A NUMERICAL VENTURE INTO THE MENAGERIE OF COHERENT STRUCTURES OF A GENERALIZED BOUSSINESQ EQUATION

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1. INTRODUCTION

We consider a generalized Boussinesq equation which is a model for the one-dimensional dynamics of phases in martensitic alloys. The natural difference approximation that coincides with the discrete form of the model is employed and then Newton's quasilinearization of the nonlinear terms is performed. In order to adequately represent the localized solitary-wawe solutions up to 20000 grid points are used in calculations.

Two distinct classes of solutions are found. To the first class belong oscillatory pulses whose envelopes are localized waves. The second class consists of smoother localized solutions that are either kinks or bell-shaped "bumps" depending on the amplitude of the initial condition. The amplitude of a bump decrease with time while its support increases. An appropriate self-similar scaling is found analytically and confirmed by the direct numerical simulations to high accuracy.

2. POSING THE PROBLEM

Following [1],[2],[3],[4] we consider the one-dimensional model of an atomic chain in which the longitudinal displacements couple to the shear strain. Upon introducing relative displacements the Euler-Lagrange equations for variation of the governing functional adopt the form

$$(2.1)\qquad \frac{d^2}{dt^2}S_n = c_T^2(S_{n+1}-2S_n+S_{n-1}) - (S_{n-1}^3-2S_n^3+S_{n+1}^3) + (S_{n+1}^5-2S_n^5+S_{n-1}^5) - \beta(S_{n+2}-4S_{n+1}+6S_n-4S_{n-1}+S_{n-2}) ,$$

whose continuum limit is

$$(2.2)\qquad S_{tt} = c_T^2 S_{\xi\xi} - (S^3)_{\xi\xi} + (S^5)_{\xi\xi} - \alpha S_{\xi\xi\xi\xi} .$$

In equation (2.1) the spatial variable is defined as $\xi=X/a$ (where a is the distance between the atoms). $X_n=na$ stands for the distance and $\alpha=\beta-0.5\ c_T^2$. The differential form hints at the name - "a generalized Boussinesq equation" in the sense that (2.2) has more complicated nonlinearity than the original Boussinesq equation [5]. The continuum limit provides also the clue how the boundary conditions are to be posed. The natural boundary condition for the Lagrangian functional in differential form is $S_{\xi\xi}=0$. Since the index "*1*" refers to the first atom of the chain and "*N*" - to the last one, then for the discrete version of the system the natural boundary conditions can be represented as follows

$$S_0-2S_1+S_2=0\ , \quad S_{N-1}-2S_N+S_{N+1}=0\ . \tag{2.3}$$

where in order to properly discretize the natural conditions we introduce into consideration two "artificial" members of the chain with indices "*0*" and "*N+1*", respectively. We also consider the physically most typical situation when the boundary points are held fixed, namely

$$S_1=0\ , \qquad S_N=0\ . \tag{2.4}$$

3. ALGORITHM

In order to successfully treat the problem of localized solutions (henceforth called "coherent structures") the first requirement for the algorithm is to be fast enough allowing computations with large number of "grid points" N in order to provide room for a structure to move without interacting with other structures or with the boundaries. The second major requirement is for strong temporal stability in the sense that the different kinds of computational errors do not amplify timewise even for large values of time increments. The last requirement is crucial because some of the properties of the individualized localized solution can be recognized only after very long temporal evolution.

It is convenient to introduce the auxiliary function

$$Q_i = c_T^2 S_i - S_i^3 + S_i^5 - \beta(S_{i-1}-2S_i+S_{i+1})\ , \quad i=1,\dots N\ . \tag{3.1}$$

and to recast (2.4) in the form

$$\frac{d^2}{dt^2} S_i = (Q_{i-1}-2Q_i+Q_{i+1})\ , \qquad i=2,\dots,N-1\ . \tag{3.2}$$

In terms of function Q_i, the boundary conditions adopt the simple form

$$S_1 = S_N = 0\ , \ Q_1 = Q_N = 0\ . \tag{3.3}$$

Initial conditions are imposed both for function S and its time derivative, say functions s_i and σ_i. We use the superscript n to denote the current time step on a staggered time mesh $t_n=(n-0.5)\tau$ where τ is the time increment. Then the initial conditions are approximated to second order as follows

$$S_i^0 = s_i - \frac{\tau}{2}\sigma_i\ , \qquad S_i^1 = s_i + \frac{\tau}{2}\sigma_i\ . \tag{3.4}$$

The main objective in devising the algorithm is to have a stable scheme that would allow us to march with large time increments τ. For this reason we chose a fully implicit scheme. At the time step *(n+1)* we use a consistent Newton's quasilinearization of the terms on the right-hand side of (3.1) according to the formulae:

$$S_i^3\Big|^{n+1} = 3S_i^{n2}S_i^{n+1} - 2S_i^{n3} + O(\tau^2)\ , \tag{3.5a}$$

$$S_i^5\Big|^{n+1} = 5S_i^{n4}S_i^{n+1} - 4S_i^{n5} + O(\tau^2)\ , \tag{3.5b}$$

$$S_i^2\Big|^{n+1} = 2S_i^{n}S_i^{n+1} - S_i^{n2} + O(\tau^2)\ . \tag{3.5c}$$

The strongly implicit scheme requires also that the time derivative of (3.2) be approximated at time step *(n+1)*. At the first step (number *2*) following the two initial steps, one can have only a first-order approximation of the second derivatives over three steps:

$$\frac{d^2}{dt^2}S_i\Big|^2 = \frac{1}{\tau^2}(S_i^2-2S_i^1+S_i^0) + O(\tau)\ . \tag{3.6a}$$

At all of the next steps *(n>2)* we employ the following four-step scheme with second-order approximation

$$\frac{d^2}{dt^2}S_i\Big|^{n+1} = \frac{1}{\tau^2}(2S_i^{n+1}-5S_i^{n}+4S_i^{n-1}-S_i^{n-2}) + O(\tau^2)\ . \tag{3.6b}$$

Introducing the above formulas into (3.1)-(3.2) we arrive at a **coupled** system of difference equations for the two set functions S_i, Q_i, namely

$$\beta S_{i-1}^{n+1} - (2\beta+c_T^2-3S_i^{n2}+5S_i^{n4})S_i^{n+1} + \beta S_{i+1}^{n+1} + Q_i^{n+1} = 2S_i^{n3}-4S_i^{n5}\ , \tag{3.7a}$$

$$Q_{i-1}^{n+1} - 2Q_i^{n+1} + Q_{i+1}^{n+1} - \frac{2}{\tau^2}S_i^{n+1} = -\frac{1}{\tau^2}(5S_i^{n}-4S_i^{n-1}+S_i^{n-2})\ . \tag{3.7b}$$

Here the set functions of steps *n*, *n-1* and *n-2* are thought of as being known. Eqs (3.7) are valid for all interior points $i = 2, \ldots, N-1$ and are coupled through the boundary conditions (3.3).

The most important feature of the system (3.7) is that upon introducing the composite set function

$$W_{2i-1} \equiv Q_i^{n+1}\ , \quad W_{2i} \equiv S_i^{n+1}\ , \qquad i = 1,\ldots,N\ , \tag{3.8}$$

and after fairly obvious manipulations the said system can be recast as a *five*-diagonal system for the new set function W_k where $1<k<2N$. The band structure allows us to use highly efficient specialized solvers, e.g., the one developed in [6].

IV. RESULTS

To start with we set $c_L = 1$, $\beta = 1$. It is easily seen that the particular values of these parameters are not so important and by changing the value of the time increment τ we can select most of the principal cases by means of simply rescaling the dependent and independent variables. Due to the strong implicity, the scheme turns out to be stable for a wide range of time increments, $10^{-6}<\tau<10^{6}$, and for a wide range of amplitudes of initial conditions. As it should have been expected the computations with larger τ's led us to the smoother solutions spreading wider in the region under consideration.

The smooth solutions persisted in our calculations when the time increment τ was larger than 5. It goes without saying that we did verify whether the same shape of coherent structure is obtained if the calculation are conducted with different $\tau>5$ (say $\tau=10$ and $\tau=100$). We discovered that what mattered was the interplay between the time increment and the amplitude of the initial condition. When the latter is "moderate" in comparison with τ then the homoclinics of the shape of Airy functions appeares as shown in Fig.1. When the initial amplitude is relatively small the pentic nonlinearity is swithched off even on the earliest stages and then the symmetric homoclinics shown in Fig.2 appeared. Conversely when the amplitude was large enough, then the balance between the two nonlinear terms yielded the kink-shaped structure (heteroclinics) shown in Fig.3.

An interesting feature of the homoclinics is that their shape is not preserved timewise while the heteroclinics (kinks) are stationary patterns. The former decrease in amplitude with time while their support increases and after a sufficiently long time the solution eventually gets on a self-similar track discussed in the next section.

A completely different Universe appeared when the time increments were small enough (say $\tau\leqslant 1$ for $\beta=1$) and allowed development of more complicated "wiggled" shapes. It is more convenient to consider the case $\tau=0.1$, $\beta=0.01$, since the spatial span of the structures is smaller. In the sequence of Figures 4 one sees the development of a "pulse" that has smooth shape in the right-hand side of the interval but in the course of its time evolution spans larger portions of the left-hand side of the interval with its wavy "tail".

The complete classification of the different creatures inhabiting the generilized Boussinesq equation goes far beyond the scope of the present short note. A more systematic account is due elsewhere.

V. THE SELF SIMILAR STAGE

The results of the previous section suggest that for large times some of the solutions tend to adopt a self-similar shape in the sense that their amplitude decreases with time while the length-scale of the support increases. Being reminded that at large times for the decaying solutions one has $S^5\ll S^3$ we found a self-similar scaling of the following type

$$(5.1)\qquad S = t^{-\alpha}s(\eta), \quad \eta \equiv t^{-\delta}(x-c_T t) \quad \text{where } \alpha = \delta = \frac{1}{3}\,.$$

Respectively, the equation for the scaled function s reads

$$(5.2) \qquad \frac{2}{3}c_T^2(4s'+\eta s'') = -(s^3)'' - \beta s'''' .$$

Here the primes stand for differentiation with respect to the similarity variable η. It is interesting to note that such self-similar solutions were found both for Burgers' equation [7] and Korteweg-de Vries' equation [8].

It goes beyond the frame of the present work to attempt a direct solution to (5.4). Rather we shall check whether the time dependent solution of the previous section conforms with the asymptotic law (5.1). Let us define the length of support L_s as the distance from the point where the maximum of the structure is situated to the point where the amplitude is 1/100 of the maximum. The definition is appropriate for all of the structures which decay monotonically in the right portion of the region under consideration. In Table 1 we present for the solution from Fig.1 the amplitude and support as a function of dimensionless time after a certain moment of time that we call $t=0$. Next to the column of numerical results we also present in Table 1 the approximation for A and L_s of the type

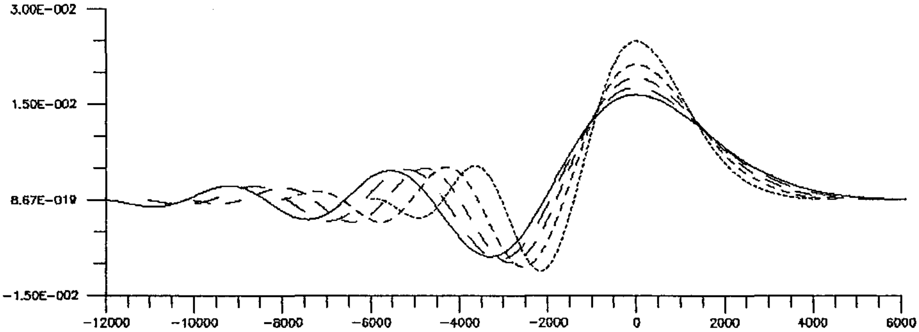
$$(5.3) \qquad A = a(t+a_0)^{-1/3} , \qquad L_s = b(t+a_0)^{1/3} .$$

where the constants a, b and a_0 are defined so as to provide a best in the least-square sense fit to observations from numerical simulations. It is clearly seen from Table 1 that the asymptotic self-similar powers are in excellent agreement with the data for both the amplitude A and support L_s the difference being less than 1% save the moment $t=0$ which in fact is "too early a moment" to be treated as an asymptotic stage.

TABLE 1. $a_0 = 2.76.10^4$; $a = 1.011$; $b = 63.3$

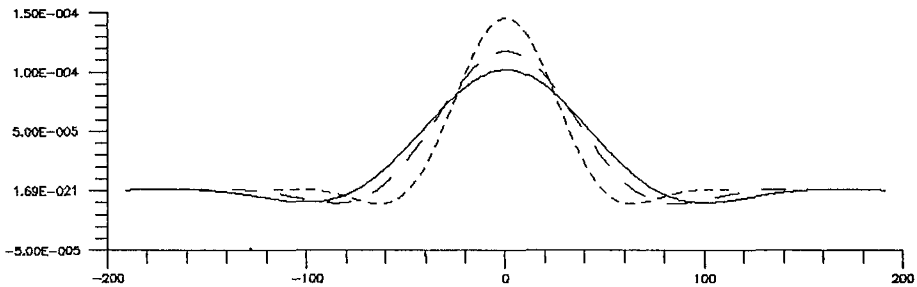
time	amplitude	approxim.	%	support	approxim.	%
0	0.033063	0.033445	1.14	1866	19139	2.503
20000	0.027840	0.027894	0.19	2281	22948	0.601
40000	0.024881	0.024818	0.255	2587	25792	0.301
60000	0.022767	0.022765	0.0106	2804	28119	0.279
80000	0.021265	0.021257	0.0378	3002	30113	0.308
100000	0.020095	0.020083	0.0597	3183	31873	0.315
120000	0.019139	0.019132	0.0377	3343	33458	0.083
140000	0.018337	0.018338	0.0082	3492	34905	0.042
160000	0.017658	0.017662	0.0244	3632	36241	0.217
180000	0.017066	0.017076	0.0583	3763	37486	0.384
200000	0.016541	0.016560	0.117	3884	38653	0.484

In Fig.5 are shown the rescaled results for the shape of coherent structure. One sees that the similarity is beyond any doubt. The same holds for the second kind of homoclinic solutions (Fig.6) which means that the expanding self- similar solutions are inherent in Boussinesq dynamics.



time=40000; time=80000; time=100000;
time=12000; time=140000;

Fig. 1



time=51000; —time=200000; time=400000.

Fig. 2

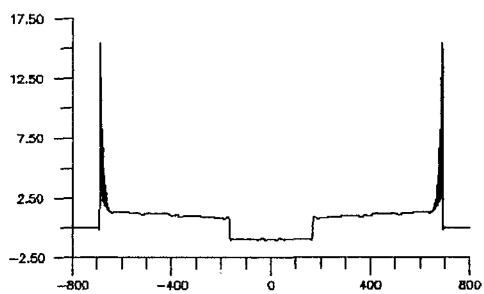


Fig. 3a

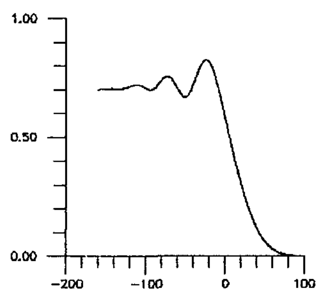


Fig. 3b

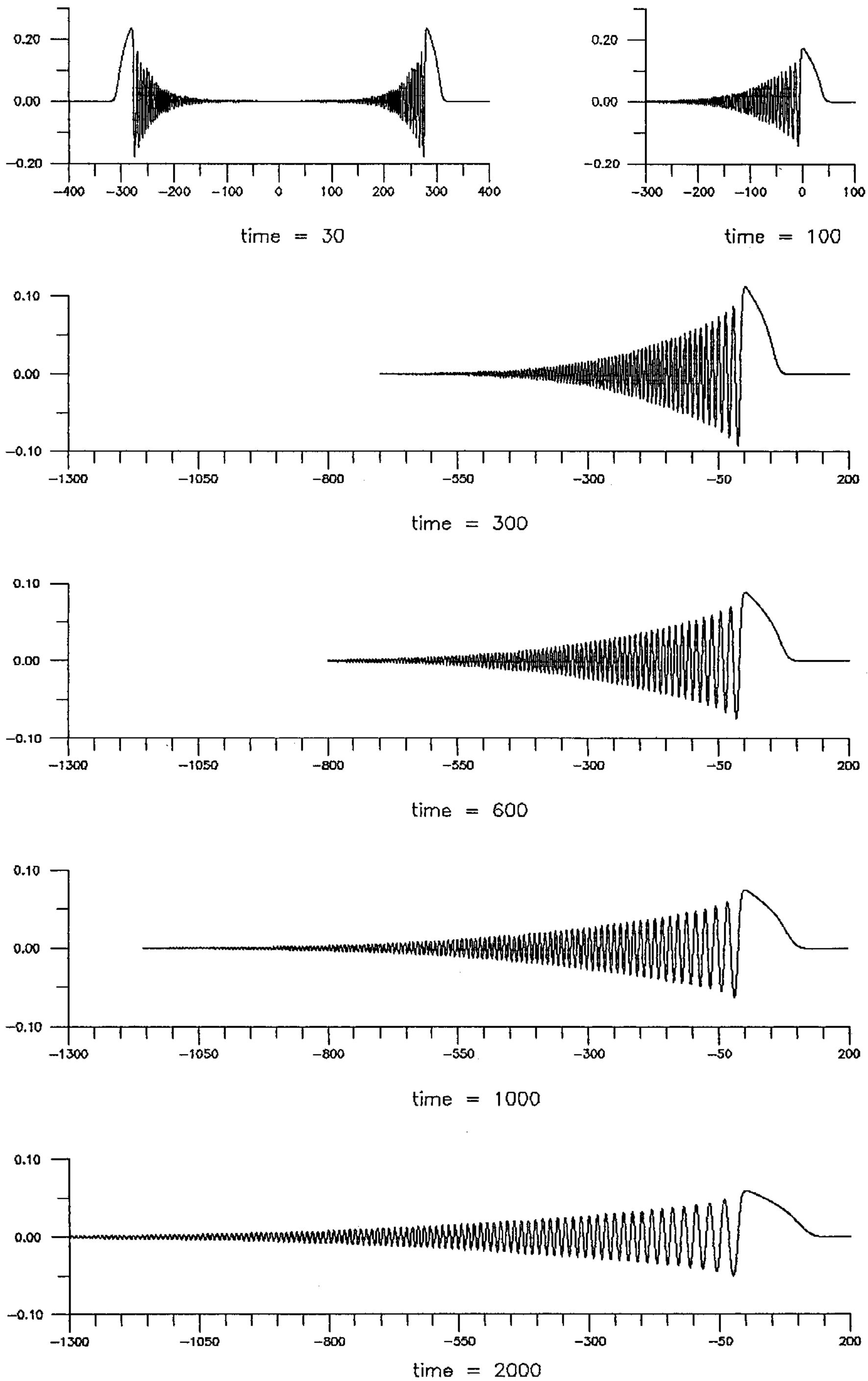
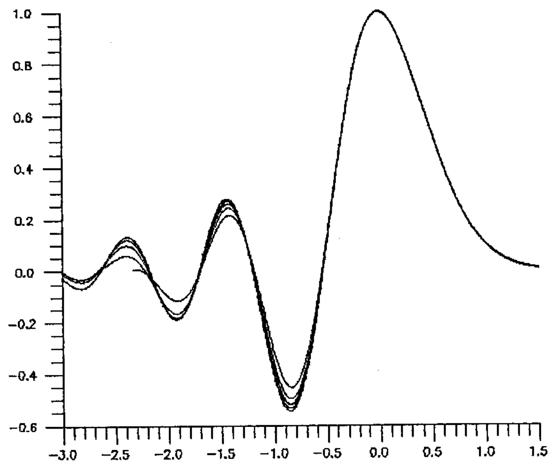
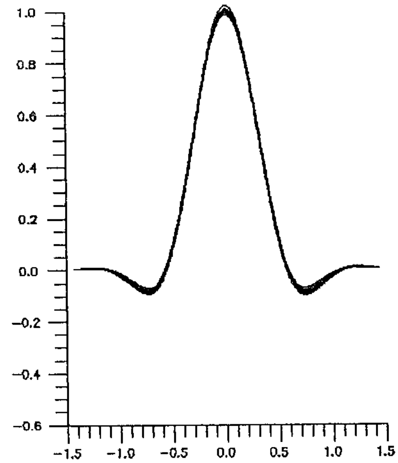

0.20
0.00
−0.20
−400
−300
−200
−100
0
100
200
300
400
time = 30
0.20
0.00
−0.20
−300
−200
−100
0
100
time = 100
0.10
0.00
−0.10
−1300
−1050
−800
−550
−300
−50
200
time = 300
time = 600
time = 1000
time = 2000

Fig. 4



time from 40000 to 200000

Fig. 5



time from 51000 to 400000

Fig. 6

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