TN-81-21

TN-81-02

NLPDE A program for integrating nonlinear partial differential equations

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1981

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# ABSTRACT

We describe a computer program to solve nonlinear partial differential equations of the type  $\frac{\partial F}{\partial \zeta} = N(F) + D(F)$  where N is some nonlinear operator and D stands for a linear dispersive operator. The numerical algorithm uses the partially corrected Adams-Bashforth method for time integration and Fast Fourier Transform (FFT) routines for space integration. The KdV equation is solved as an illustration.

#### INTRODUCTION

The purpose of t is note is to provide a detailed description of a computer program that has been developed to numerically integrate nonlinear partial differential equations of the type

$$\frac{\partial F}{\partial T} = N(F) + D(F) \tag{1}$$

where N is some nonlinear operator and D stands for a linear dispersive operator. Many wave propagation problems in plasma physics as well as in other systems yield such equations. Some familiar examples are the Korteveg de Vries (KdV) equation for ion acoustic or magnetohydrodynamic waves in plasmas, the Nonlinear Schrodinger (NLS) equation for high frequency Langmuir waves, the complex modified KdV equation for lower hybrid waves etc. Several numerical schemes are now available for the solution of these equations. Some of them are based on the finite-difference method (Zabusky & Kruskal 1965; Greig and Morris 1976) which reduces the partial differential equation to an appropriate set of algebraic equations. Alternatively Fourier expansion methods have also been employed (Schamel & Elsasser 1976; Watanabe et al 1977) which take advantage of the extremely efficient Fast Fourier Transform (FFT) techniques. Some hybrid methods have also been proposed (Gazdag 1973; Tappert 1974; Canosa and Gazdag 1977).

The present program is based on one such hybrid method where the time integration is done by using the partially corrected Adams-Bashforth scheme (Gazdag 1976) and the space operator is split up into a linear and nonlinear part (Tappert 1974). The space integration is mainly carried out in the Fourier space but the nonlinear terms are computed by getting back into real space representation. To prevent

aliasing when computing the nonlinear term only the n/2 lowest Fourier modes are retained, where n is the number of grid points in the space coordinate. The accuracy of the integration is gauged by keeping a check on how well the constants of motion are conserved.

In the following sections we illustrate the algorithm by considering a specific equation, namely the Korteveg de Vries equation. A listing of the program written in Fortran IV which is suitable for use on the present IBM 360/44 system at PRL is given at the end. The program can be adapted to solve other equations of type (1) by suitably changing the nonlinear terms and the coefficients of the linear operator; these parts are indicated by appropriate comment cards. The plotting subroutines are specific to the PRL machine and should be suitably replaced for running on other systems. A typical integration time for a single time step  $\Delta t$  of .001 and n = 512 for the KdV equation is less than 2 secs.

## THE ALGORITHM

The KdV equation may in general be written as

$$\frac{\partial \varphi}{\partial \tau} + \beta \varphi \frac{\partial \varphi}{\partial \xi} + \delta^2 \frac{\partial^3 \varphi}{\partial \xi^3} = 0$$
 (2)

where  $\mathcal{T}$  is the time variable and  $\xi$  a suitably constructed space variable.  $\beta$  and  $\delta$  are constant coefficients (e.g.  $\beta$  = 1 and  $\delta^2$  = 1/2 for ion acoustic waves in plasmas). Note that Eq. (2) is invariant under the scaling transformation

$$\xi \to \lambda \xi$$
;  $\tau \to \lambda^3 \xi$  and  $\varphi \to \lambda^2 \varphi$ 

This invariance is useful for example, to normalize the scale length  $\lambda$  in the  $\xi$  direction to unity. There is an alternate scaling given by Berezin & Karpman (1966) which can convert all initial conditions to

a unit-amplitude unit-width type of initial condition. To see this, consider a class of initial conditions of the form '

- 
$$\varphi(\xi_0) = \varphi_0 f(\xi/L)$$
 (3)

where  $\varphi_c$  is the initial amplitude, L is the width and  $f(\xi/L)$  is the functional form of the initial pulse (viz. a square pulse, half sine pulse, secant hyperbolic pulse etc.). The following new set of variables

$$\xi = \xi/L$$
 ;  $\hat{T} = \varphi_0 T/L$  and  $\hat{\varphi} = \varphi/\varphi_0$  (4) changes the KdV equation (2) to

$$\frac{\partial \vec{\varphi}}{\partial \vec{\xi}} + \beta \vec{\varphi} \frac{\partial \vec{\varphi}}{\partial \vec{\xi}} + \frac{\delta^2}{\sigma^2} \frac{\partial^3 \vec{\varphi}}{\partial \vec{\xi}^3} = 0$$

$$\sigma^2 = \varphi_0 L^2$$
(4)

where

Under the given transformation, all initial conditions are transformed to the same initial condition i.e. unit amplitude, unit-width functions. Initial conditions with same numerical values of evolve identically in the scaled co-ordinate system though differently in the laboratory system. This scaling applies for all time and not merely in the asymptotic region. With the use of appropriate scaling parameter the initial condition can be simply described by the functional form of unit width and the behavior in laboratory co-ordinates can be recovered by multiplying the space, time and amplitude in the scaled

Scaling parameter for amplitude =  $\frac{1}{\sqrt{2}}$  Scaling parameter for time =  $\frac{1}{\sqrt{2}}$  Scaling parameter for space = L

co-ordinates by the scaling parameters given below:

In case, the calculations are to be carried out without this scaling, the scaling parameter of may be set equal to unity and

initial condition may be specified by its correct amplitude and width.

Fourier transforming Eq (2) gives us

$$\frac{\partial \varphi_k}{\partial \tau} - i k^3 S^2 \varphi_k + i k \langle \varphi^2 \beta / 2 \rangle_k = 0$$
 (5)

where

$$\varphi_{k} = \int \varphi(\xi, \tau) \exp(-ik\xi) d\xi \qquad (6)$$

is the kth. Fourier component of  $\varphi(\xi, \zeta)$  and

$$\langle \varphi^2 \beta / 2 \rangle_k = \frac{\beta}{2} \int_{-\infty}^{\infty} \varphi^2(\xi, \tau) \exp(-ik\xi) d\xi$$
 (7)

is the kth component of the nonlinear term.

Equn. (5) consists of a linear part

$$\frac{2\varphi_k}{2\tau} - i k^3 \delta^2 \varphi_k$$

and a nonlinear part  $-ik < \beta \varphi^2/2 >_k$  which can be treated as a source term. Thus we can treat the linear part exactly by writing

$$Q_k(\tau) = \overline{Q}(\tau) \exp(i\Omega\tau)$$
 (8)

where  $\Omega = k^3 \delta^2$  From (8) we can get by Taylor expansion

$$\varphi(\tau + \Delta \tau) = \left[ \frac{\partial \varphi_{k}}{\partial \tau} \right|_{\tau} \Delta \tau + \frac{1}{2} \frac{\partial^{2} \varphi_{k}}{\partial \tau^{2}} \right|_{\tau} \Delta \tau^{2} + - \left[ exp \left[ i\Omega(\tau + \Delta \tau) \right] \right] \tag{9}$$

The derivatives can be evaluated from the equation for  $\overline{\varphi}(\zeta)$  which can be obtained by substituting (8) in (5)

$$\frac{\partial \bar{\varphi}_{k}}{\partial \tau} = -ik S_{k}(\tau) \exp(-i\Omega \tau)$$
 (10)

where  $S_{k}(\tau) = \langle \varphi^{\beta} \beta_{2} \rangle_{k}$  If  $\Delta \tau$  is chosen such that  $S_{k}(\tau)$  does not vary significantly in this interval then (10) can be integrated to yield

 $\overline{\varphi(z+\Delta z)} = \overline{\varphi(z)} + \frac{k}{\Omega} S_{k}(z) \left[ \exp(-i\Omega \Delta z) - i \right] \exp(-i\Omega z)$ (11)

Hence the second term of equation (9) may be written as  $\frac{\partial \overline{\varphi}_{k}}{\partial \tau} \exp(i\Omega\Delta\tau).\Delta\tau = \left[\overline{\varphi}_{k}(\tau+\Delta\tau) - \overline{\varphi}_{k}(\tau)\right] \exp(i\Omega\Delta\tau)$ 

$$= \frac{k}{2} \left[ 1 - \exp(i2\Delta t) \right] s(t) \exp(-i2t) (12)$$

Similarly the higher derivatives can be evaluated by using equation (11). Note that the nonlinear term  $S_k(\tau)$  is a convolution term and hence it is convenient to first go back to real space, construct the nonlinear term and then take its Fourier transform. To prevent aliasing errors only the n/2 lowest Fourier modes are retained. The solution to equation (5) can then be obtained in terms of the Taylor series of equation (9) and truncating the series at an appropriate term. An inverse Fourier transform then yields the solution to the KdV equation. The method involves a single-step time differencing scheme.

It has however been shown (Gazdag 1973) that this method of using truncated Taylor series is unstable if the truncation is effected by neglecting time derivatives higher than first  $(\Im \overline{\varphi}_k/\partial \zeta)$  and second  $(\Im \overline{\varphi}_k/\partial \zeta)$ ; however, it is stable if the truncation is done by neglecting derivatives higher than  $\Im \overline{\varphi}_k/\partial \zeta^3$  and  $\Im \overline{\varphi}_k/\partial \zeta^4$ . Thus for stable calculations it would be necessary to calculate second and third time derivatives at each step, which may become rather involved.

In order to avoid this difficulty, following Gazdag (1976) we have used a two-step time differencing scheme, which yields stable accurate solutions, with the evaluation of only first time derivatives.

The scheme consists of (1) a predictor step, followed by (2) a corrector step. For this purpose we write equation (12) as

$$\frac{\partial \overline{\varphi_k}}{\partial \zeta} | \exp(i\Omega \Delta \zeta) \cdot \Delta \zeta = G_k(\zeta) - \frac{k}{\Omega} \left[ 1 - \exp(i\Omega \Delta \zeta) \right] S_k(\zeta)$$

$$= \exp(-i\Omega \zeta) \cdot \Delta \zeta = (i + 1) + \exp(-i\Omega \zeta) \cdot (i + 1)$$
(13)

Then if results obtained from predictor step are denoted by super script by then the predictor step according to partially corrected second-order Adams-Bashforth Scheme (Gazdag 1976) is given by

$$\overline{Q}_{k}^{p}(\tau+\Delta \tau) = \overline{P}_{k}(\tau) \exp(i\Omega \Delta \tau) + (3G_{k}^{p}(\tau) - G_{k}^{p}(\tau-\Delta \tau))/2$$
(14)

and the corrector step

$$\overline{Q}(\tau+\Delta \tau) = \frac{\overline{q}(\tau) \exp(i\Omega \Delta \tau) + (G_{k}^{\dagger}(\tau) + G_{k}^{\dagger}(\tau+\delta \tau))/2.}{(15)}$$

Equations (14) and (15) correspond to equations (8) and (9) of Gazdag (1976) respectively. In the first time step the predictor is calculated according to the equation

$$\overline{\varphi}_{k}^{(\tau+\Delta\tau)} = \overline{\varphi}(\tau) \exp(i2\Delta\tau) + G_{k}(\tau)$$
 (16)

and for subsequent time steps equations (14) and (15) are used to obtain predicted and corrected values for  $\overline{\varphi}_{k}$ . Inverse transform according to the equation

$$\varphi(\tau+\Delta\tau)\xi) = -\frac{1}{\sqrt{2\pi}} \operatorname{Ke} \left[ \overline{\varphi}(\tau+\Delta\tau) \exp\left[i(s2\tau+k\xi)\right] dk \right]$$
(17)

then yields the solution of KdV equation at a given time step (T+AT).

To check the accuracy of the integration, the conservation of the following invariant quantities are monitored.

$$I_1 = \int \varphi(\xi, \tau) d\xi \tag{18}$$

$$I_2 = \int_{-\infty}^{+\infty} \varphi^2(\xi, \tau) d\xi \tag{19}$$

$$I_3 = \left( \frac{\varphi(\xi, \zeta)}{2} - \left( \frac{\partial \varphi}{\partial \xi} \right)^2 \right) d\xi$$
 (29)

These constants are conserved to better than 1 part in 106 and are sensitive to the size of the time-step used. The time step should be chosen to satisfy  $\pi^3 \delta^2 k_{\text{max}}^3 \Delta \tau \leq 1$ . (Abe and Inoue, 1980). DESCRIPTION OF THE PROGRAM: "NLPDE"

#### a) Main Program.

In the main program the constants and functions are n initialised the input parameters are read, the differential operator, the exact time development operator "UL" (corresponding to the dispersion relation of the differential equation) and the multiplicative factors of the nonlinear operator, "UNL" are calculated and stored. Fourier transform is initialised through subroutine "PREFFT" and the initial value problem is defined through a given functional form. After transforming the initial condition to k space, the time development calculations are carried out and results are printed/plotted at regular predetermined intervals. The program makes use of the following aubroutines: PREFFT, FFT, NLROP, RESOUT

# b) Subroutine NLROP (PHI, DPHI)

This subroutine calculates the nonlinear part of the time derivative by first carrying out a Fourier transform to real space, then evaluating the nonlinear term of the differential equation and then carrying out a Fourier transform of this term to k space. This subroutine uses the subroutine FFT. The nonlinear part of the derivative of PHI is returned in DPHI. PHI is not destroyed.

# c) Subroutine PREFFT (EXPF, EXPB).

This subroutine initialises the Fourier Transform by calculating the exponential functions EXPF and EXPB for the forward and backward Fourier Transform and stores these functions. It also calculates and

stores the parameters MIXUP which unscramble the Fourier co-efficients. This subroutine must be called before a first call of the subroutine FFT.

# d) Subroutine FFT (A, B, EXPT, INV)

This subroutine calculates the Fourier Transform of the function "A". The transform is returned in function "B" and function "A" is not destroyed during the transformation. The values of integer INV and function EXPT determine the nature of the transform. INV = 1 and EXPF yield a Fourier transform from real space to k-space and INV = -1 and EXPB give a transform from k-space to real space.

## e) Subroutine RESOUT (IT)

This subroutine is called when it is desired to print out the results at any given time IT. It transforms the function from k-space to real space, evaluates its real part and prints/plots the value of the function at various space points. In addition to printing/plotting the function at time IT, it also calculates the invariants and prints out their values. The subroutine makes use of the subroutines PLOT and SCAL which are provided with system IBM 360/44 at PRL and suitable modification, would be necessary for its use with any other system.

## DESCRIPTION OF FUNCTIONS & PARAMETERS USED.

F (X) : Functional form of the initial pulse

DT : Time Step

 $L \equiv 2 \times \times N$ : Defines the number of grid points.

XMN, XMX : Limits of space coordinates

AMP : Initial Amplitude of the function F

WIDTH : Initial width of the function F

X1 : Initial position of maximum of F

TMX : Maximum Number of Time Steps.

IDIAG : Number of Time Steps that elapse between each

print out.

SIGMA : Berezin - Karpman Scaling Factor.

CAY(I) : K - vector

DIF (I) : Differential Operator.

UL (I) : Linear Operator

UNL (I) : Multiplicative factor of Non linear Operator.

X (I) : Space coordinates.

F (I) : Function values at space points.

PSI (I), PSIP (I) : Fourier Coefficients; corrected and predicted

values.

RINV 1, RINV 2 : Invariants

RINV 3.

# ACKNOWLEDGEMENT:

We would like to thank  $Mr.\ V.R.$  Choksi for his assistance in the computations.

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PROGRAM - ! NUPDE! -
         IT SOLVES THE FIRST CADER IN TIME PARTIAL DIFFERENTIAL EQUATION
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         25,215
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           H. C. THOO
             COMMON JTET /M. M1xUP(512)
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            0.7 = 0.4001
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  JEE FORMATE SEC.4)
            REPOIS. IZ4 ITMX. TO TAG. XMN. XMX. N. OT
       HATRE (6, NDARME)
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      SICHA-6.0 CORRESPONDS TO EXACT SCLITZRY SOLUTION.
      FUNCTION SCALES AS AMPLITUDE, THE SPACE AS WIDTH AND THE TIME
      AS INTOTHIAMPI STUDE 1.
       INTIAL CONDITIONS WITH SAME VALUE OF SIGMA PROPAGATE SIMILARLY
       IN SCALED SPACE-TIME BUT DIFFERENTLY IN LABORATORY.
      SCALING MAY BE REMOVED BY DEFINING SIGNARIO
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IF (TAMP .LT . O) GOTO PO CONTROL

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14 X= 1.5
    YMN--0.6
    en en e
   YYX-Co5.
    Y'4N=-1.0
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    SCAL TO WIDTH/AMP
    STEMM-SULPHDAMS+SI
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 SET UP DEFFERENTIAL OPERATOR AND TRUNCTION PARAMETER
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   1 #1114202
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7 CONTINUE
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TE SCALING IS NOT USED THE INITIAL VALLE FUNCTION SECULO HE DEFINED
WITH CORRECT AMPLITUDE AND WINTHO
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  13.-L)+X9+NPX+1L1X
  TX-(L)X=(LK
  IF [ABS(XJ116LF.1.C) GO TO 5
 F. J = 0 . O
  FO TO E
E FI=[1.0+5[N[P]*[XJ]+0.5]]]/2.0
  F.J=-F1
FIJECMPL XIFJ. C. O.
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I CONTINUE

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TRANSFORM INITIAL CONDITION TO K-SPACE.
    CALL FETTE-PST-EXPF-FRWD1
    NPLOT- 0
    7 * (
    CALL RESOUTETA
  FIND FIRST TIME STEP FOR PST
    CALL NUROPIPSI . GO I
    ho frei 6. seciptivi . Rinvz . Rinv3
996 FORMATE 191=1 GELE.9, 112+1 F15.9, 113+1 F15.9)
    1.1=10107
 10 PS IP (T #=PST( T ##UL (T #+GO(T #
  THE TURNATOR
    T0188T=1.TMX
    CALL NEMPPEPEPERE
    C3287=1.1
  CAZCAG FOUATION G
    P$1171=P$1(1)*UL(1)+0.5*(GC(1)+GP(1))
    [41] -- 6711
    COLT 1= GOLT1
  ERZDAG FOUNTION B
    PC 1P(1)=PC111)+UL111+0.5+13+GC111-GN11)+
 28 CONTINUE
    TUNDOMODIT. ID IAGI
    IF (TMOD.NE.O)GOTO188
    CALL RESOUTETA
    RRITEL 6.898 IR INVI .RINV2 .RINV3
LEE CONTINUE
123 F7PMATC1X.315/(3F12.4)}
    FORMAT(216,2F8.4.15.E10.4)
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   COMPLEX EXPEREXPRICTIONL
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CALL FATIPHI.FPHI.CXPB.BKWD1

FPFT1T3=(FPHT1T1++2)/2.00

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   COMPLEX EXPELLI-EXPELLI
   TWOP T#6.2821852C7179
   K=2**N
   K2=K/2
   0310L=1.K
   19-1-1
   LL = 0
   E7111=1.N
   JP=19/2
   KTT=[8-24]9
   LP=JA
11 il=2*ll•K↑↑
   MIXUPLL I-LE+1
IC CONTINUE
   EG12KHSTA=1,K2
   C=CDS(TWDPT+(KHFTA-1)/K)
   S=SIN(TWOPI+(KHFTA=1)/K)
   EXPERKHETAT CMPL X1C.51
   EXPRIKHETA I=CMPL XIC :- 51
12 CANT INUE
   RETURN
   EMP
   SUPROUTINE FETIA. P. EXPT. INVI
   COMMONITETINIM EXUPESIZE
  COMPLEX ACTION(11.EXPT(11.80.81
  K= 2**N
  K]=1
  KC-2
  Enit =1*K
  L9*MTXUP({ }
T FILENALUMS
  EO SMER GE = 1 . N
  FORK Date 1.K1
  KFFT3=[KP~13#K/KC+1
```

C74JeKP.K.KO

[AF=4X]T9X=+[9L]8=f8

```
P(J)=90+91
P(J)=180-81
CONTINUE

KI=KO
KO=2*KI
TF(*NV.*NE.*I)GOTOIC
STK
R=1/S
COTCL=1.K
C P(L)=9(L)*0
IC CONTINUE
RETURN
END
```

TRANSFORM TO X SPACE AND CALCULATE INVAPIANT 2

```
CALL FET(PSI, FPSI, EXPB, PKWD)
CRET=1.L
EPHISQ=FPSITIA+COAJG(FPSITIA)
RINV2=RINV2+FPHISC
FINV2*RINV2*D/L
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FRINT OUT VALUES OF FUNCTIONS

```
haitel6, coi

haitel6, coi

la-1/4

coitel,

i la-1

k-1+14

k-1+14

haitel6, coil, allia, allia, alkia, baitel6, coil, allia, alkia, baitel6, coil, allia, alkia, baitel6, coil
```

CAUCULATE INVARIENTS 1 AND 3

```
R*NV1=00,00
    P INV 3= 0.
    201=1.1
    SINVIMP INVIAY( ) + DVL.
    COS ! [ 1 1 == D | F ( I 1 * 0 5 [ ( I 1
    W=DDST(T)*CDNJC(DDST(F))
 20 RINV34RINV3+[Y[]]++3++DX3-W+DFLD
  CALCULATE MAXIMUM OF FUNCTION TO HE PLOTTED
    YMN=0
    0 -X PY
    1.1 *L01 *D
    IL | Y = 4 HY I MMY = 7 J = I L ) Y } 7 I
    ICIYEK MY 6 NO LLIYI NI
 10 CONTINUE
    IF (YMX & GT & LOC ) STOP
    TM THE ARMY MY
    YMAXWA INTOYMXI
    YMN =YMIN+AINTI[YNN-YMIN1+10.0-1.01/10.0 :
    YM X= YMA X +A TMTEE YM X- YMA X | 41 C+ C+1+ O | / 1 O+ O
    YL # 2.00
    YOULLYM X-YMN 1/YL
    XL = 10e 00
    JX \ L NMX -X MX ] = PX
    M = 3.0
    YD= [ YM X- YMN 1 / YL
    CALL PLOTER, NMX, XMX, XL, YD, YMX, YL, YD,
                  CALL SCALL
    PUET 07 4 = 1 . 1
    TALL PLATISO.XIIII.Y(III)
STO CONTINUE
    CALL PLATISSI
    1F (NP) 77 .50.21607060
    NPLOT=NPLOT+1
    TYAKEYMXAYE
    CALL PLOTICO, XMA, YMAX)
    BOLLOW
 (C NOLUTEO
    DAUSFIPLEASE APPAAGE THE PLOTTER-PEN ON THE NEXT FAGE!
SCA FREMATE ! THE THIRD INVARIENT IS ! E15.91
    FORMATI . THE INTEGRAL OF PHI SQUARED IS' E15.91
915
                                                71 MF = 1 F5 . 21
                               VEL2= 1F5.2.1
900
    FORMATI VELI = * FF. 2 . 1
    F7P43*(1H1)
901
    F7FM4T (1x, 4( 13, 4x, F1C, 4, 15x))
962
                   TYME TO! F11.41
     EDRMAT ( 1
903
    R"TURN
```

ľ

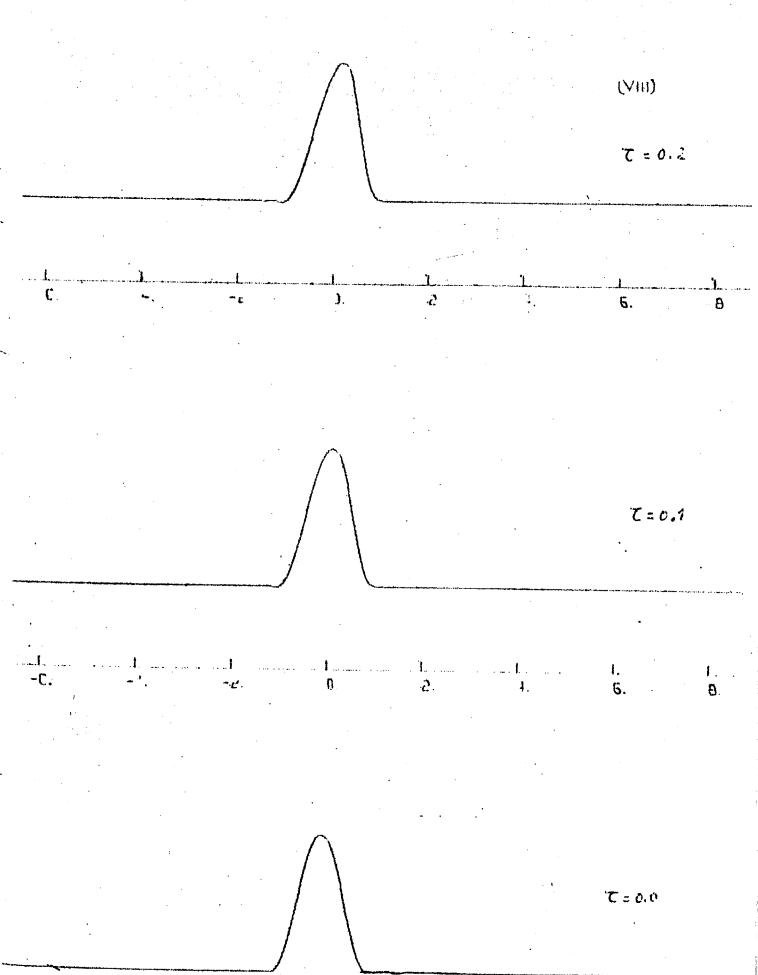
C

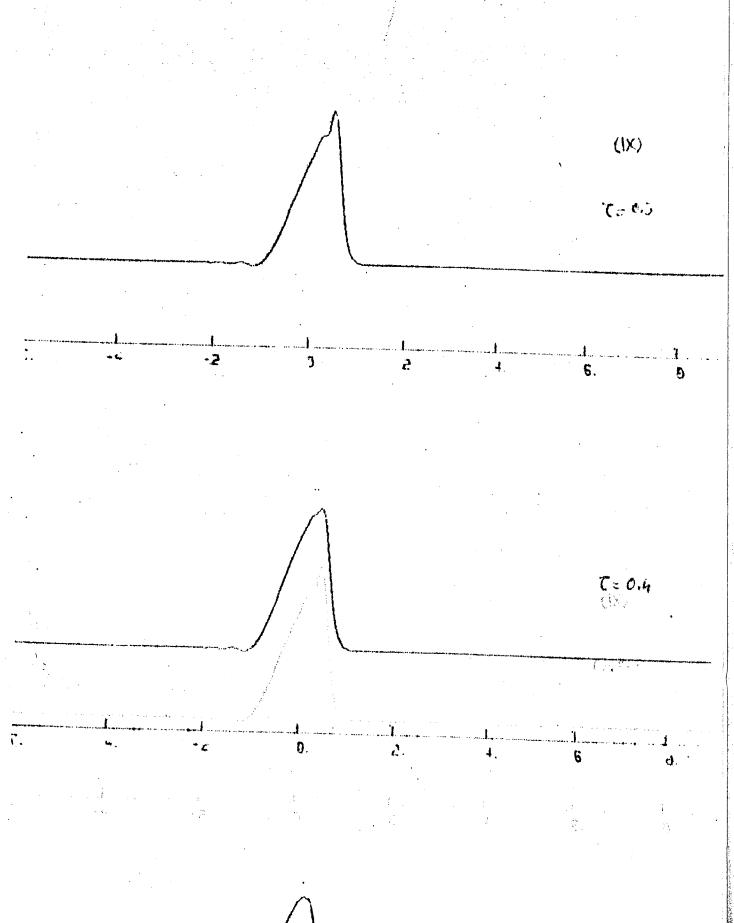
FMF

## ANNEXURE II

# Caption to figures.

In subsequent figures we show the evolution of a single sinusoidal positive pulse as obtained by the numerical solution of the KdV equation. Amplitude, time and space are normalised according to Berezin-Karpman scaling and the scaling factor is  $\sigma^{-2} = 250$ . The process of steepening at the front edge and breaking of the initial perturvation into a number of solitons is clearly demonstrated.





T=0.3

