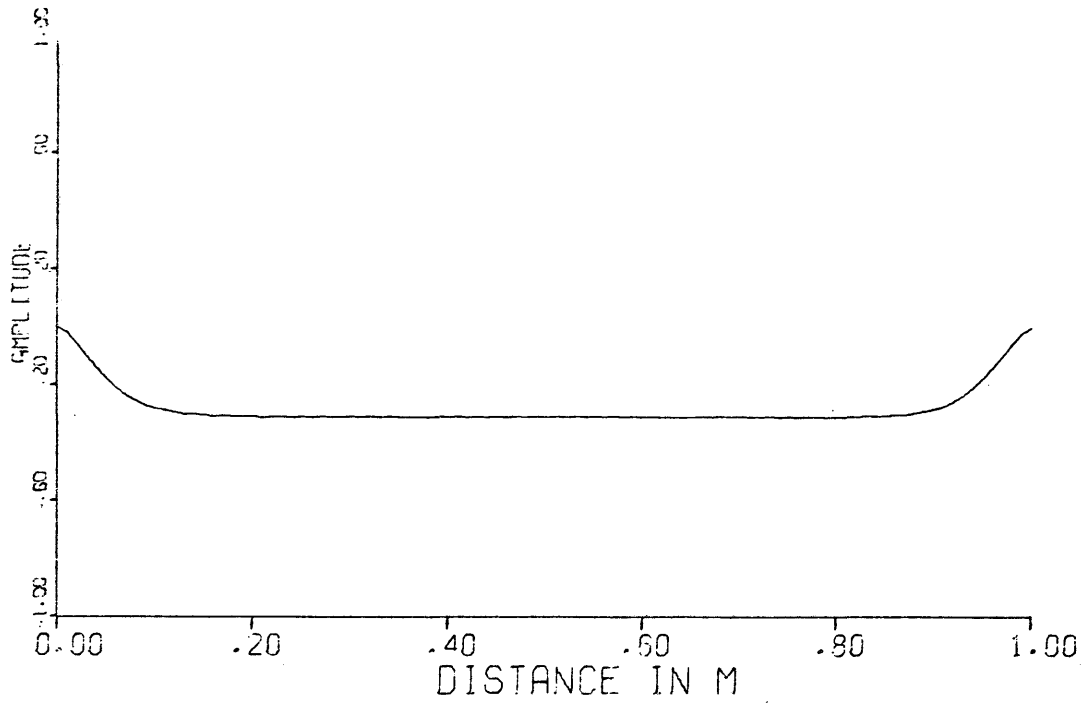
Configuration at  $T = 0.040$  sec



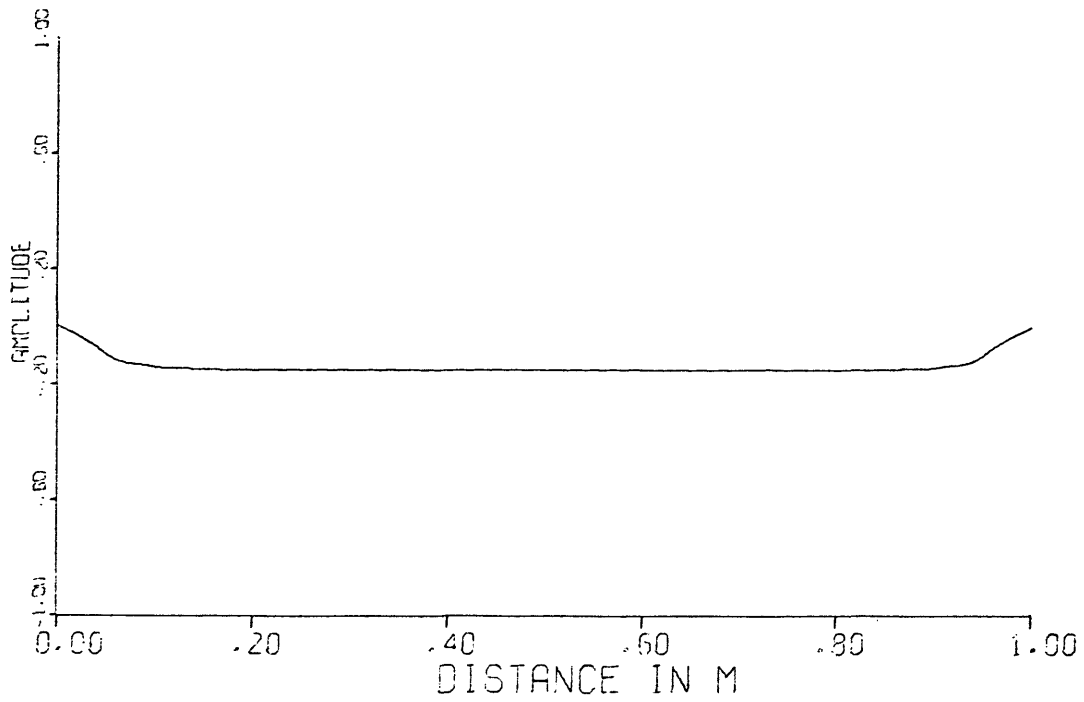
Configuration at  $T = 0.100$  sec



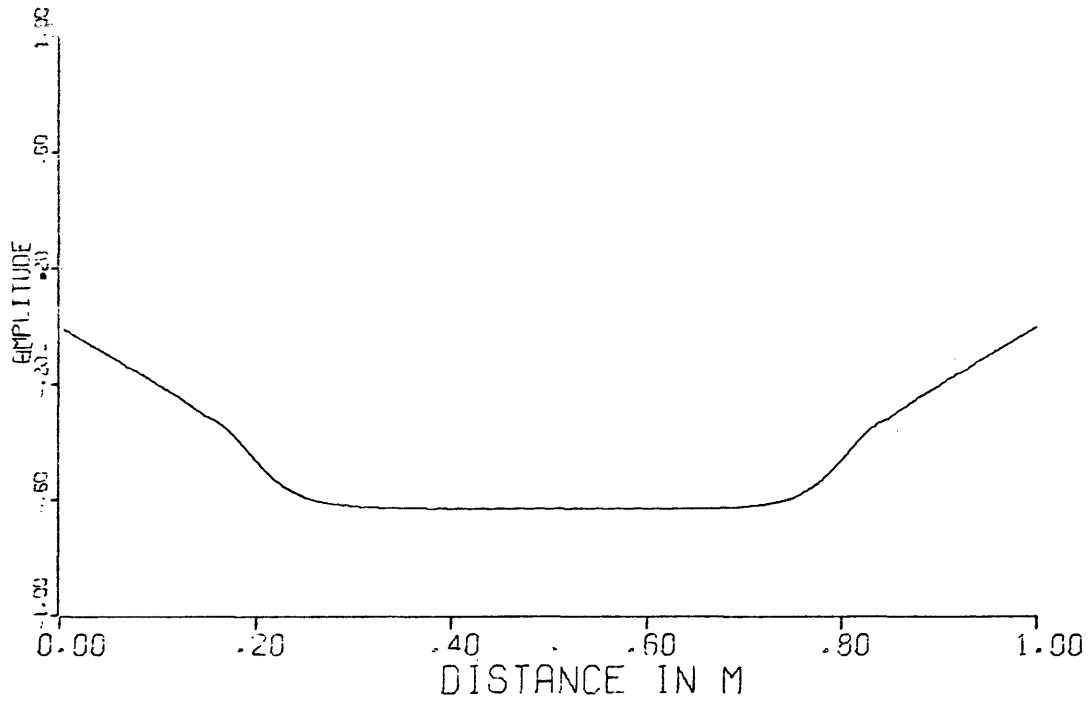
Configuration at  $T = 0.080$  sec



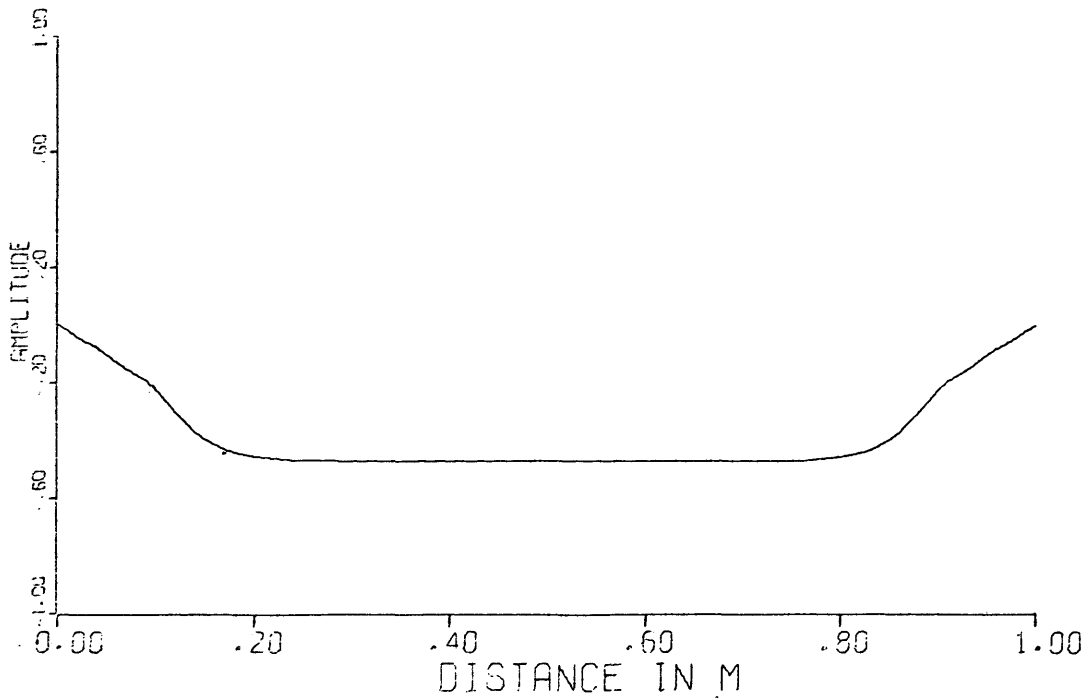
Configuration at  $T = 0.140$  sec



Configuration at  $T = 0.120$  sec



Configuration at  $T = 0.180$  sec



Configuration at  $T = 0.160$  sec

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## b) Variational method

Since  $\sum_{om}$  and  $\sum_{Nm}$  are zero for all  $m$ , the eq. (64) reduces to

$$b_{k,m+1} = -b_{k,m-1} + \left[ 2 - \frac{20v^2}{\lambda^2} D_{kk} \right] b_{km} \quad (65)$$

$m = 1, 2, \dots, M$   
 $k = 1, 2, \dots, N$

The solution of the problem is as follows: given the coefficients  $b_{k0}$  and  $b_{k1}$ ,  $k = 1, 2, \dots, N$ , we calculate by means of eq. (65) the coefficients  $b_{km}$  at the  $m$ th. configuration,  $m = 3, 4, \dots, M$ . Having obtained these coefficients, we calculate, using eq. (51), the  $m$ th. configuration of the string.

The variational method is based upon having continuity of the function  $\xi(x, m \Delta t)$  and its derivative at all times, so we cannot use the same example as in part (a), due to the fact that the first configuration of the string has a discontinuity in its derivative at  $x = 0.50$  m. Instead, we will use a first configuration that has the shape of a sine wave.

The following data were used:

DELTA X = 0.1 m

DELTA T = 0.002 sec

LENGTH OF THE STRING = 1 m

WAVE PROPAGATION VELOCITY = 4 m/sec

COEFFICIENTS AT THE FIRST CONFIGURATION:  $b_{k0}$ ,  $k = 1, 10$

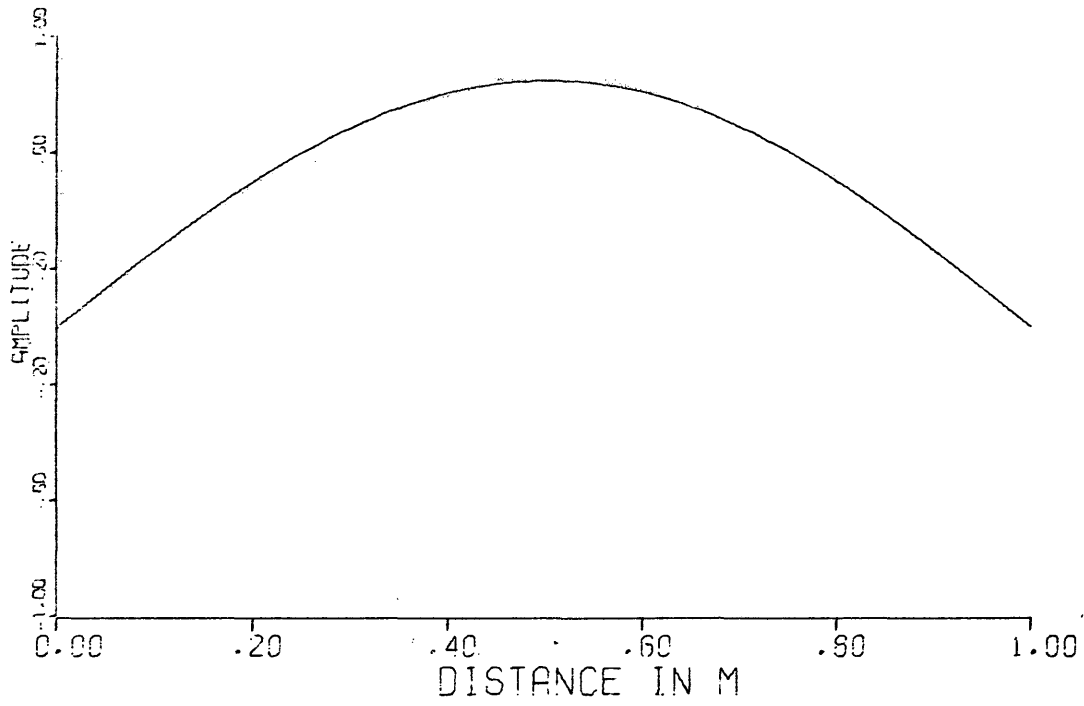
3.14159      2.98784      2.54161      1.84659      0.97081  
 0.00000      -0.97081      -1.84659      -2.54161      -2.98784

COEFFICIENTS AT THE SECOND CONFIGURATION:  $b_{k1}$ ,  $k = 1, 10$

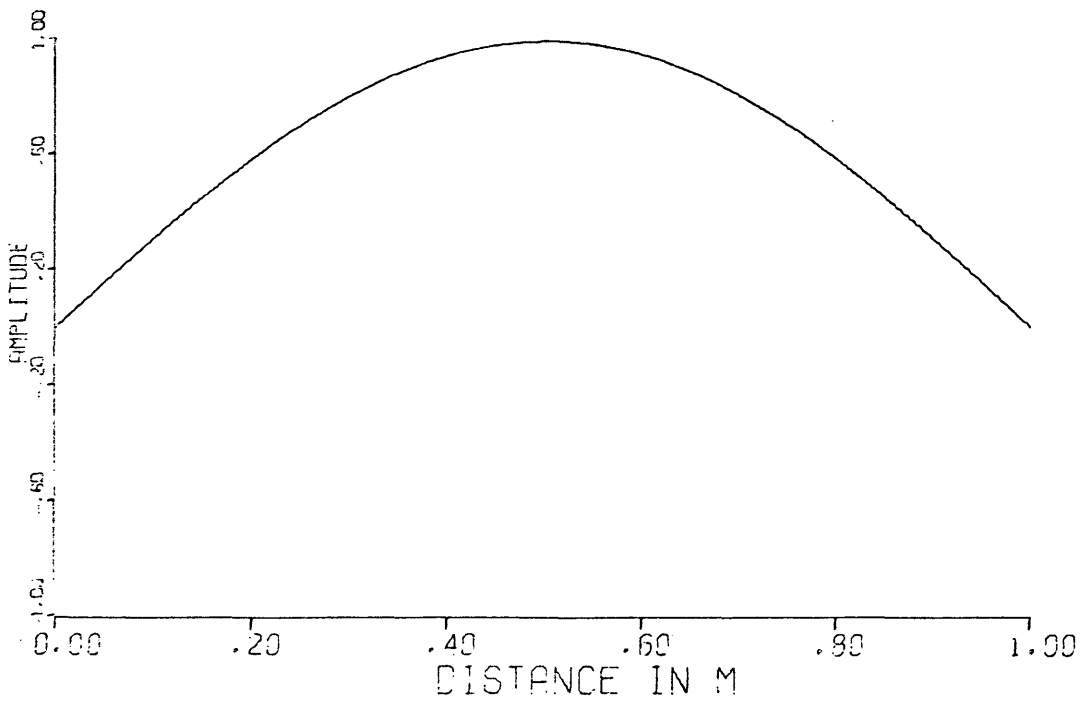
The coefficients at the second configuration are calculated so that the initial velocity of the string is zero.

Note that we divide the total length of the string into 10 intervals, making the sampling in the x direction ten times greater than the one used in the finite differences method.

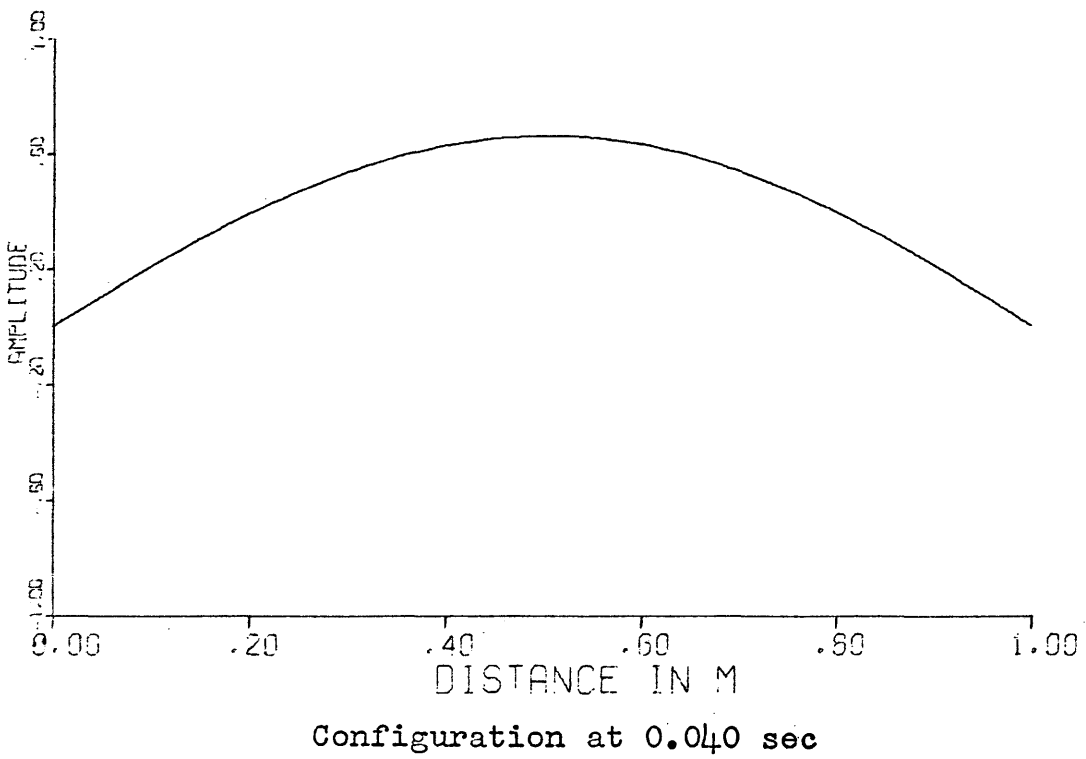
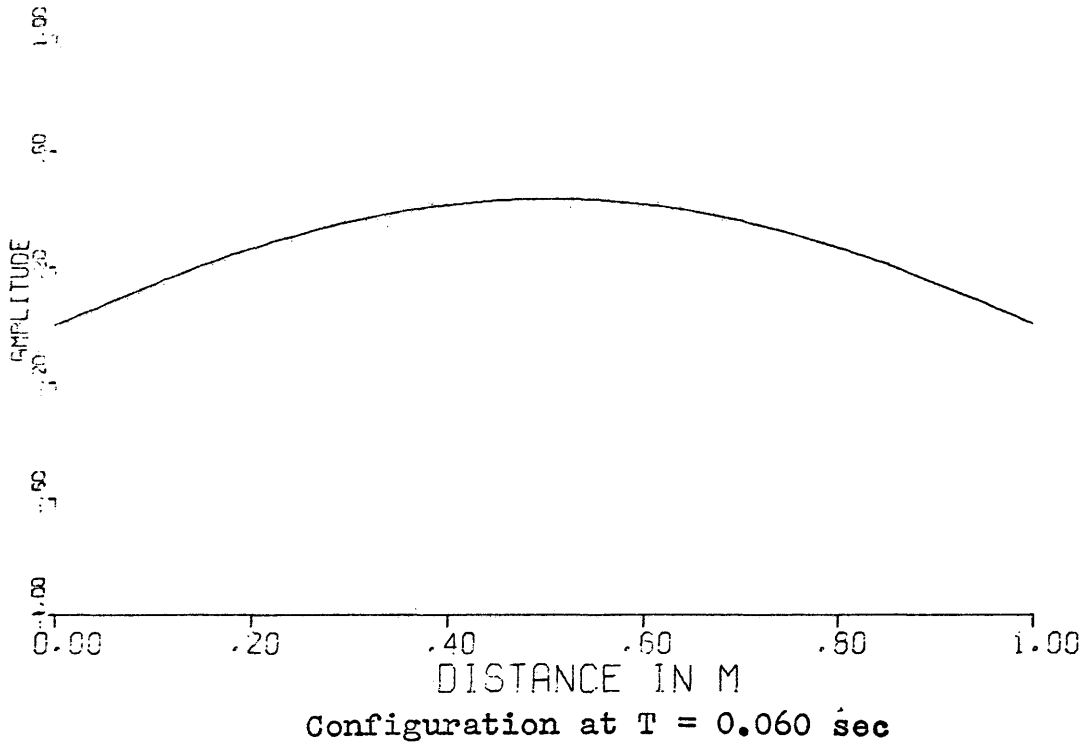
We show in the next five pages the configuration of the string at time step  $0.020 k \Delta t$ ,  $k = 0, 1, 2, \dots, 9$ .

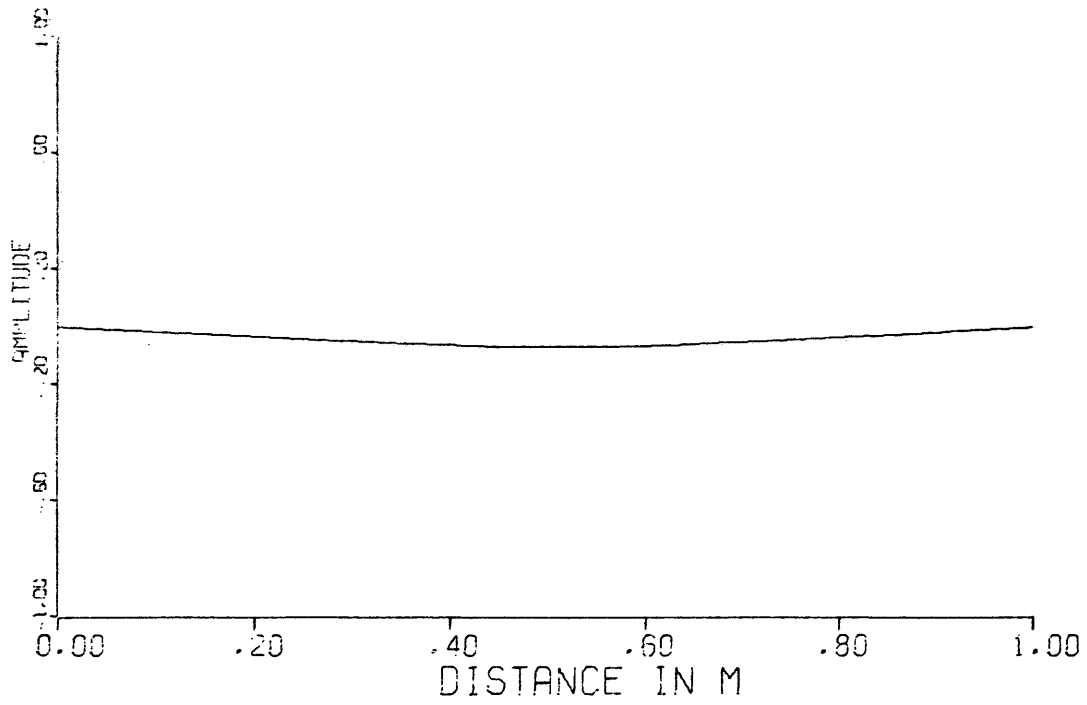


Configuration at T = 0.020 sec

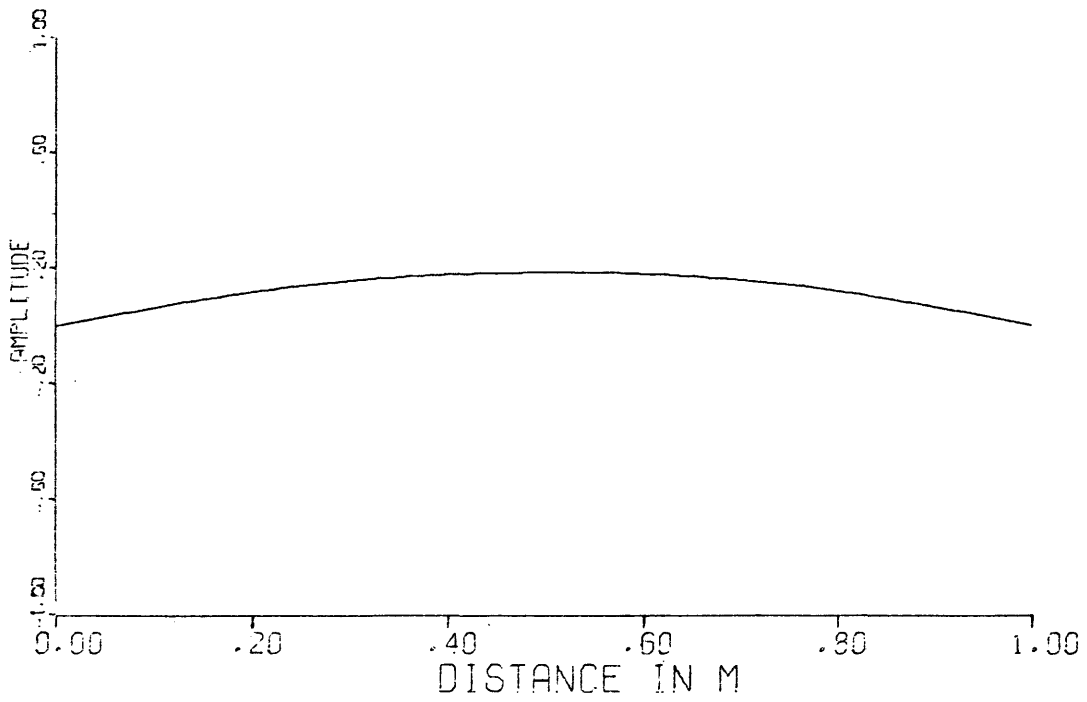


Configuration at T = 0.000 sec

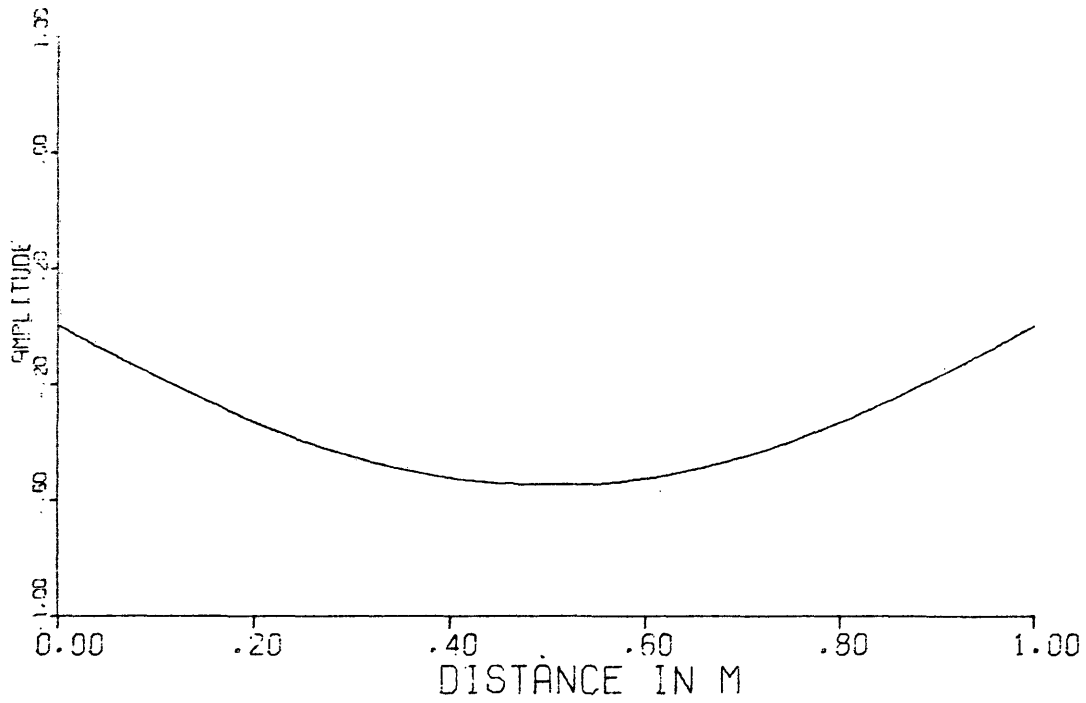




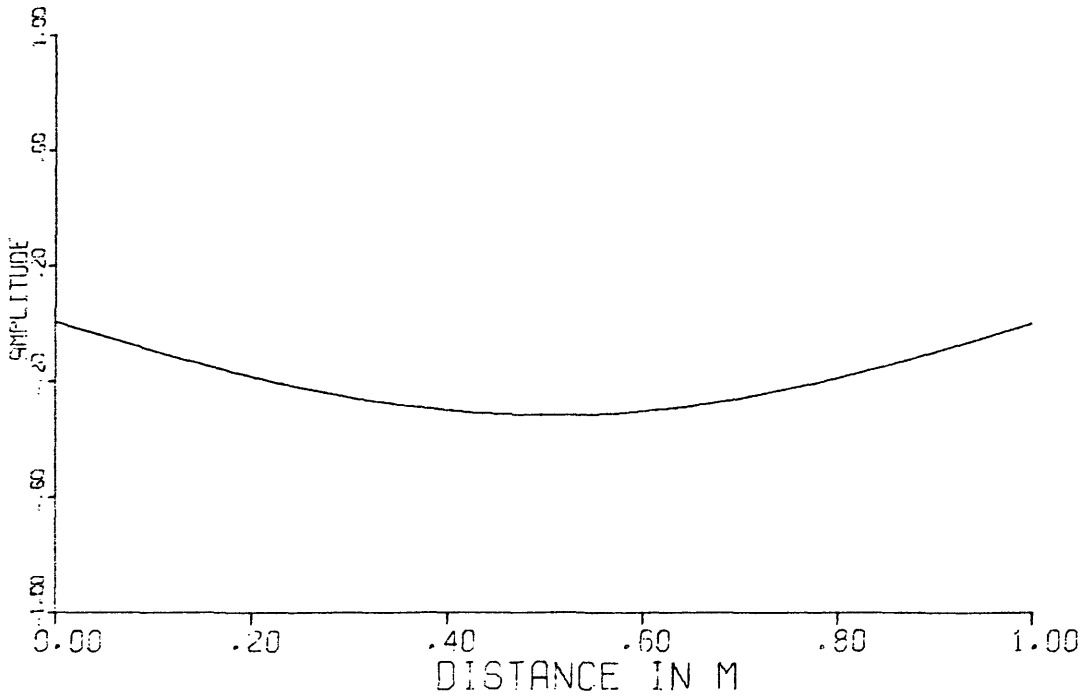
Configuration at  $T = 0.100$  sec



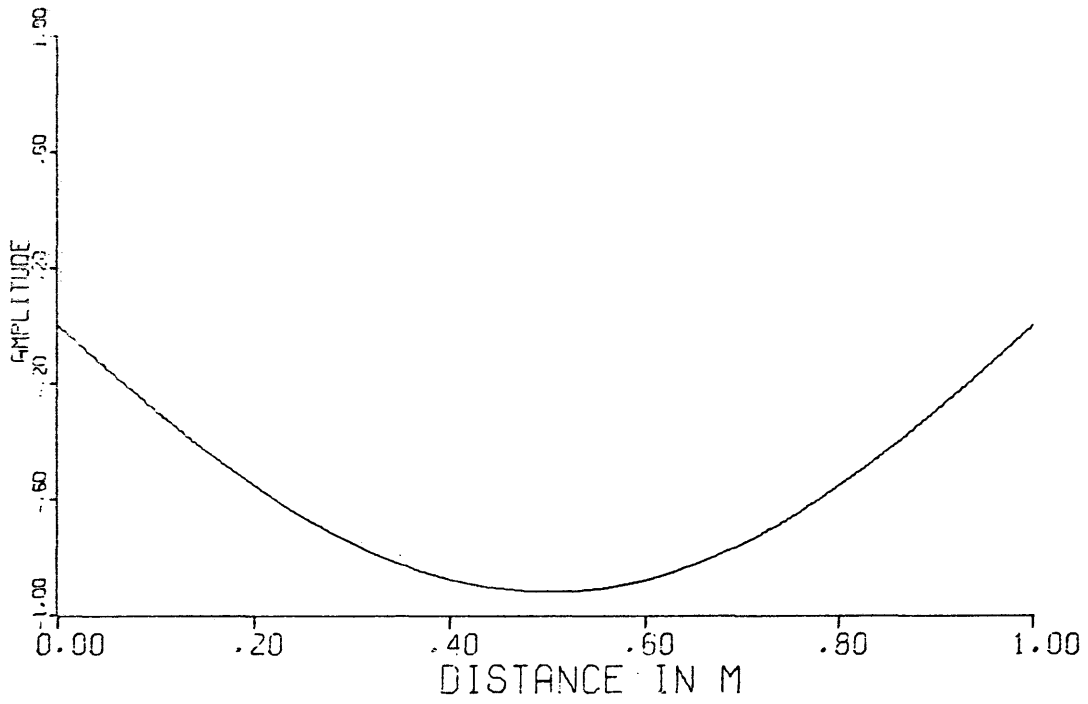
Configuration at  $T = 0.080$  sec



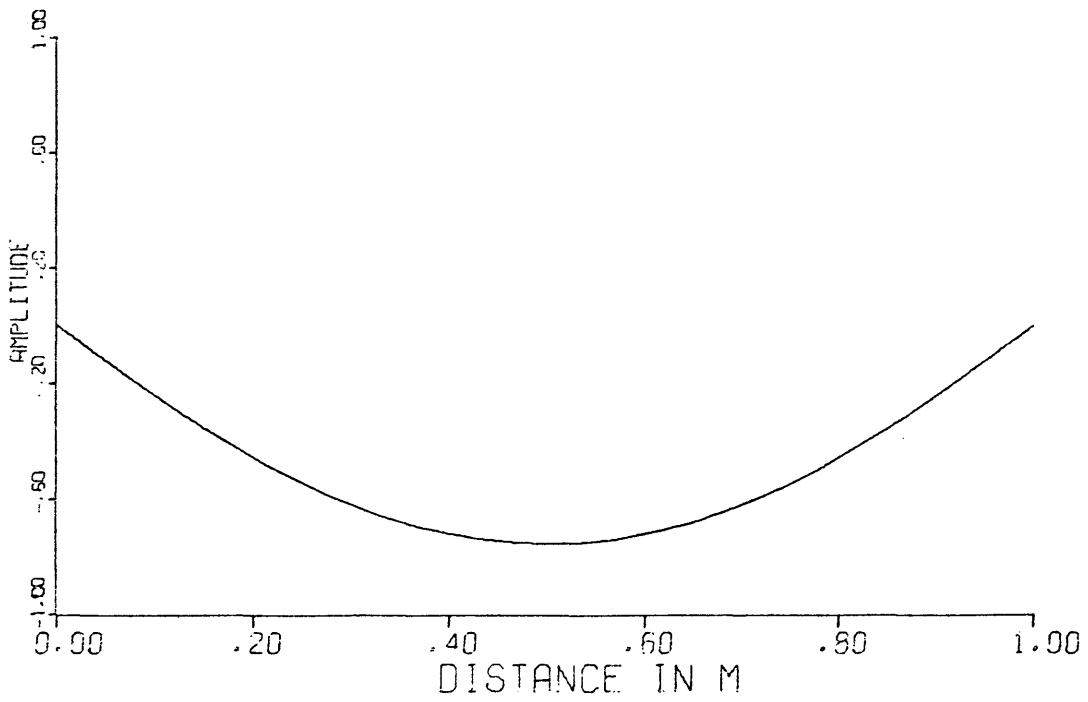
Configuration at T = 0.140 sec



Configuration at T = 0.120 sec



Configuration at T = 0.180 sec



Configuration at T = 0.160 sec

Second Example: Vibrating string with one end free and the other fixed

Consider a vibrating string problem with a free end at  $x = 0$  and a fixed end at  $x = l$ . In this case we excite the system at the free end with the function  $\xi(0,t)$ .

Any numerical formulation has its own difficulties with respect to stability, accuracy, and choice of the sampling interval in both the space and time directions. One way to test the response of a numerical algorithm with respect to the frequency content of the driving function  $\xi(0,t)$  is to excite the system first with an impulse  $\delta(t)$ . According to wave propagation theory, the function is seen to be a disturbance travelling in the  $x$  direction with velocity  $v$ . Thus if we take the Fourier Transform of  $\xi(x,t)$  for a fixed  $x$ , which is obtained in the numerical formulation we should obtain, in theory, a white spectrum. The part of the spectrum that is flat is the region where we can obtain accurate solutions; thus in order to accomplish this result, we must excite the system with driving functions whose Fourier spectrum is within this region.

We show in Fig. 3, the behavior of the variational formulation. We note that the flat spectrum is obtained between 0 and 50 hertz. In order to be on the safe side, we are going to experiment with a transient sine wave, which has a period of 40 ms.

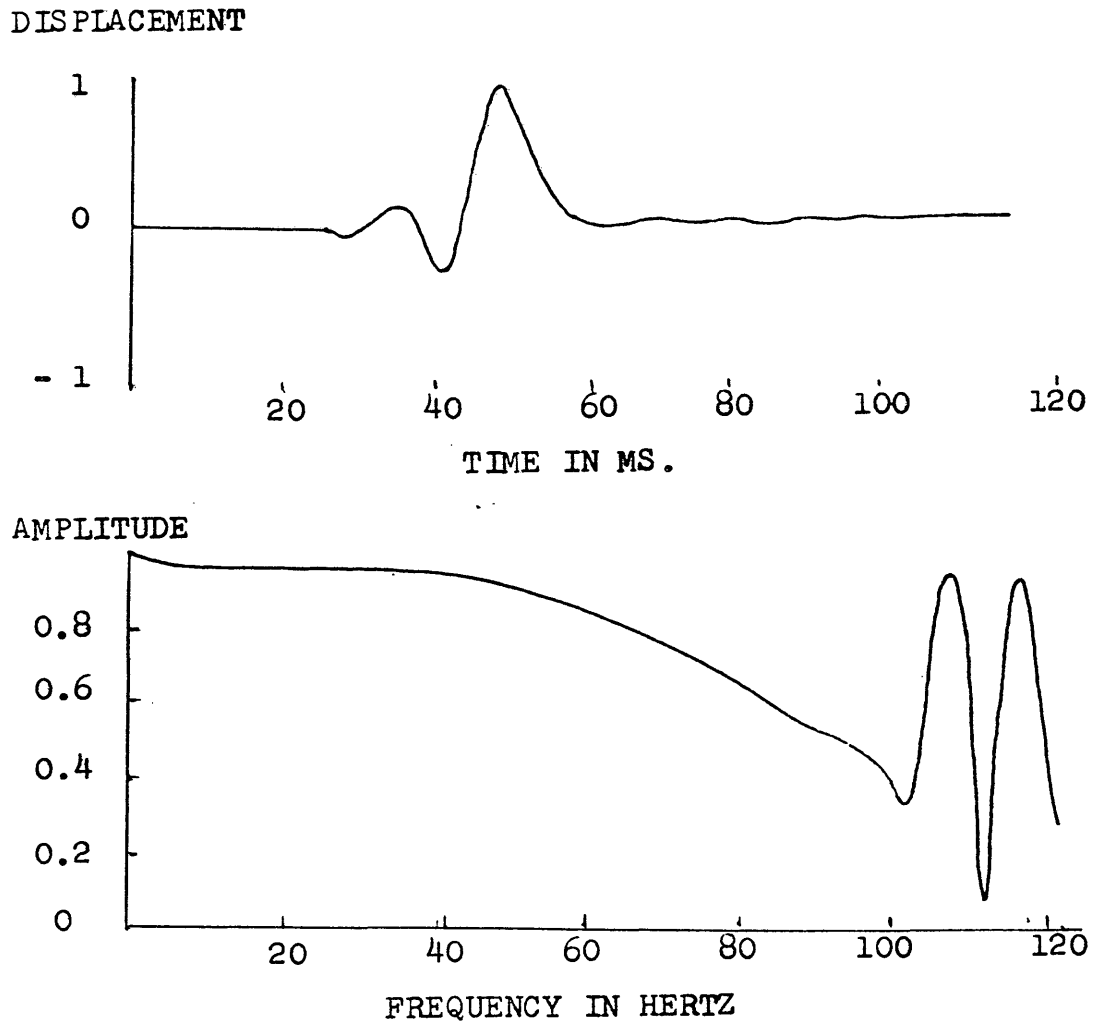


Figure 3. Impulse response and its Fourier spectrum at the distance of 0.2 m when the function of the system is an impulse.

a) Finite differences method

The method of solution is similar to that of the case in which we have fixed boundary conditions.

The following data were used:

DELTA X: 0.005 m

DELTA T: 0.001 sec

LENGTH OF THE STRING = 1 m

WAVE PROPAGATION VELOCITY = 4 m/sec

BOUNDARY CONDITION AT  $x = 0$

$$\xi_{0m} = \sin(50\pi m \Delta t) \quad 0 \leq m \leq 40$$

$$= 0 \quad m > 40$$

FIRST CONFIGURATION:

$$\xi_{n0} = 0, \quad n = 0, 200$$

SECOND CONFIGURATION:

$$\xi_{n1} = 0 \quad n = 0, 200$$

b) Variational method

Since  $\xi(N, m)$  is zero for all  $m$ , the eq. (64) reduces

to

$$b_{k, m+1} = -b_{k, m-1} + \left[ 2 - \frac{20v^2}{\lambda^2} D_{kl} \right] b_{lm}$$

$$- \frac{20v^2}{h \lambda^2} Q_k \xi_{0m} + \frac{2}{h} \left( -\xi_{0, m-1} + 2\xi_{0m} - \xi_{0, m+1} \right) P_k$$

$k = 1, 2, \dots, N$   
 $m = 1, 2, \dots, M$

We obtain from this equation the coefficients  $b_{km}$ , and then we follow the same procedure outlined for the case of fixed boundary conditions.

The following data were used:

DELTA X = 0.02 m

DELTA T = 0.001 sec

LENGTH OF THE STRING = 1 m

WAVE PROPAGATION VELOCITY = 4 m/sec

BOUNDARY CONDITION AT  $x = 0$

$$\xi_{0n} = \sin(50\pi m \Delta t) \quad 0 \leq m \leq 40$$

$$= 0 \quad m > 40$$

COEFFICIENTS AT THE FIRST CONFIGURATION

## COEFFICIENTS AT THE SECOND CONFIGURATION

$$b_{11} = -17.643$$

$$b_{ni} = 0 \quad n = 2, 50$$

The coefficient  $b_{11}$  was obtained by fitting the quadratic between the grid points  $\xi_{01}$  and  $\xi_{11}$ .

We show in Fig. 4 the plot  $x$  vs  $t$ . which reveals that the wave propagation velocity  $v$  is conserved through the process.

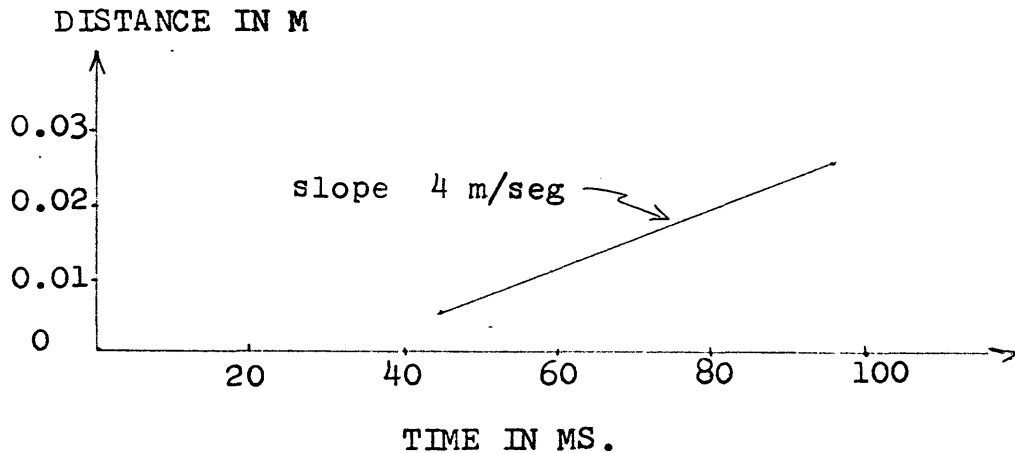
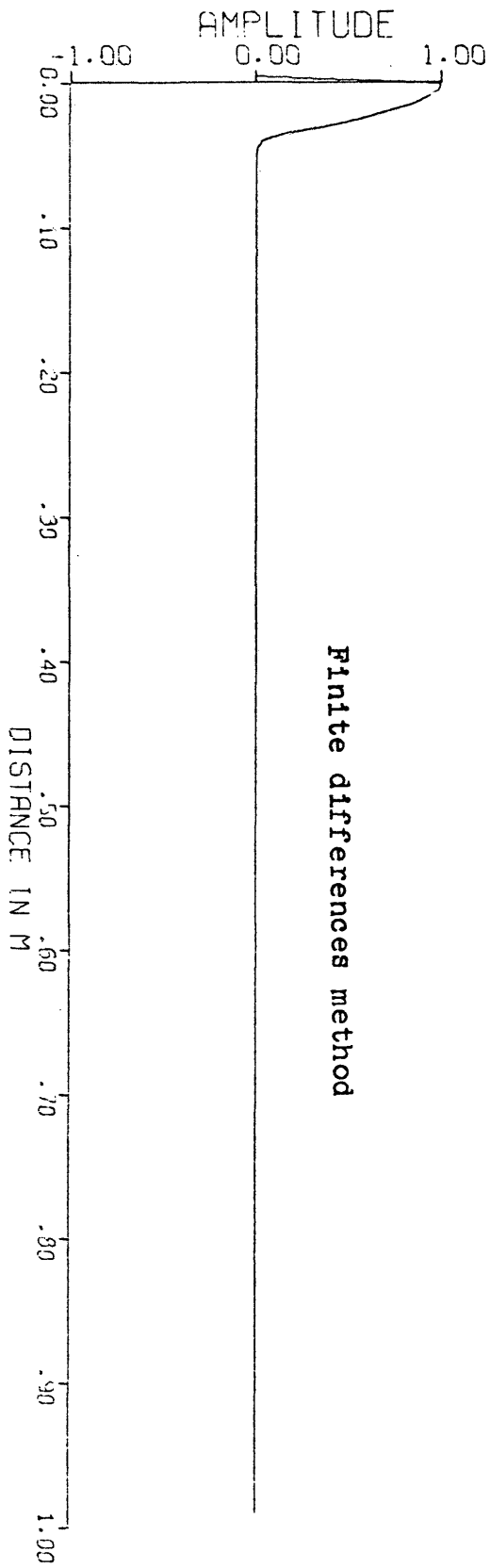
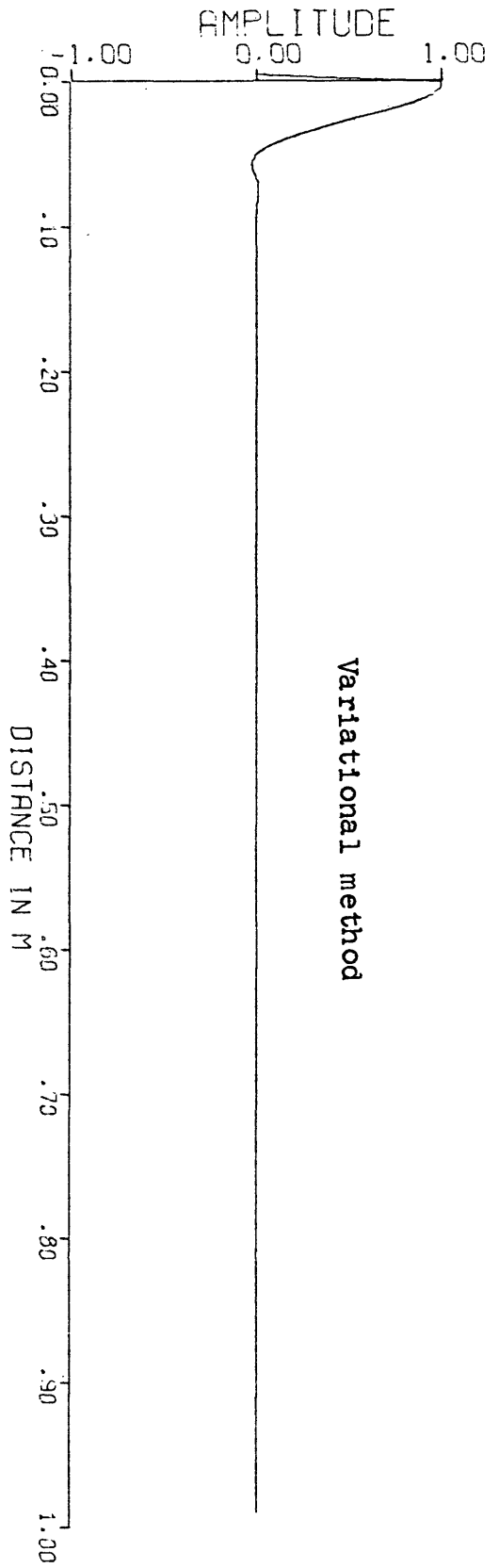


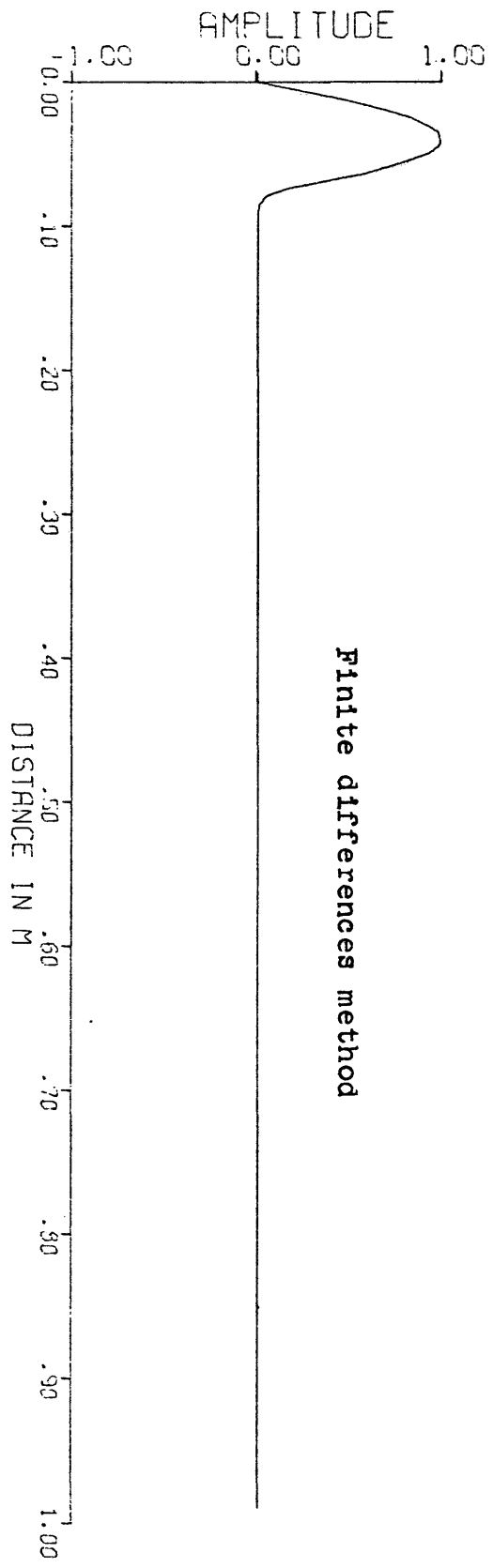
Figure 4. Distance-time plot showing that the wave propagation velocity is conserved in the numerical calculations.

Note that we divide the length of the string into 50 intervals, thus making the sampling interval in the  $x$  direction four times greater than the one used in the finite differences method. In the next ten pages follow the configuration of the string as the time goes on.

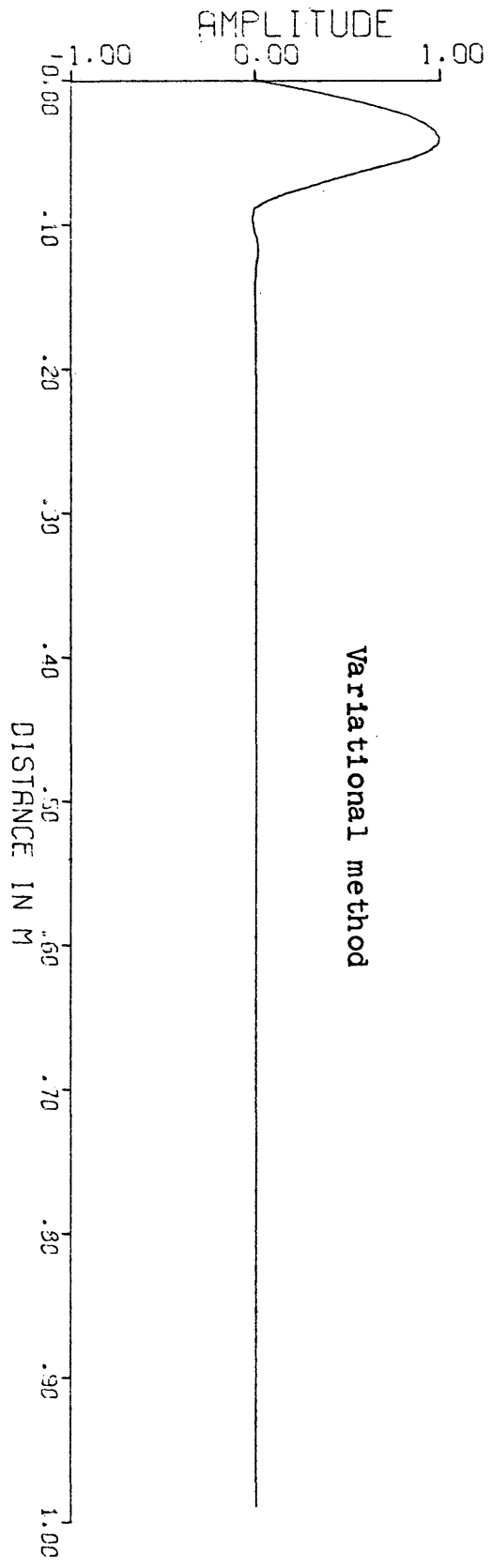


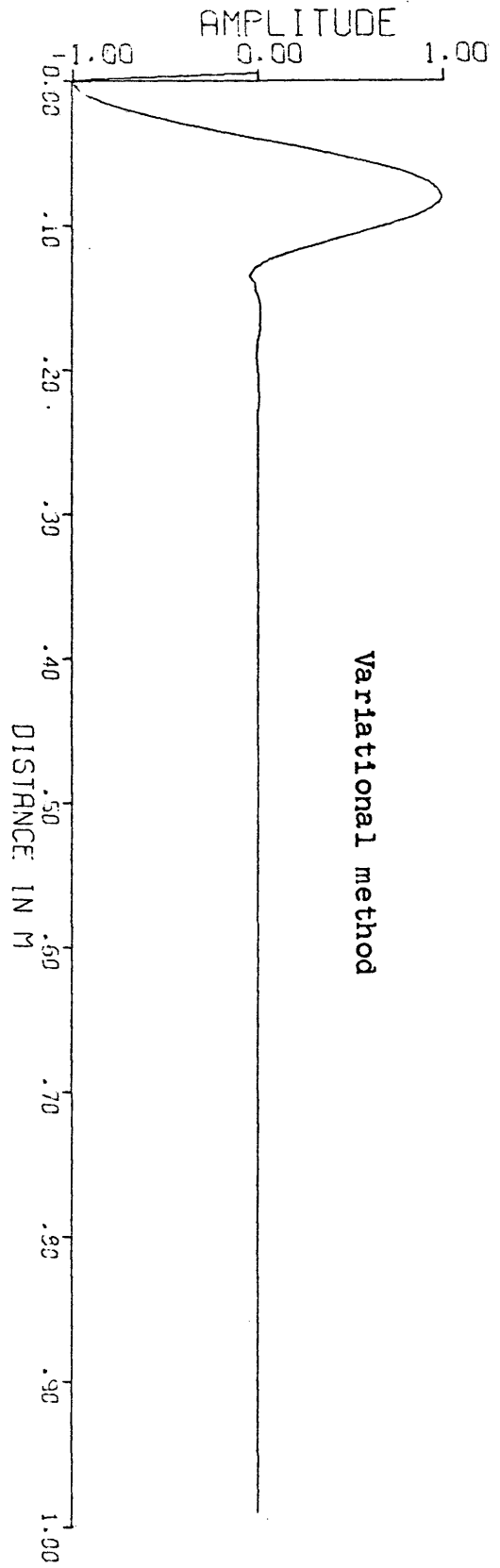
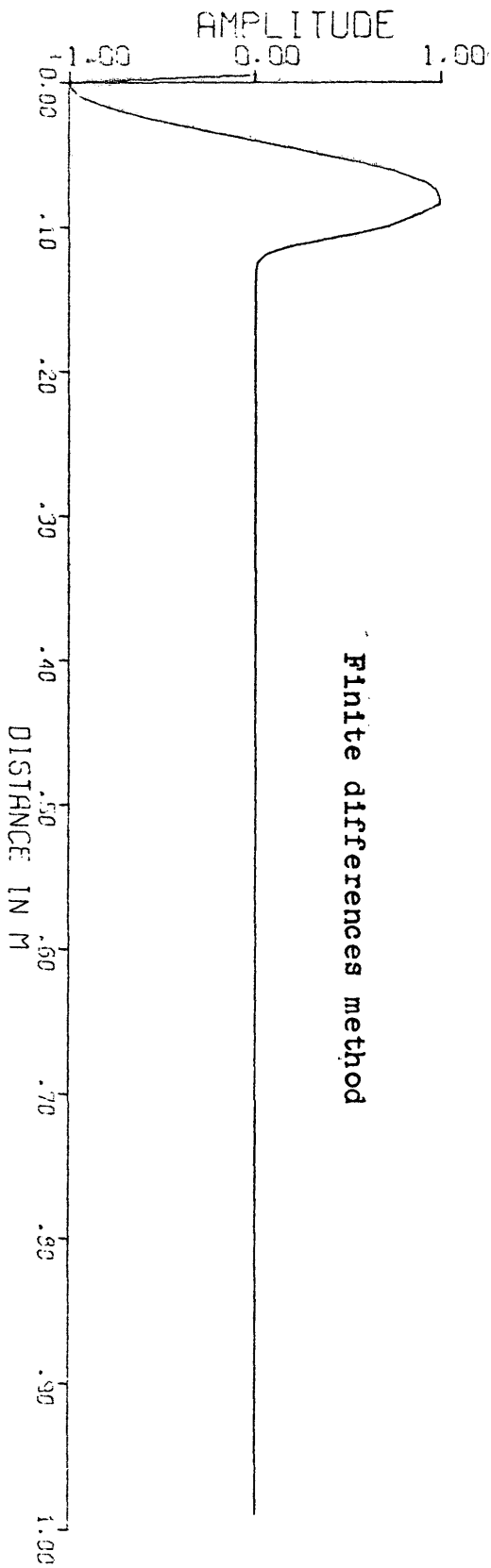
Configuration at  $T = 0.010$  sec.

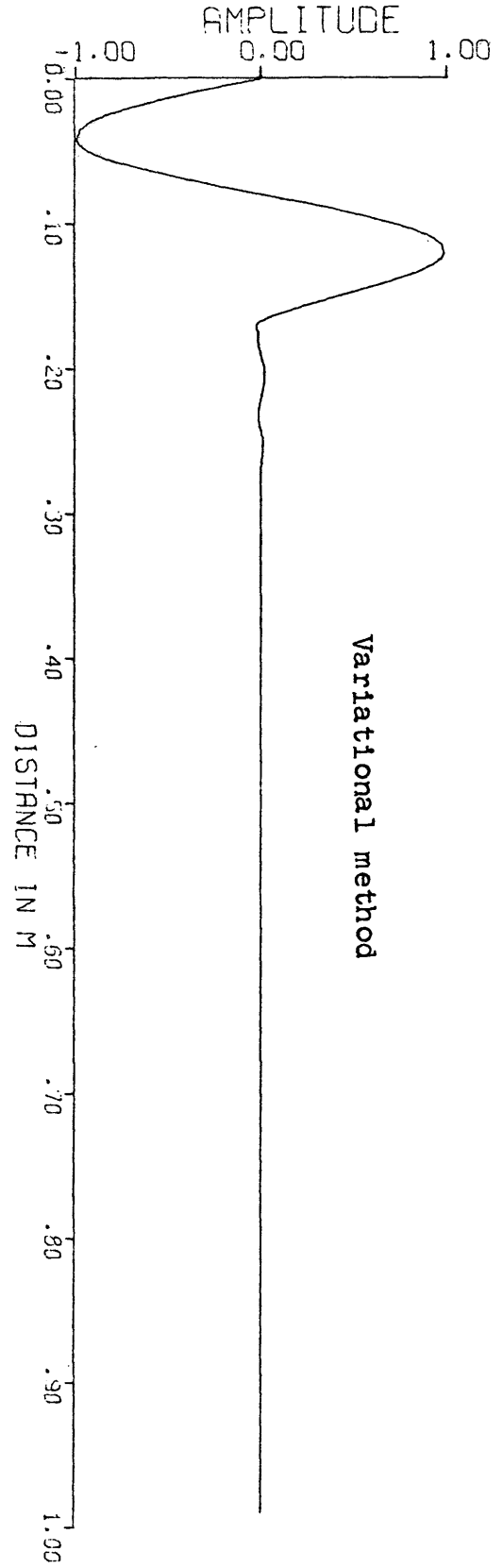
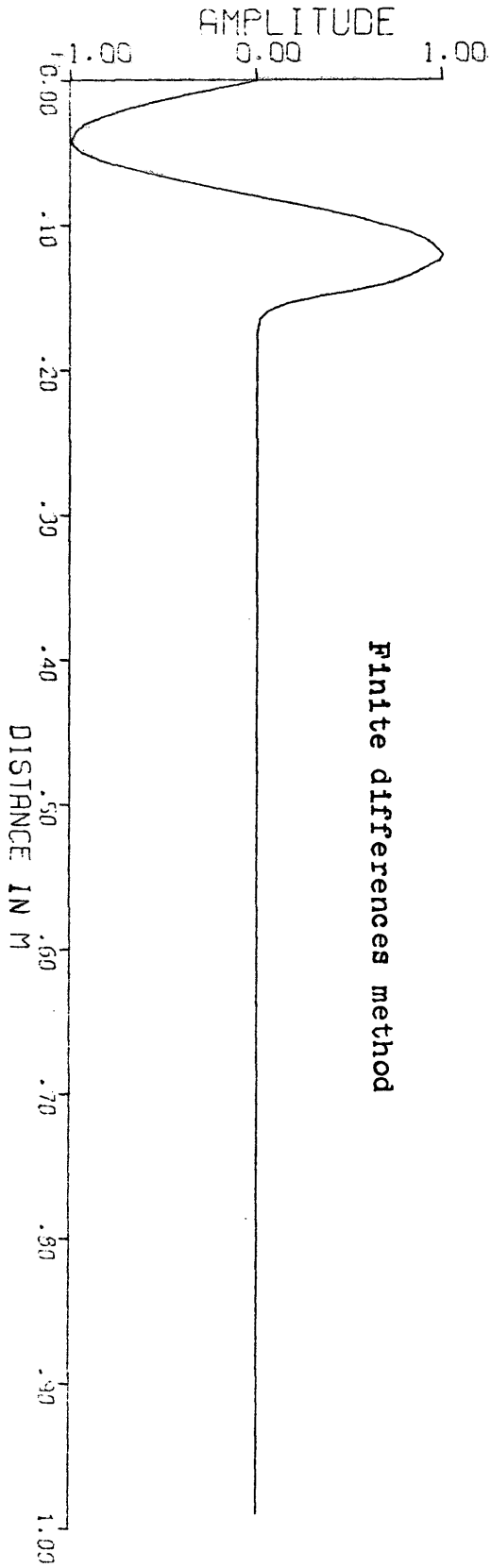


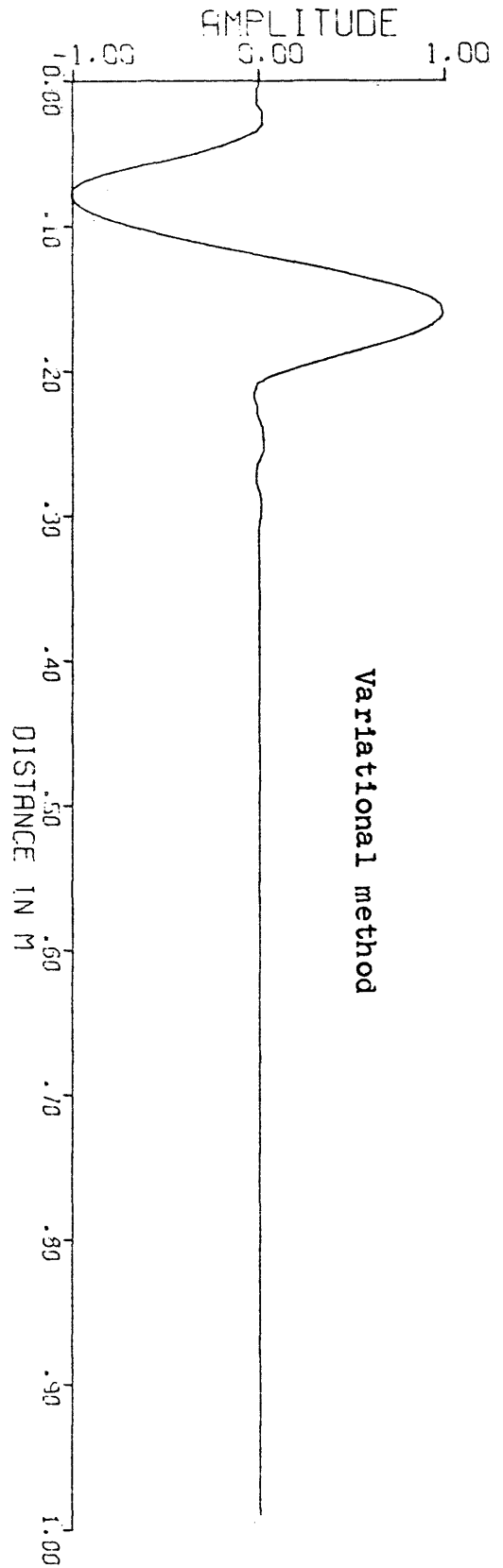
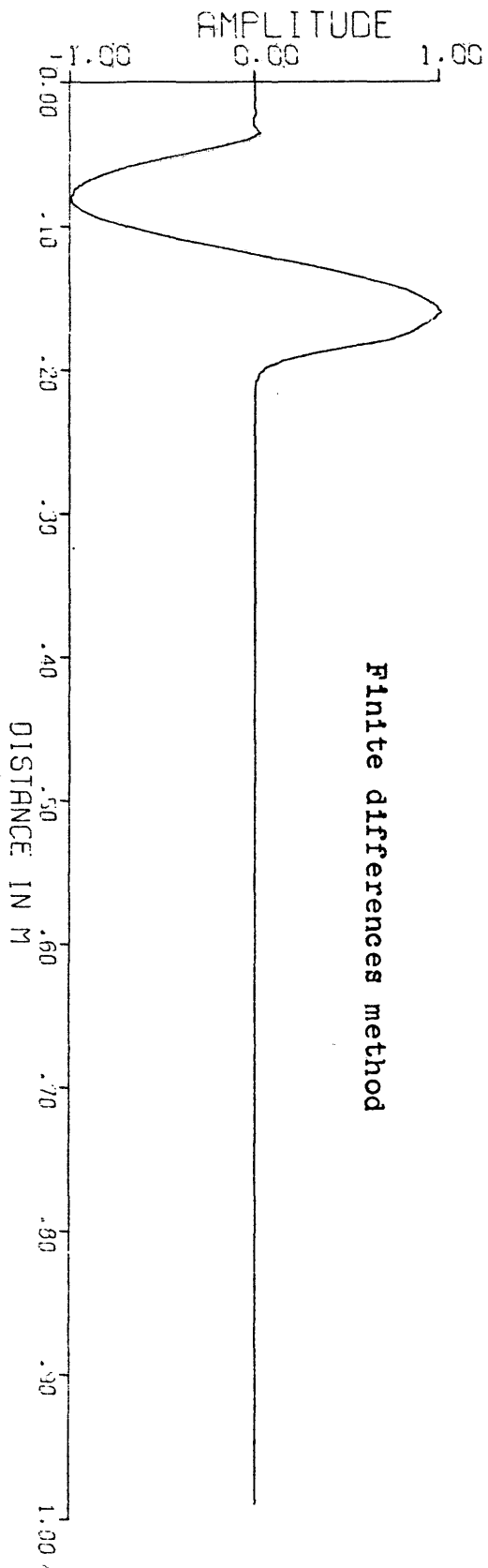


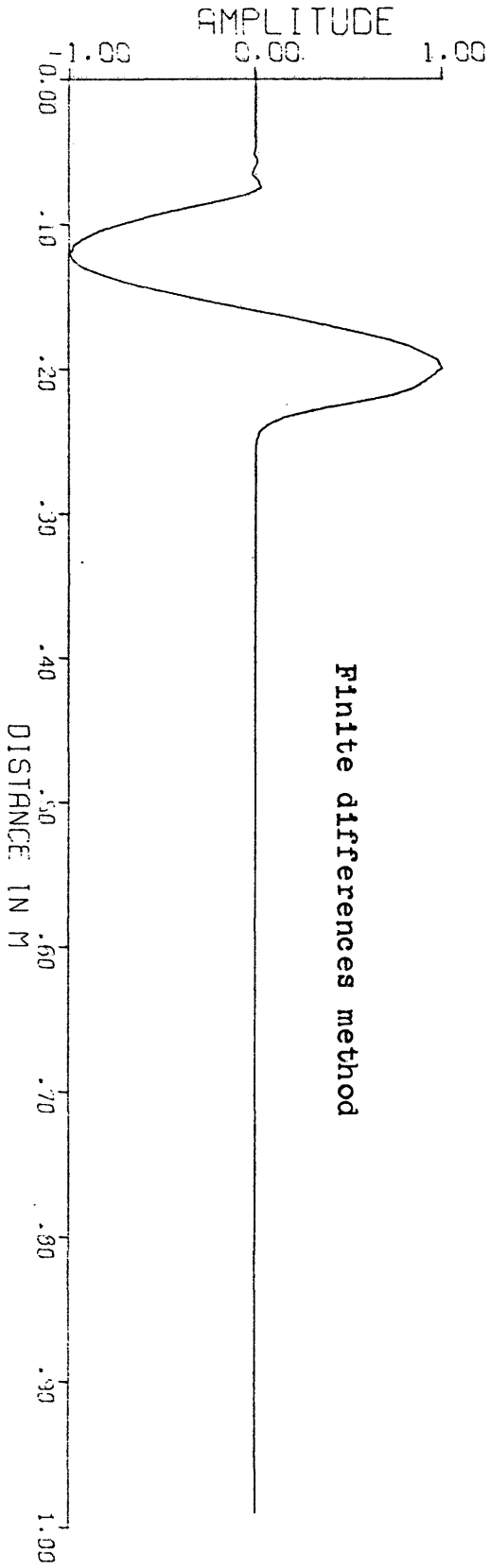
Configuration at  $T = 0.020$  sec



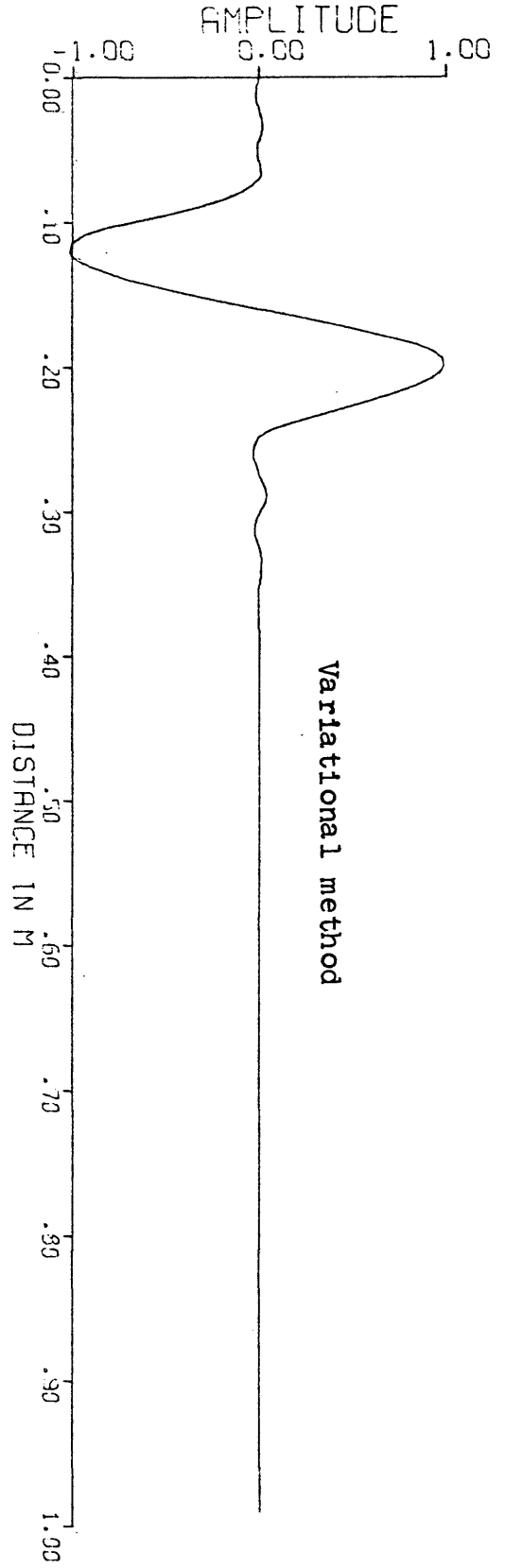


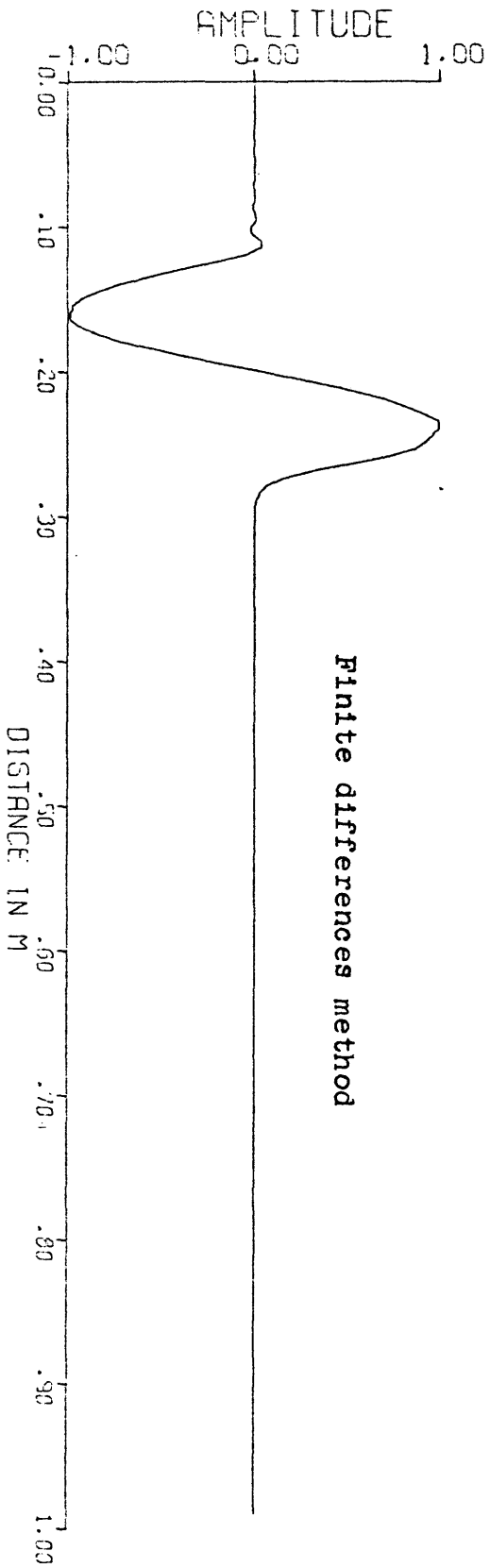




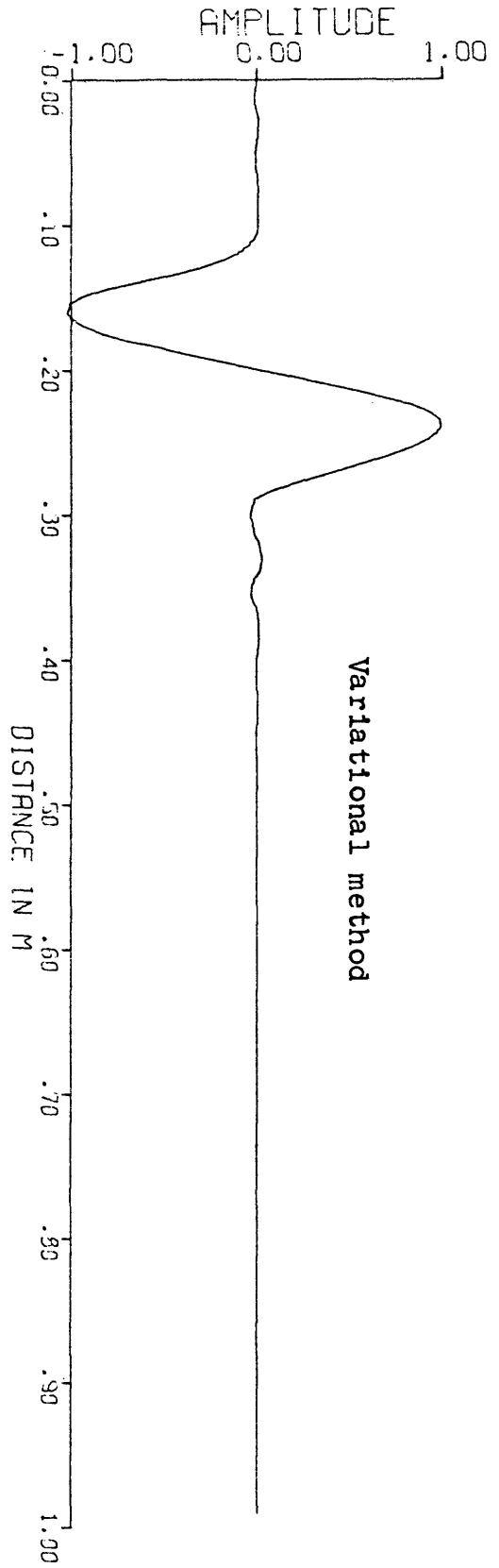


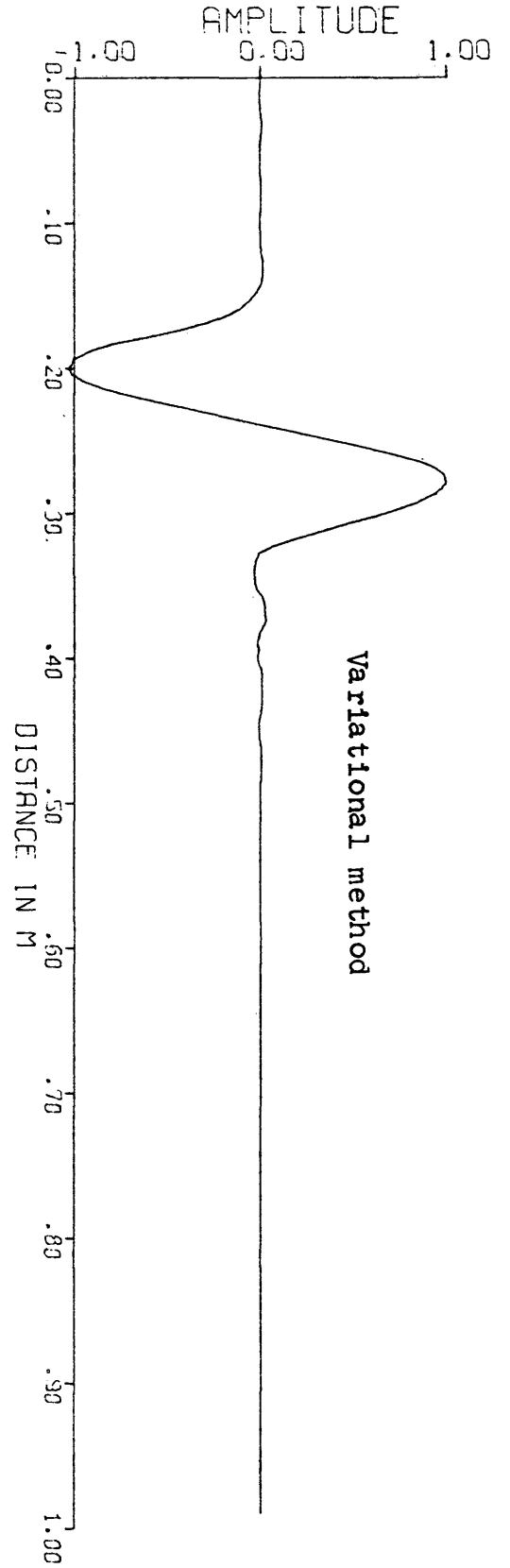
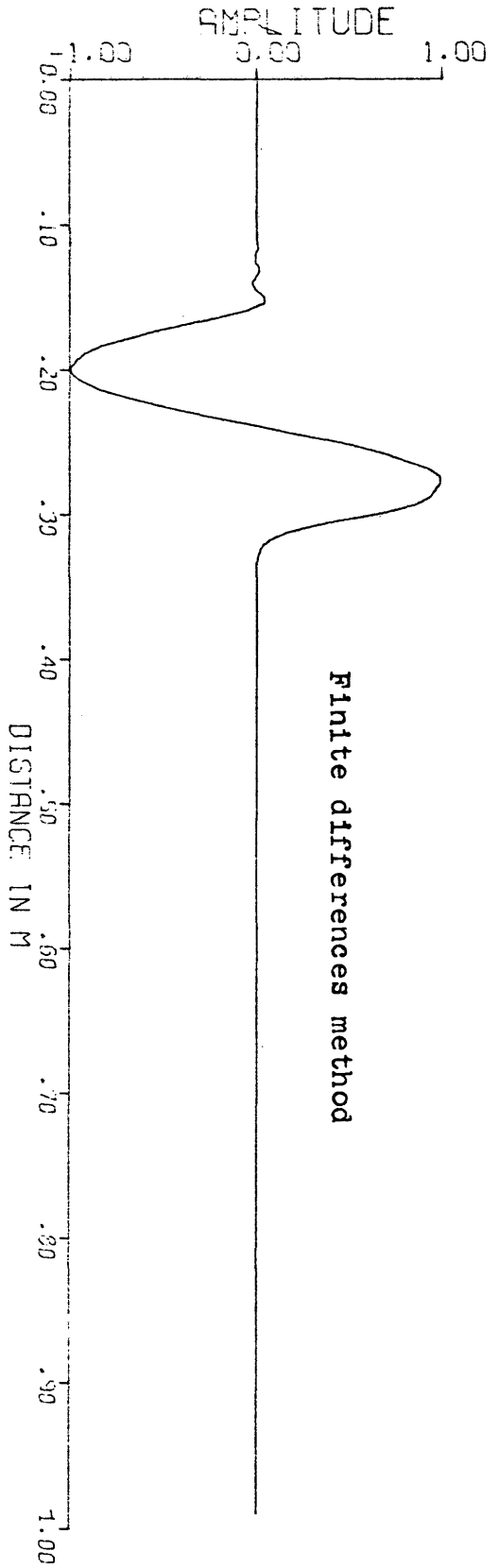
Configuration at  $T = 0.060$  sec.



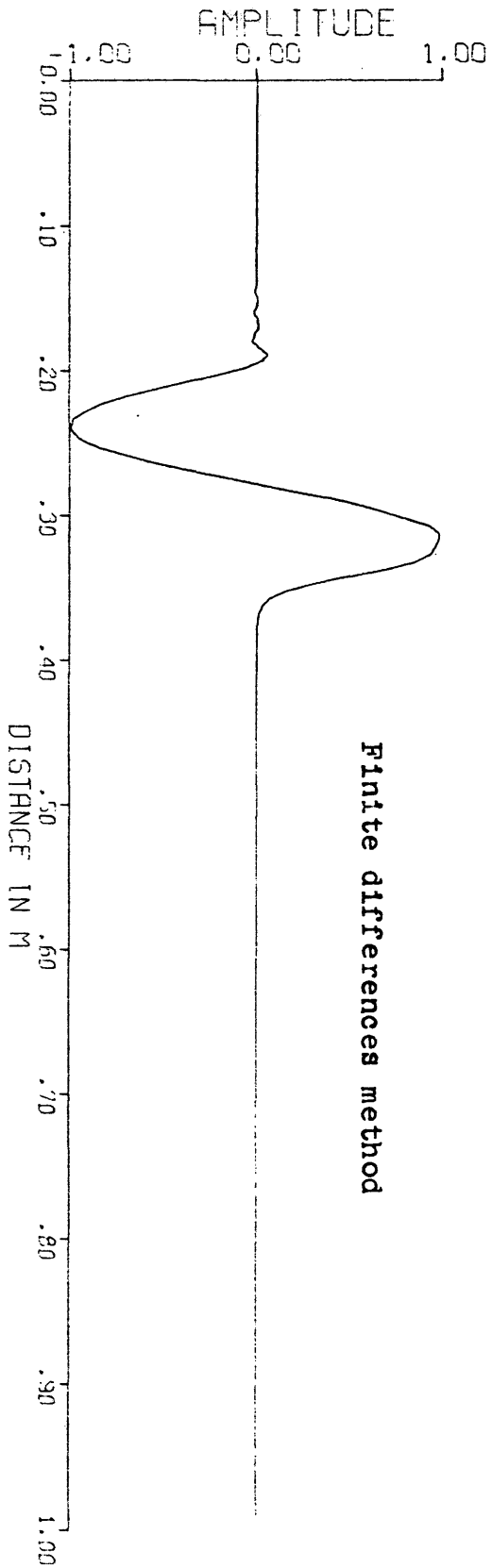


Configuration at  $T = 0.070$  sec.

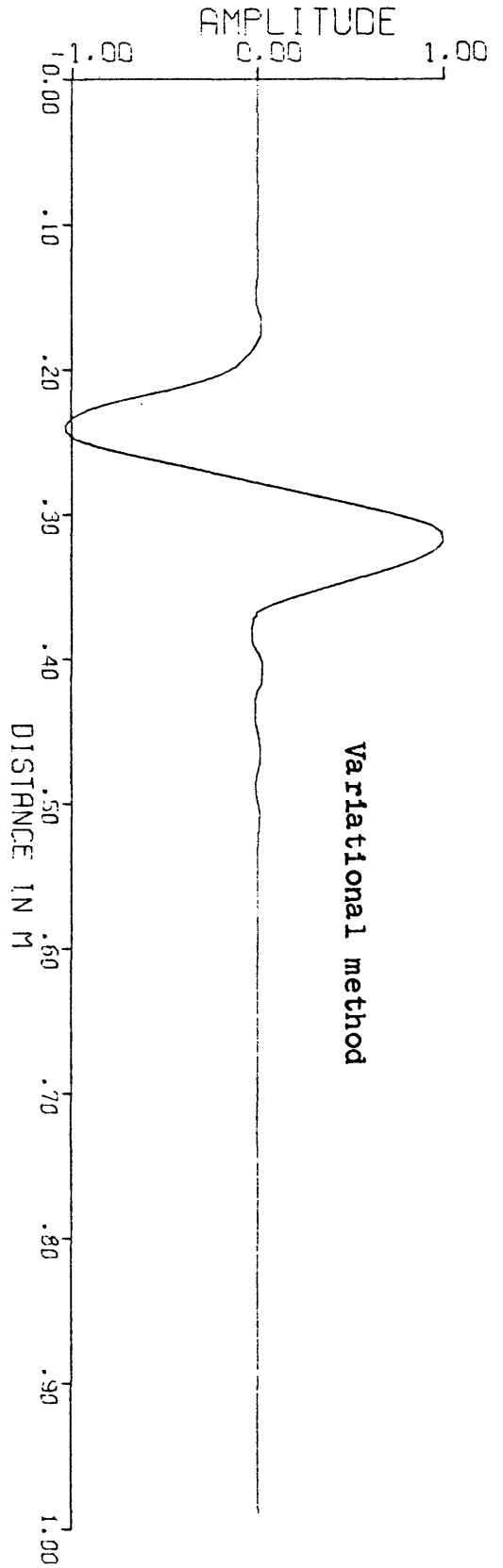


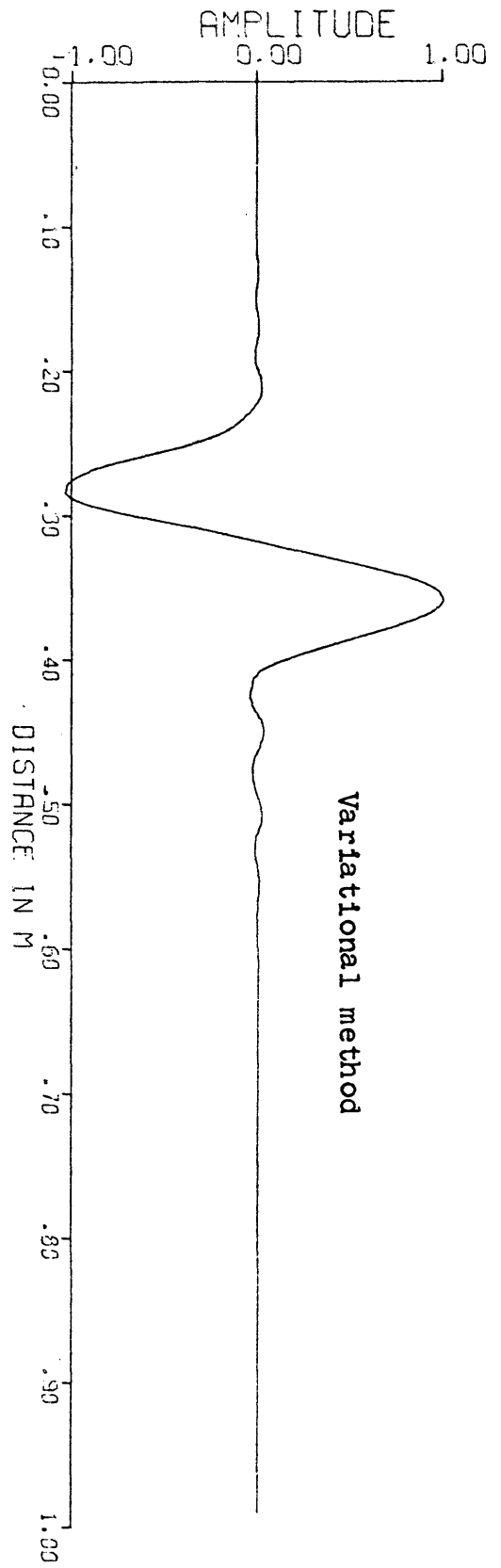
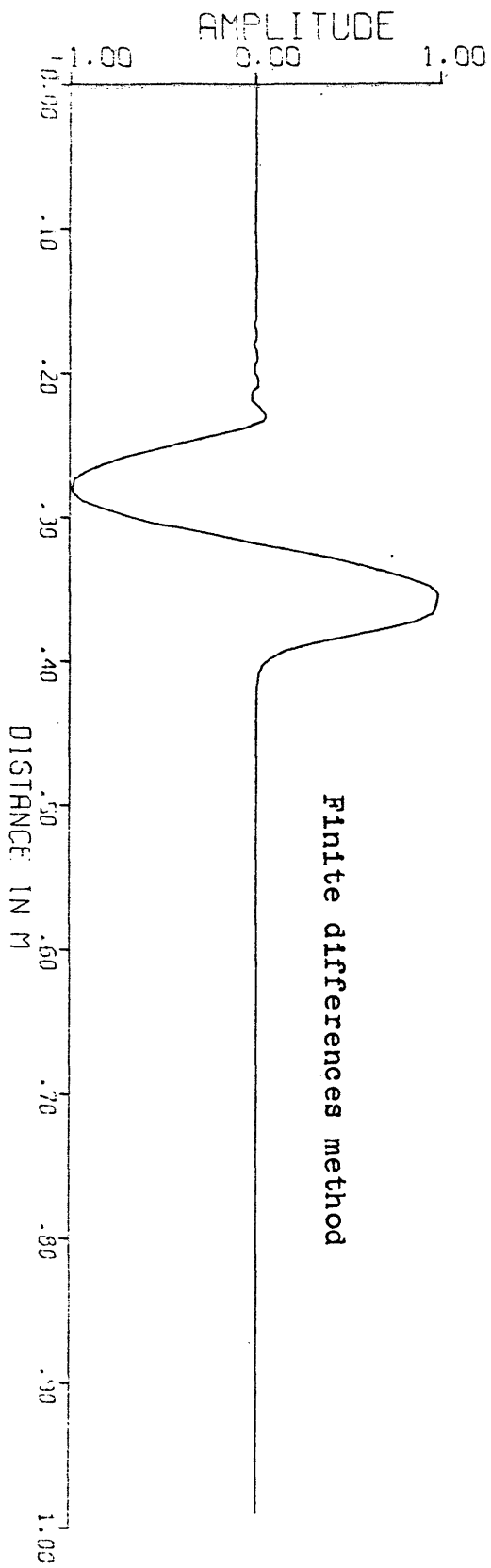


Configuration at 0.080 sec .



Configuration at  $T = 0.090$  seg.





Configuration at  $T = 0.100$  sec .

DISCUSSION OF THE RESULTS

In this section, I discuss the numerical results obtained from the methods described in the previous section.

The work was done in the PDP-10 computer of The Colorado School of Mines. The computer time involved in the calculations is presented in the following table:

	Finite differences method	Variational method
Vibrating string with fixed boundary conditions	35'	33'
Vibrating string with one end free and the other fixed	1'04''	1'01''

From this table, we can see that the computer time is approximately the same in both techniques.

The digital Fourier Transform  $F(n\Delta f \Delta t)$  of a function  $f(t)$ , for which there are  $2N+1$  samples, is defined as

$$F(n\Delta f \Delta t) = \sum_{m=-N}^N f(m\Delta t) e^{-2\pi j n \Delta f m \Delta t} \Delta t$$

In order to find the range of values of  $\Delta t$ , which can give accurate solutions, we see from Fig. 5. that we must have all the frequency components of the driving function less or at less equal than the cutoff frequency. This frequency is defined as the maximum frequency where the variational formulation is still accurate. Therefore the following inequality must be satisfied:

$$n \Delta f \Delta t \leq N \Delta f \Delta T$$

where  $n$  = maximum frequency component of the driving function,

$N$  = cutoff frequency

$\Delta T$  = temporal sampling interval used in exciting the system with an impulse.

$\Delta t$  = temporal sampling interval which can give accurate solutions.

From last inequality, we obtain

$$\Delta t \leq (N \Delta T) / n$$

Experimentation carried out with the variational method showed that this formulation was stable if  $(\Delta x / \Delta t) \gg v$ , where  $v$  is the wave propagation velocity. The range of values examined were for  $\Delta x$  from 0.02 m. through 0.1 m. and for  $\Delta t$  from 0.001 sec. through 0.010 sec.

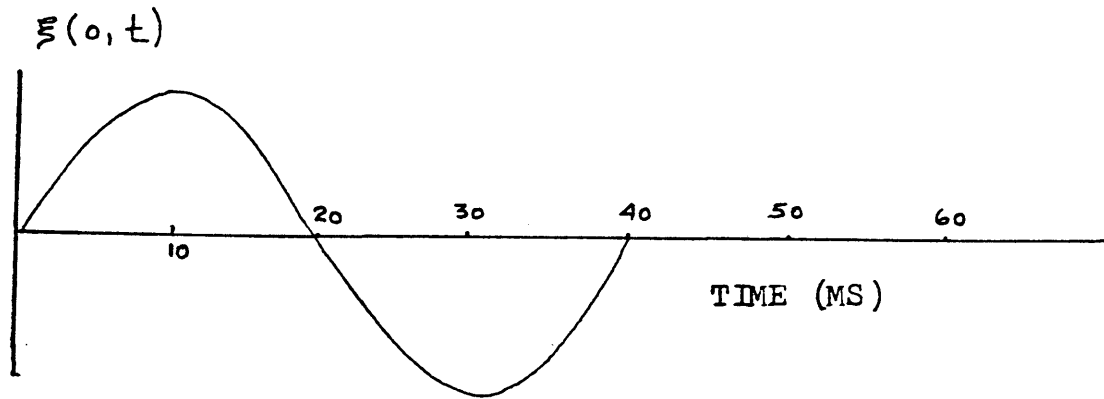


Figure 4.- Driving function used in the second example.

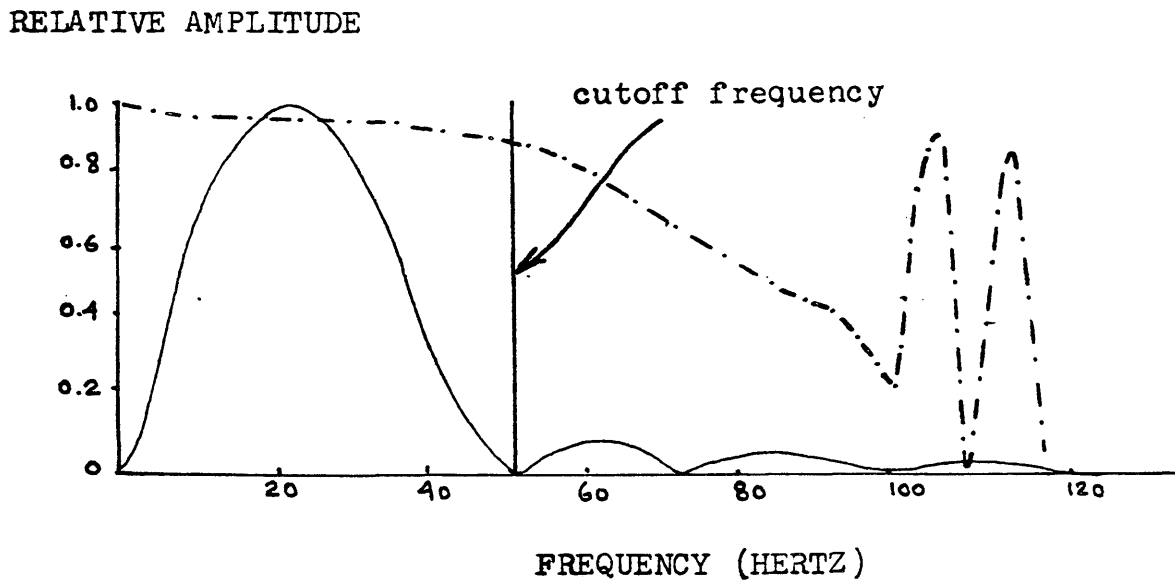


Figure 5.- — Fourier Amplitude Spectrum of the driving function.

----- Fourier Amplitude Spectrum obtained when the system is driven with an impulse.

Having determined  $\Delta t$ , the lower bound of  $\Delta x$  is found such the stability criteria holds and its upper bound is selected small enough that the quadratic approximation provides a reasonable fit to the initial disturbance between grid points.

The generalization of the method to more than one dimension is feasible if the problem possesses spherical or cylindrical symmetry. The integration in a volume presents serious difficulties for a body of arbitrary shape.

Further investigation of the variational method involving the use of higher order polynomials to fit the grid points is suggested.

APPENDIXEvaluation of the integral (55).

The integral (55) reads:

$$I_n = \int_0^l \left[ -\xi(x,0) + 2\xi(x,\Delta t) - \xi(x,2\Delta t) \right] \frac{\partial \xi(x,\Delta t)}{\partial b_{n_1}} dx$$

Index 1 in  $\frac{\partial \xi(x,\Delta t)}{\partial b_{n_1}}$  refers to the partial differentiation with respect to coefficients at the conclusion of the first time step.

In order to solve the integral (55), we must divide the integration from 0 to  $l$  into  $N$  intervals and fit the quadratic to each grid point. Thus we obtain:

$$I_n = \sum_{j=1}^N \int_{(j-1)h}^{jh} \left[ -\eta(x,0) + 2\eta(x,\Delta t) - \eta(x,2\Delta t) \right] K_{jn} dx$$

where  $K_{jn} = \frac{\partial \eta_j(x,\Delta t)}{\partial b_{n_1}}$

The array  $K_{jn}$  can be generated by application of its definition (A-2) to eq. (51),

$$K_{11} = -\frac{x^2}{2h} + x$$

$$K_{j1} = \frac{h}{2} \quad j = 2, 3, \dots, N-1$$

$$K_{jj} = -\frac{1}{2h} [x - (j-1)h]^2 + [x - (j-1)h] + \frac{h}{2} \quad , j = 2, 3, \dots, N-1$$

$$K_{ij} = h \quad \begin{array}{l} i = 3, 4, \dots, N-1 \\ j = 2, 3, \dots, N-2 \quad i > j \end{array}$$

$$K_{N1} = -\frac{1}{2h} [x - (N-1)h]^2 + \frac{h}{2}$$

$$K_{Nj} = -\frac{1}{h} [x - (N-1)h]^2 + h \quad , j = 2, 3, \dots, N-1$$

$$K_{NN} = -\frac{3}{h} [x - (N-1)h]^2 + [x - (N-1)h] + \frac{h}{2}$$

$$K_{j, j+1} = -\frac{1}{2h} [x - (j-1)h]^2 \quad , j = 1, 2, \dots, N-1$$

$$K_{ij} = 0 \quad \begin{array}{l} i = 1, 2, \dots, N-2 \\ j = 3, 4, \dots, N \quad j > i+1 \end{array}$$

(A-3)

If we define

$$\alpha_{nm} = \sum_{j=1}^N \int_{(j-1)h}^{jh} \eta_j(x, m \Delta t) K_{jn}(x) dx \quad (A-4)$$

then the integral (A-2) can be written as

$$I_n = -\alpha_{n0} + 2\alpha_{n1} - \alpha_{n2} \quad (A-5)$$

Now using eq. (51) and (A-3), we evaluate the quantities  $\alpha_{nm}$

$$\begin{aligned}
 \alpha_{1m} = & \left( h^3/120 \right) \left( 16 b_{1m} + 9 b_{2m} \right) + \frac{1}{3} h^2 \xi_{0m} + \\
 & \left( h^3/120 \right) \left( 30 b_{1m} + 50 b_{2m} + 10 b_{3m} \right) + \frac{1}{2} h^2 \xi_{0m} + \\
 & \left( h^3/120 \right) \left( 30 b_{1m} + 60 b_{2m} + 50 b_{3m} + 10 b_{4m} \right) + \frac{1}{2} h^2 \xi_{0m} + \\
 & \text{-----} \quad \text{(A-6)} \\
 & \left( h^3/120 \right) \left( 30 b_{1m} + 60 b_{2m} + \dots + 60 b_{N-2,m} + 50 b_{N-1,m} + 10 b_{Nm} \right) \\
 & \quad + \frac{1}{2} h^2 \xi_{0m} + \\
 & \left( h^3/120 \right) \left( 16 b_{1m} + 32 b_{2m} + \dots + 32 b_{N-1,m} + 23 b_{Nm} \right) \\
 & \quad + \frac{3}{5} h^2 \xi_{0m} + \frac{1}{15} \xi_{Nm}
 \end{aligned}$$

Here, all the intervals contribute to  $\alpha_{1m}$ , since  $K_{j1} \neq 0$  for  $j = 1, 2, \dots, N$ .

$$\begin{aligned}
 \alpha_{2m} = & \left( h^3/120 \right) \left( 9 b_{1m} + 6 b_{2m} \right) + \frac{1}{6} \xi_{0m} h^2 + \\
 & \left( h^3/120 \right) \left( 50 b_{1m} + 86 b_{2m} + 19 b_{3m} \right) + \frac{5}{6} \xi_{0m} h^2 + \\
 & \left( h^3/120 \right) \left( 60 b_{1m} + 120 b_{2m} + 100 b_{3m} + 20 b_{4m} \right) + \xi_{0m} h^2 + \\
 & \left( h^3/120 \right) \left( 60 b_{1m} + 120 b_{2m} + 120 b_{3m} + 100 b_{4m} + 20 b_{5m} \right) + \xi_{0m} h^2 + \\
 & \text{-----} \quad \text{(A-7)} \\
 & \left( h^3/120 \right) \left( 60 b_{1m} + 120 b_{2m} + \dots + 120 b_{N-2,m} + 100 b_{N-1,m} + 20 b_{Nm} \right) + \xi_{0m} h^2 + \\
 & + \left( h^3/120 \right) \left( 32 b_{1m} + 64 b_{2m} + \dots + 64 b_{N-1,m} + 46 b_{Nm} \right) + \frac{8}{15} \xi_{0m} h^2 \\
 & \quad + \frac{2}{15} \xi_{Nm} h^2
 \end{aligned}$$

Here all the intervals contribute to  $\alpha_{2m}$  since  $K_{j2} \neq 0$  for  $j=1,2,\dots,N$ .

$$\begin{aligned} \alpha_{3m} = & (h^3/120) (10b_{1m} + 19b_{2m} + 6b_{3m}) + \frac{1}{6} \sum_{0m} h^2 + \\ & + (h^3/120) (50b_{1m} + 100b_{2m} + 86b_{3m} + 19b_{4m}) + \frac{5}{6} \sum_{0m} h^2 + \\ & + (h^3/120) (60b_{1m} + 120b_{2m} + 120b_{3m} + 100b_{4m} + 20b_{5m}) + \sum_{0m} h^2 + \\ & + \frac{\text{-----}}{(h^3/120) (60b_{1m} + 120b_{2m} + \dots + 120b_{N-2,m} + 100b_{N-1,m} + 20b_{Nm}) + \sum_{0m} h^2} \\ & + (h^3/120) (32b_{1m} + 64b_{2m} + \dots + 64b_{N-1,m} + 46b_{Nm}) + \frac{8}{15} \sum_{0m} h^2 + \frac{2}{15} \sum_{Nm} h^2 \end{aligned}$$

(A-8)

Here the intervals which contribute to  $\alpha_{3m}$  are  $j=2,3,\dots,N$ .

$$\begin{aligned} \alpha_{km} = & (h^3/120) (10b_{1m} + 20b_{2m} + \dots + 20b_{k-2,m} + 19b_{k-1,m} + 6b_{km}) + \frac{1}{6} \sum_{0m} h^2 \\ & + (h^3/120) (50b_{1m} + 100b_{2m} + \dots + 100b_{k-1,m} + 86b_{km} + 19b_{k+1,m}) + \frac{5}{6} \sum_{0m} h^2 \\ & + (h^3/120) (60b_{1m} + 120b_{2m} + \dots + 120b_{km} + 100b_{k+1,m} + 20b_{k+2,m}) + \sum_{0m} h^2 \\ & + \frac{\text{-----}}{(h^3/120) (60b_{1m} + 120b_{2m} + \dots + 120b_{N-2,m} + 100b_{N-1,m} + 20b_{Nm}) + \sum_{0m} h^2} \\ & + (h^3/120) (32b_{1m} + 64b_{2m} + \dots + 64b_{N-1,m} + 46b_{Nm}) + \frac{8}{15} \sum_{0m} h^2 + \frac{2}{15} \sum_{Nm} h^2 \end{aligned}$$

$k = 4, 5, \dots, N-1$ .

(A-9)

Here, the intervals which contribute to  $\alpha_{km}$  are  
 $j = k - 1, k, k + 1, \dots, N$

$$\alpha_{Nm} = \left(\frac{h^3}{120}\right) (10b_{1m} + 20b_{2m} + \dots + 20b_{N-2,m} + 19b_{N-1,m} + 6b_{Nm}) + \left(\frac{h^2}{6}\right) \xi_{0m} \\ + \left(\frac{h^3}{120}\right) (23b_{1m} + 46b_{2m} + \dots + 46b_{N-1,m} + 34b_{Nm}) + \frac{23}{60} \xi_{0m} h^2 + \frac{7}{60} \xi_{Nm} h^2 \quad (\text{A-10})$$

Here the intervals which contribute to  $\alpha_{Nm}$  are  
 $j = N - 1, N.$

Let us write the vectors  $\alpha_{nm}$  as

$$\alpha_{nm} = \frac{h^3}{120} R_{nk} b_{km} + \frac{h^2}{60} \xi_{0m} T_n + \frac{h^2}{60} \xi_{Nm} V_n \quad (\text{A-11})$$

where the matrix  $R_{nk}$ , the vector  $T_n$ , and the vector  $V_n$  are to be determined from eq. (A-6) through (A-10) as a function of  $N$ .

Substituting this last equation into eq. (A-5), we obtain

$$I_n = \frac{h^3}{120} R_{nk} (-b_{k0} + 2b_{k1} - b_{k2}) + \frac{h^2}{60} (-\xi_{00} + 2\xi_{01} - \xi_{02}) T_n + \frac{h^2}{60} (-\xi_{N0} + 2\xi_{N1} - \xi_{N2}) V_n \quad (\text{A-12})$$

Now, we proceed to calculate the matrix  $R_{nk}$ . We find the first row of this matrix from eq. (A-6),

$$\begin{aligned} R_{11} &= 32 + 30(N-2) \\ R_{12} &= 91 + 60(N-3) \\ R_{ij} &= 92 + 60(N-j-1), \quad j = 3, 4, \dots, N-1. \end{aligned} \quad (\text{A-13})$$



$$\begin{array}{cccccccc}
 \begin{array}{c} \sum_{22} \\ \downarrow \end{array} & & & & & & & \begin{array}{c} \sum_{2,N-1} \\ \swarrow \end{array} \\
 & N-3 & N-4 & N-5 & \cdot & N-J-1 & \cdot & 0 \\
 & & N-4 & N-5 & \cdot & N-J-1 & \cdot & 0 \\
 & & & & \cdot & \cdot & \cdot & 0 \\
 & & & & \cdot & \cdot & \cdot & \cdot \\
 & & & & & N-J-1 & \cdot & 0 \\
 & & & & & & \cdot & 0 \\
 & & & & & & \cdot & 0 \\
 & & & & & & & \begin{array}{c} \sum_{N-1,N-1} \\ \swarrow \end{array}
 \end{array}$$

(A-17)

Therefore, using the eq. (A-13) through (A-17), we can generate all the elements of the matrix  $R_{nk}$ .

The vector  $S_n$  involves the boundary condition at  $x = 0$  and is:

$$\begin{aligned}
 S_1 &= 36 + 30(N-2) \\
 S_n &= 92 + 60(N-n-1), \quad n = 2, 3, \dots, N-1 \\
 S_N &= 33
 \end{aligned}$$

(A-18)

The vector  $V_n$  involves the boundary condition at the end point  $x = l$  and is

$$\begin{aligned}
 V_1 &= 4 \\
 V_2 &= 8, \quad n = 2, 3, \dots, N-1 \\
 V_N &= 7
 \end{aligned}$$

(A-19)

Evaluation of the Integral (56)

The integral (56) reads:

$$J_n = \int_0^l \frac{\partial \xi(x, \Delta t)}{\partial x} \frac{\partial^2 \xi}{\partial x \partial b_{n1}} dx$$

As we calculate integral (55) analogously, we divide the integration from 0 to  $l$  into  $N$  intervals and fit a quadratic to each grid point. Thus we obtain

$$J_n = \sum_{j=1}^N \int_{(j-1)h}^{jh} L_j(x) M_{jn}(x) dx \quad (\text{A-20})$$

where

$$L_j(x) = \frac{\partial \eta_j(x, \Delta t)}{\partial x} \quad (\text{A-21})$$

$$M_{jn}(x) = \frac{\partial^2 \eta_j(x, \Delta t)}{\partial x \partial b_{n1}} \quad (\text{A-22})$$

The array  $L_j$  can be generated by applying its definition to eq. (51),

$$L_j = \frac{b_{j+1} - b_{j1}}{h} \left[ x - (j-1)h \right]^2 + b_{j1}, \quad j=1, 2, \dots, N-1$$

$$L_N = \left[ \frac{b_{11} + 2b_{21} + \dots + 2b_{N-1,1} + 3b_{N1}}{h} \right] \left[ x - (j-1)h \right]^2 +$$

$$+ \frac{2(\xi_{N1} - \xi_{01})}{h^2} \left[ x - (j-1)h \right]^2 + b_{N1} \quad (\text{A-23})$$

The array  $M_{jn}$  can be generated applying eq. (A-22) to eq. (A-23) to yield the result

$$M_{jj} = \frac{-[x - (j-1)h]}{h} + 1, \quad j = 1, 2, \dots, N-1$$

$$M_{NN} = -\frac{3[x - (N-1)h]}{h} + 1, \quad M_{j, j+1} = -\frac{[x - (j-1)h]}{h}$$

$$M_{ij} = 0 \quad \begin{array}{l} i = 2, 3, \dots, N-1 \\ j = 1, 2, \dots, N-2 \end{array} \quad i > j \quad (A-24)$$

$$M_{i, j} = 0 \quad \begin{array}{l} i = 1, 2, \dots, N-2 \\ j = 3, 4, \dots, N \end{array} \quad j > i+1$$

$$M_{N1} = -\frac{x - (N-1)h}{h} \quad \text{and} \quad M_{Nj} = -\frac{2(x - (N-1)h)}{h}$$

$$j = 2, 3, \dots, N-1$$

Applying the eq. (A-24) to eq. (A-20), the integrals  $J_n$  can be generated to yield the result

$$J_1 = \frac{h}{6} \left[ 2b_{11} + b_{21} \right] +$$

$$\frac{h}{6} \left[ 2b_{11} + 4b_{21} + \dots + 4b_{N-1,1} + 3b_{N1} \right] - \frac{2}{3} \left( \sum_{N1} - \sum_{01} \right) \quad (A-25)$$

Here, each row corresponds to each interval integration with non-zero value. In this case, these intervals are  $j = 1$  and  $j = N$ .

$$J_n = \frac{h}{6} [b_{n-1,1} + 2b_{n1}] + \frac{h}{6} [2b_{n1} + b_{n+1,1}] + \frac{h}{6} [4b_{11} + 8b_{21} + \dots + 8b_{N-1,1} + 6b_{N1}] - \frac{4}{3} (\xi_{N1} - \xi_{01}) \quad (A-26)$$

$n = 2, 3, \dots, N-1$

Here, the intervals with a non-zero integration value are  $j = n-1, n, N$ .

$$J_N = \frac{h}{6} [b_{N-1,1} + 2b_N] + \frac{h}{6} [3b_{11} + 6b_{21} + \dots + 6b_{N1}] - (\xi_{N1} - \xi_{01}) \quad (A-27)$$

Here, the intervals with a non-zero integration value are  $j = N-1, N$ .

Let us write the vector  $J_n$  as

$$J_n = \frac{h}{6} U_{nk} b_{k1} + \frac{1}{6} T_n (\xi_{01} - \xi_{N1}) \quad (A-28)$$

where the matrix  $U_{nk}$  and the vector  $T_n$  are to be determined as a function of the number of intervals  $N$ .

From eq. (A-25) through (A-27), one finds that the matrix  $U_{nk}$  is symmetric and is:

$$U = \begin{vmatrix} 4 & 5 & 4 & \cdot & \cdot & \cdot & 4 & 3 \\ & 12 & 9 & 8 & \cdot & \cdot & 8 & 6 \\ & & 12 & 9 & 8 & \cdot & 8 & 6 \\ & & & \cdot & 9 & \cdot & \cdot & \cdot \\ & & & & \cdot & \cdot & 8 & \cdot \\ & & & & & \cdot & 9 & 6 \\ & & & & & & 12 & 7 \\ & & & & & & & 8 \end{vmatrix} \quad (A-29)$$

and the vector  $T_n$  is

$$T_1 = 4$$

$$T_n = 8, \quad n = 2, 3, \dots, N-1$$

$$T_N = 6$$

(A-30)

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