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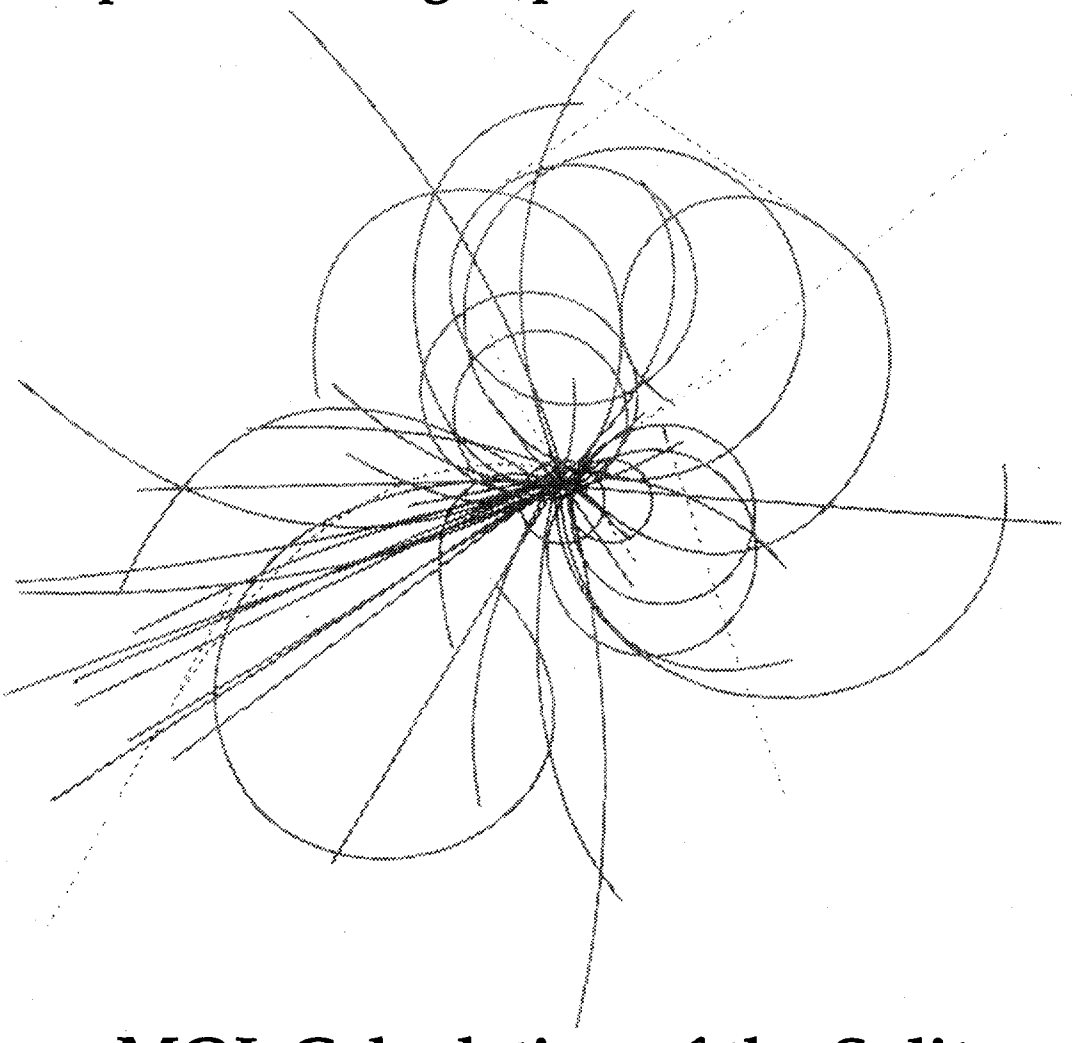

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MOL CALCULATION OF THE SOLITONS OF THE CUBIC SCHRÖDINGER EQUATION

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The cubic Schrödinger equation (CSE) is a complex (in the mathematical sense) nonlinear partial differential equation (PDE) with a known analytical solution. Further, the solution consists of solitons (traveling waveforms that do not change shape with time or position) that are very sharp spatially. Thus the CSE is a stringent test problem for any numerical procedure. We report here the results of a method of lines (MOL) solution using second-derivative, finite-difference approximations for spatial second derivatives that accommodate Dirichlet and Neumann boundary conditions without approximation of the boundary conditions.

The CSE

The CSE in one dimension is

$$\mathrm{i}u_t + u_{xx} + \mathrm{Q}|u^2|u = 0 \,, \tag{1}$$

where subscripts in t and x denote partial derivatives with respect to these independent variables, *e.g.*, $u_t = \partial u/\partial t$; t is an initial value variable, and x is a boundary value variable. Therefore, Eq. (1) requires one initial condition and two boundary conditions; $\mathrm{i} = \sqrt{-1}$ and Q is a given constant; $u = u(x, t)$ is therefore complex.

An exact solution [2], [3] to Eq. (1) is

$$u(x, t) = \sqrt{2}\, \exp\{\mathrm{i}(0.5x + 0.75t)\}\, \mathrm{sech}(x - t) \,. \tag{2}$$

It follows immediately from Eq. (2) that

$$|u(x, t)| = \sqrt{2}\, \mathrm{sech}(x - t) \,, \tag{3}$$

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which is the equation for a soliton travelling from left to right with unit velocity and a maximum amplitude of $\sqrt{2}$.

We take as the initial condition for Eq. (1)

$$u(x, 0) = \sqrt{2} \exp\{i(0.5x)\} \operatorname{sech}(x) , \tag{4}$$

which follows directly from Eq. (2). The boundary conditions are taken as

$$u(-\infty, t) = u(\infty, t) = 0 . \tag{5)(6}$$

For a numerical solution on a spatial grid of finite length, we actually use

$$u(-30, t) = u(70, t) = 0 . \tag{7)(8}$$

Eqs. (7) and (8) allow for movement of the soliton from left to right, yet for the interval of t used in the calculations, the soliton does not come close enough to the finite boundaries at $x = -30$ and $x = 70$ to depart significantly from a zero value; *i.e.*, Eqs. (7) and (8), and (5) and (6) are essentially equivalent.

To program Eq. (1), we write u as a complex variable:

$$u = v + iw . \tag{9}$$

Substitution of u from Eq. (9) in Eq. (1), and separation into real and imaginary parts, gives the two real coupled PDEs:

$$v_t + w_{xx} + Q(v^2 + w^2)w = 0 \tag{10}$$

$$w_t - v_{xx} - Q(v^2 + w^2)v = 0. \tag{11}$$

The initial conditions for Eqs. (10) and (11) follow directly from Eq. (4):

$$v(x, 0) = \sqrt{2} \cos(0.5x) \operatorname{sech}(x) \tag{12}$$

$$w(x, 0) = \sqrt{2} \sin(0.5x) \operatorname{sech}(x) . \tag{13}$$

Homogeneous Dirichlet boundary conditions follow from Eqs. (7) and (8):

$$v(-30, t) = w(-30, t) = 0 \tag{14)(15}$$

$$v(70, t) = w(70, t) = 0 . \tag{16)(17}$$

Eqs. (10) to (17) are the problem system.

MOL Solution of the CSE

The essential features of a MOL solution of Eqs. (10) to (17) are:

(1) The discretization of the spatial derivatives, v_{xx} and w_{xx}, in Eqs. (10) and (11).

(2) The integration of the temporal derivatives, v_t and w_t, in Eqs. (10) and (11), which are transformed into ordinary derivatives as a result of feature (1).

We focus attention on feature (1), and accomplish feature (2) with an established ODE integrator, RKF45 [1]. The discretization of the spatial derivatives v_{xx} and w_{xx} is accomplished by finite differences for second-order derivatives, as described by Schiesser [4]. These finite-difference approximations: (1) do not involve approximations of either Dirichlet or Neumann boundary conditions, (2) are second- and fourth-order correct (higher-order approximations can easily be developed), and (3) can easily by implemented in a general-purpose differentiation routine. We now illustrate these properties through the MOL solution of Eqs. (10) to (17).

A subroutine for calculating the MOL temporal derivatives is listed in Program 1.

```
      SUBROUTINE DERV
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (NG=400)
      COMMON/T/          T,      NSTOP,      NORUN
     1      /Y/    V(0:NG),    W(0:NG)
     2      /F/   VT(0:NG),   WT(0:NG)
     3      /S/   VX(0:NG),   WX(0:NG), VXX(0:NG), WXX(0:NG),V2W2(0:NG),
     4             X(0:NG)
     5      /C/         XL,         XR,          Q,      ROOT2,       SSET
     6      /I/         IP
C...
C...  PDES
C...
C...  V
C...   XX
         NL=1
         NU=1
         IF(NORUN.EQ.1)CALL DSS042(XL,XR,NG+1,V,VX,VXX,NL,NU)
         IF(NORUN.EQ.2)CALL DSS044(XL,XR,NG+1,V,VX,VXX,NL,NU)
C...
C...  W
C...   XX
         NL=1
         NU=1
         IF(NORUN.EQ.1)CALL DSS042(XL,XR,NG+1,W,WX,WXX,NL,NU)
         IF(NORUN.EQ.2)CALL DSS044(XL,XR,NG+1,W,WX,WXX,NL,NU)
C...
C...  ODES AT THE BOUNDARIES
         VT(0)=0.0D0
         WT(0)=0.0D0
         VT(NG)=0.0D0
         WT(NG)=0.0D0
C...
C...  ODES AT THE INTERIOR POINTS
      DO 10 I=1,NG-1
```

```
C...
C...        V**2 + W**2
            V2W2(I)=V(I)**2+W(I)**2
C...
C...        EQUATION (10)
            VT(I)=-WXX(I)-Q*V2W2(I)*W(I)
C...
C...        EQUATION (11)
            WT(I)= VXX(I)+Q*V2W2(I)*V(I)
10      CONTINUE
        RETURN
        END
```

Program 1. Subroutine DERV for the Calculation of the Temporal Derivatives of Eqs. (10) and (11).

The following points can be noted about subroutine DERV (reading from top to bottom):

(1) The number of spatial intervals in x, NG, is 400.

(2) v and w are in arrays V(0:NG) and W(0:NG) in COMMON/Y/.

(3) v_t and w_t are in arrays VT(0:NG) and WT(0:NG) in COMMON/F/.

(4) v_x, w_x, v_{xx}, and w_{xx} are in arrays VX(0:NG), WX(0:NG), VXX(0:NG), and WXX(0:NG) in COMMON/S/.

(5) $v^2 + w^2$ and the grid in x are in arrays V2W2(0:NG) and X(0:NG) in COMMON/S/.

(6) v_{xx} is first calculated; NL = 1 and NU = 1 specifies Dirichlet boundary conditions at $x = -30$ and $x = 70$.

(7) The call to DSS042 (for the first run with NORUN = 1) calculates v_{xx} from v over the 401 point grid. v_x in array VX(0:NG) is used only if Neumann boundary conditions are specified (NL = 2 and/or NU = 2). DSS042 contains second-order finite differences to calculate second derivatives. DSS044 contains fourth-order finite differences. Thus, a comparison between the results for the two orders can easily be made. w_{xx} is then calculated in the same way.

(8) The temporal derivatives are zeroed at the boundaries, *i.e.*, $v_t(-30, t) = w_t(-30, t) = v_t(70, t) = w_t(70, t) = 0$.

(9) v_t and w_t are calculated in DO loop 10 at interior grid points 1 to 399. This coding again illustrates one of the positive features of the MOL: the close correspondence between the equations, in this case Eqs. (10) and (11), and the coding. Also, the code is very compact considering the complexity and nonlinearity of the PDEs.

(10) The 802 temporal derivatives are sent to the ODE integrator through COMMON/F/ (in this case, RKF45).

As indicated previously, this is a stringent test problem since the traveling soliton has a very sharp spatial variation as illustrated by the solution for the second run in Figure 1. (The solitons moving left to right are for $t = 0$ (centered at $x = 0$), 5, 10, . . . , 30.) Also, the peak of the soliton where the curvature is most extreme should have a value of $\sqrt{2} = 1.41412$; this peak value for the first and second runs, for both single and double precision coding of this problem (which was run on a computer with a 32-bit word in single precision Fortran), is tabulated in Table 1.

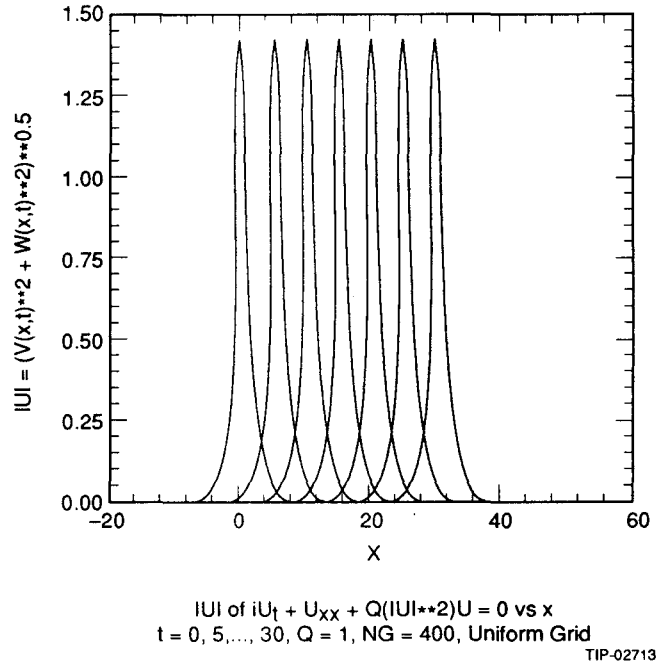

Figure 1. Solution of the Cubic Schrödinger Equation by Fourth-Order Finite Differences in the MOL.

The principal conclusions from the results in Table 1 are: (1) for this problem at least, the computer wordlength had little effect, and (2) the fourth-order differentiation formulas (in DSS044) were clearly more effective than the second-order formulas (in DSS042) in preserving the peak height of the solitons as they moved left to right; however, when the four solutions were plotted (two wordlengths × two spatial differentiators = four solutions), the differences were almost imperceptible.

Table 1. Effect of the Order of the Spatial Differentiator and Computer Wordlength on the MOL Solution to Eqs. (10) and (11).

DSS042	$O(\Delta x^2)$	single	1.41910 (t = 10) 1.37941 (t = 20) 1.31159 (t = 30)
DSS044	$O(\Delta x^4)$	single	1.41522 (t = 10) 1.41523 (t = 20) 1.41501 (t = 30)
DSS042	$O(\Delta x^2)$	double	1.41910 (t = 10) 1.37943 (t = 20) 1.31165 (t = 30)
DSS044	$O(\Delta x^4)$	double	1.41522 (t = 10) 1.41523 (t = 20) 1.41499 (t = 30)

Summary

The CSE is a stringent test problem for PDE numerical algorithms. However, an accurate MOL solution could be computed using library routines and a minimum of problem-specific coding; also, the computer run times were modest. Two complete Fortran programs (for single and double precision), including subroutines DSS042 and DSS044, are available on request from the author (on a DOS-formatted, 3.5-in., 1.44-MB diskette).

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