Computer Modelling Wave Propagation

Carlo Cattani, Università di Roma La Sapienza, P.le A. Moro 5, I-00185 Roma (Italy), carlo.cattani@uniroma1.it
Luis Manuel Sánchez Ruiz, Universidad Politécnica de Valencia, ETSID, E-46022 Valencia (Spain), lmsr@mat.upv.es

Abstract — In recent years the application of computer algebra systems devoted to Mathematics and Physics have become very popular both in instruction and scientific research. In this paper some issues arising in solving and modelling mathematical and physical problems in wave propagation will be discussed. In particular, computer algebra systems make easy to provide at the same time a large amount of data to be analyzed and a qualitative model and simulation. Very complicated problems of qualitative theory of partial differential equations or computer simulation of physical problems, such as the nonlinear wave propagation require a lot of tedious (some time impossible) analytical computations if done by hand. This is drastically smoothened with computation systems which increase our ability in doing both numerical and symbolic computations, and also making easy the animation of physical problems. The impact of modelling with a computer algebra system, both in teaching and in research, will be discussed giving some examples in the linear and nonlinear wave propagation.

Index Terms — Computer Modelling, Nonlinear, Wave Propagation.

INTRODUCTION

In recent years many scientific results have been based on computer simulation, [1]-[3], in a such way that the theoretical framework was subsequently supported. The amount and difficulty of problems that we can handle now with very little effort by properly using the mathematical software at our disposal, such as MATHEMATICA, MATLAB or DERIVE, [10]-[12], to name some of the most commonly used, is something that we have to take advantage of. Is is noteworthy to mention that the most famous proof such as the 4 colour theorem and the Fermat last theorem take consistently advantage of a computer algebra system.

Computer modelling is successfully based on the following features:

- Visualization.
- Complex computations, both symbolic and numeric.
- Easy approach to sophisticated mathematical tools, even with a little mathematical background.
- Possibility to experience a large amount of mathematical computations in a limited time interval.

However, together with these successfull performances of computer algebra systems, some other physical-technical characteristics of this approach should be considered. A computer simulation is a virtual experiment whose results are taken to guarantee the expected results of a theoretical model. Indeed the virtual experiment made by a computer algebra system may enjoy more advantages than a real experiment such as:

- The virtual experiment is cheaper compared to the real experiment in which all the physical constraints must be included in the simulation, and whose realization may require the construction of sophisticated tools, with extremely expensive pure materials.
- The virtual experiment may be repeated many times with different initial conditions. In fact, the change on the initial conditions of the real experiment, may require the modification of the hardware and mean a long time delay.
- The observation time may be chosen, compatibly with the mathematical stability of the simulation, as large as possible. Thus allowing the forecasting of the evolution in time of the system for a large time \( t \) while in a real experiment it is impossible to make a test up to a time \( t \) greater than our life time (or the life of the instruments).

Another disadvantage in the real experiment (versus computer simulation) is that the realization of the experiment, even if it is accurately done, obliges us to neglect some details whose numerical values are estimated to be small with respect to the numerical results of the experiment. This is true if the time duration of the experiment is also “small”, so that the influence of higher infinitesimal order quantities may be neglected, but if the time range of the experiment is significantly high, then the contribution of the “infinitesimal” or “higher infinitesimal order” terms should not be neglected. Moreover in general the virtual experiment (computer simulation) allows to study complex models so that the effects of the experiment might open new frontiers in the theoretical analysis. We will see in the following that some effects and theoretical prediction, in the linear and nonlinear wave propagation [4]-[7] can be detected only by computer modelling.
LINEAR WAVES PROPAGATION IN SOLID MIXTURES

As a first example we consider wave propagation in solids. The theory of solid mixture can be constructed similar to the classical theory of elasticity. The main hypothesis on mixtures is that the microstructure of a multi-component composite (we will consider in the following a two component, also called two phase materials) can be described using a medium, whose particles simultaneously interact each other at each geometric point of a domain.

In particular we consider a two phase solids, i.e. a material with the microstructure described by the microstructural theory of second order – linear theory of two-phase mixture. Both interacting continua permit finite deformations and displacement not infinitely small. But according to the general theory of interacting and interpenetrating continua the relative displacements of one phase with respect to the other phase in each point of the medium may only infinitely small. So that the conservation of the continuity of the medium holds.

As strain tensor we consider the nonlinear symmetric Green strain tensor, and for the stress the asymmetric Piola-Kirchhoff stress tensor. The interaction model is taken as follows: a) the basic shear force interaction for solid mixtures is the outcome of the relative motions of phases, b) the innercrossing interaction of nonlinear strains appear also in the constitutive equations. The representative volume contains the particle-granules of both phases with different mechanical properties, and each separate phase is characterized by its physical parameters. The interaction between phases is linear and reflects the interaction between mechanical fields of both phases of the mixture.

Usually, the basic assumption of isotropic media is considered, but even in this case there are not enough basic experiments to set up the fully array of physical constants. This is a fundamental problem since in the generalization to a more complex media (for example orthotropic) we do not have a sufficient number of independent experiments. Only theoretical approach is known [13], moreover the orthotropy of a mixture complicates the basic equations, which for an isotropic medium in absence of external forces are

$$\rho_{aa} \frac{\partial^2 u^{(a)}_1}{\partial t^2} - a_\alpha \frac{\partial^2 u^{(a)}_1}{\partial x^2} - a_3 \frac{\partial^2 u^{(\delta)}_1}{\partial x^2} - \beta \left( u^{(a)}_1 - u^{(\delta)}_1 \right) = 0. \tag{1}$$

Here $\rho$ is the partial density of the two-phase mixture, $u^{(a)}_1$ is the partial displacement, $a_\alpha, a_3, \beta$ are physical constants and $\alpha=1, 2, \delta=3-\alpha$.

In this case it is assumed that the plane wave runs in the direction of the $x$-axis. So that there are only two independent variables: $x$ and the time $t$.

As the initial profile at the initial moment $t=0$ we assume the initial pulse with the profile of the Mexican hat (Fig. 1),

$$u^{(a)}_1(x, 0) = B^a F(x), \quad F(x) = \left(1 - x^2\right)e^{-\frac{x^2}{2}}. \tag{2}$$

Due to the weak dispersivity of the mixture, as the medium where the wave propagation occurs, this initial pulse will propagate for a short time in the form of the solitary wave with the profile similar to the Mexican hat. In fact, for the linearity and the absence of external forces no essential distortion of the Mexican hat would appear. That is, if we assume the weak evolution of the initial profile, from the physical point of view we should expect that in a small time interval, close to the initial time, the wave should maintain more or less the initial profile as a classical harmonic wave (see Fig. 2).

This result can be obtained with a classic numerical method, giving the approximate solution of the system (2). Nevertheless some conditions are imposed on the time discretization in order to fulfill stability and convergence of the numerical method.

Since the initial profile is localized in time and is a function having the same properties of wavelets [8]-[9], one can use a family of suitable wavelets, [4]-[6], in order to reconstruct the solution which includes the initial profile (Mexican Hat). By a Galerkin method one obtains an ordinary linear differential system which gives the solution for any $t$. In doing so one can represent the wave propagation even after a long time thus obtaining the surface of Fig. 3 with a superposition of two wave modes, which cannot be seen in the initial time interval (see Fig. 2).

It should be noticed that without a computer algebra system it would be rather difficult, if not impossible to set up an experiment, lasting for a such long time. Moreover, with the computer simulation we avoid the difficult (expensive) problem of constructing a two-phase mixture which fulfills the axioms of the mathematical theoretical model.

One can argue that this virtual experiment cannot be used in the reality, because of the many restrictions on which it is based. However with this approach one can predict some unexpected phenomena that cannot be experienced nor seen from the mathematical solution. The visualization of the wave after a long time gives the full description of the physical propagation.
NONLINEAR WAVES IN ELASTIC MATERIALS

Nonlinear wave interaction in elastic materials arise when a cubic (or higher) order elastic potential is considered for hyperelastic continuum media (such as the Murnaghan potential), [7] and [15]. The nonlinear interaction is due to the presence of simultaneous quadratic and cubic deformation. These deformations are displayed mainly in the second and third harmonic generation [15]. The typical representation of the Murnaghan potential [14] is

\[ W(\varepsilon_{\text{m}}) = \frac{1}{2} \lambda (\varepsilon_{\text{m}})^2 + \mu (\varepsilon_{\text{m}})^2 + \frac{1}{3} A \epsilon_{\text{m}} \epsilon_{\text{m}} + B (\varepsilon_{\text{m}})^2 + \frac{1}{3} C (\varepsilon_{\text{m}})^3. \]  

(3)

Here \( \varepsilon_{\text{ik}} = \frac{1}{2} (u_{i,k} + u_{k,i} + u_{m,i} u_{m,k}) \) is the nonlinear Green strain tensor, \( \lambda, \mu \) are the Lame elastic constants, \( A, B, C \) are the Murnaghan elastic constants. Thus the full representation of the potential (3) in terms of the displacement vector is

\[ W = \frac{1}{2} \lambda (u_{m,m})^2 + \frac{1}{4} \mu (u_{i,k} + u_{k,i})^2 + \left( \mu + \frac{A}{4} \right) u_{i,k} u_{m,i} u_{m,j} + \]
\[ + \frac{1}{2} (\lambda + B) u_{m,m} (u_{i,k})^2 + \frac{1}{12} A u_{i,k} u_{k,m} u_{m,i} + \frac{1}{2} B u_{i,k} u_{k,m} u_{m,m} + \frac{1}{3} C (u_{m,m})^3 + \]
\[ + \frac{1}{4} \lambda (u_{m,m})^4 + \frac{1}{4} \mu (u_{i,m} u_{m,m})^2 + \frac{1}{8} A (u_{i,k} + u_{k,i}) (u_{i,m} + u_{m,i}) (u_{m,k} + u_{k,m}) + \]
\[ + (u_{i,k} + u_{k,i}) (u_{i,m} + u_{m,i}) u_{m,k} u_{m,m} + (u_{i,k} + u_{k,i}) (u_{i,m} + u_{m,i}) u_{m,k} u_{m,m} + \]
\[ + \frac{1}{2} B \left[ (u_{i,k} + u_{k,i}) u_{m,i} u_{m,m} + \frac{1}{2} (u_{i,k} + u_{k,i}) u_{m,i} u_{m,m} \right] + \frac{3}{2} C (u_{m,m})^2 (u_{m,m})^2 + \]
\[ + \frac{1}{24} A \left[ (u_{i,k} + u_{k,i}) (u_{i,m} u_{m,m}) (u_{i,k} u_{m,m}) + \]
\[ + (u_{i,m} + u_{m,m}) (u_{i,k} u_{m,m}) (u_{i,k} u_{m,m}) (u_{m,k} u_{m,m}) \right] + \]
\[ + \frac{1}{4} B \left[ (u_{i,m} u_{n,k})^2 u_{m,m} + (u_{i,k} + u_{k,i}) u_{n,n} u_{n,n} (u_{m,m})^2 + \frac{1}{12} C u_{m,m} (u_{m,m})^4 + \]
\[ + \frac{1}{24} A (u_{i,n} u_{n,k}) (u_{i,m} u_{m,m}) (u_{i,k} u_{m,m}) + \]
\[ + \frac{1}{8} B (u_{i,n} u_{n,k})^2 (u_{m,m})^2 + \frac{1}{24} C (u_{m,m})^6. \]  

(4)

We can see that in the potential appear terms of different order of nonlinearity, from the second order to the 6th. Usually in the nonlinear wave propagation only the contribution given by the second and third order of nonlinearity is considered. The higher order terms of nonlinearity are usually neglected because their contribution to the wave propagation are significantly small and practically invisible (in the real experiments) in the general wave picture. But this may fail to be true as we can see in this example.

If we restrict our analysis to only plane waves propagating along the x-axis so that the displacement is \( u_k = u_k (x, t) \), and we retain only the nonlinear terms of (4) up to the fourth order, by using the non-symmetric Kirchoff stress tensor \( t_{ik} = (\partial W/\partial u_{i,k}) \), the equations of motion are \( t_{k,k} = \rho u_{k,tt} \). Following simple computations we obtain three polarised waves - longitudinal, transverse horizontal and transverse vertical - [7] and [15],

\[ \rho u_{i,tt} - (\lambda + 2\mu) u_{i,tt} = N_1 u_{i,tt} + N_2 (u_{2,1} u_{2,1} + u_{3,1} u_{3,1}) + \]
\[ + N_3 u_{i,tt} (u_{1,1})^2 + N_4 (u_{2,1} u_{2,1} u_{1,1} + u_{3,1} u_{3,1} u_{1,1}), \]  

(5)
\[
\rho u_{2,tt} - \mu u_{2,tt,11} = N_2 \left( u_{2,11}u_{t,1} + u_{t,11}u_{2,1} \right) + \\
+ N_4 u_{2,11} \left( u_{2,1}^2 \right) + N_5 u_{2,11} \left( u_{t,11}^2 \right) + N_6 u_{2,11} \left( u_{t,1}^2 \right), \quad (6)
\]

\[
\rho u_{3,tt} - \mu u_{3,tt,11} = N_2 \left( u_{3,11}u_{t,1} + u_{t,11}u_{3,1} \right) + \\
+ N_4 u_{3,11} \left( u_{3,1}^2 \right) + N_5 u_{3,11} \left( u_{t,11}^2 \right) + N_6 u_{3,11} \left( u_{t,1}^2 \right), \quad (7)
\]

\[
N_3 = \frac{3}{2} (\lambda + 2\mu) + 6 (A + 3B + C), \quad N_4 = \frac{1}{2} \left[ 2 (\lambda + 2\mu) + 5A + 14B + 4C \right], \\
N_5 = \frac{3}{2} (\lambda + 2\mu + A + 2B), \quad N_6 = 3A + 10B + 4C.
\]

The solution \( u_k = u^*_k + u^{**}_k + u^{***}_k + \ldots \) is found by using successive approximations, \([7]\) and \([15]\). In this way, \( u^*_k \) is the first approximate solution of the linear part of the basic system (5)-(7) when all nonlinear terms on the right hand sides are neglected. Once these have been determined, the second approximation solution \( u^{**}_k \) is found from considering the system

\[
\rho \left( u^{**}_{1,tt} - (\lambda + 2\mu) u^{**}_{1,11} \right) = N_1 u^*_1 \left( u_{t,1}^* + u_{t,11}^* \right) + \\
+ N_4 u^*_2 \left( u_{t,2}^* + u_{t,21}^* + u_{t,211}^* \right) + \\
+ N_5 u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right) + \\
+ N_6 u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right), \quad (8)
\]

\[
\rho \left( u^{**}_{2,tt} - \mu u^{**}_{2,tt,11} \right) = N_2 \left( u^*_2 \left( u_{t,2}^* + u_{t,21}^* + u_{t,211}^* \right) \right) + \\
+ N_4 u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right) + \\
+ N_5 u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right) + \\
+ N_6 u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right), \quad (9)
\]

\[
\rho \left( u^{**}_{3,tt} - \mu u^{**}_{3,tt,11} \right) = N_2 \left( u^*_3 \left( u_{t,3}^* + u_{t,31}^* + u_{t,311}^* \right) \right) + \\
+ N_4 u^*_4 \left( u_{t,4}^* + u_{t,41}^* + u_{t,411}^* \right) + \\
+ N_5 u^*_5 \left( u_{t,5}^* + u_{t,51}^* + u_{t,511}^* \right) + \\
+ N_6 u^*_5 \left( u_{t,5}^* + u_{t,51}^* + u_{t,511}^* \right), \quad (10)
\]

If waves propagate only in one direction, e.g. in the direction of the \( x \)-axis, then \( u_x(x,t) = u^*_x(x,t) = 0 \) and just the quadratic nonlinearity is present. From (8), we have

\[
\rho \left( u_{1,tt} - (\lambda + 2\mu) u_{1,11} \right) = N_1 u_{1,11}, \quad (11)
\]

Hence the first approximations for the components of the displacement solution are

\[
u_1^*(x,t) = u^*_x \cos \left( k^*_1 x - \omega t \right), \quad u^*_x(x,t) = u^*_x(x,t) = 0. \quad (12)
\]

The second approximation gives the pure second harmonic with amplitudes continuously increasing with the wave propagation distance

\[
u_1^{**} (x,t) = \frac{1}{8} x \left( \frac{N_1}{\lambda + 2\mu} \right) \left( u^*_0 \right)^2 \left( k^*_1 \right)^2 \cos \left( k^*_1 x - \omega t \right). \quad (13)
\]

The solution describing the profile evolution is \( u_1(x,t) = u^*_1(x,t) + u^{**}_1(x,t) \). Substituting,

\[
u_1 (x,t) = u^*_0 \cos \left( k^*_1 x - \omega t \right) + \frac{1}{8} x \left( \frac{N_1}{\lambda + 2\mu} \right) \left( u^*_0 \right)^2 \left( k^*_1 \right)^2 \cos \left( k^*_1 x - \omega t \right). \quad (14)
\]

In particular, if we fix the parameters and constants in order to analyze the function

\[
u_1 (x,t) = 10^{-4} \cos \left( 0.005x - 10^{-5} t \right) + \frac{3}{8} x 10^{-7} \cos \left( 0.01x - 10^{-5} t \right).
\]
the first approximation
\[ u_1'(x, t) = 10^{-4} \cos \left( 0.005x - 10^5t \right) \]
provides the characteristic profile of wave propagation even for large values of the space and time coordinates (Fig. 4).

The amplitude of the second approximation contribution, being less than \(10^{-4}\),
\[ u_2''(x, t) = \frac{3}{8} x10^{-7} \cos \left( 0.01x - 10^7t \right), \]
seems to be neglectable (Fig. 5). However when we combine together the first and second approximation, the influence of the second approximation on the basic trend will be neglectable for small values of \(x\), but it becomes more and more evident on the wave profile, for large values of \(x\) (Fig. 6).

**CONCLUSION**

The needs of future Engineering professionals follow the trend, and perhaps with more emphasis, of the need of learning that many of the things that we learn will become obsolete in a short period of time, and that there is an urgent need of doing things and solving problems with efficency and quickness. Thus traditional Mathematics taught on blackboards and just mimicking the techniques to solve mathematical problems might be an option to save the day, or the academic year, but it would not be fair to our students who would find scenarios in the real world very different from the ones learnt at the university. The proliferation of new technologies and mathematical software have complicated, and made much easier at the same time, our daily task of preparing our future engineers. We are just at the threshold of a revolution in the teaching and research of Mathematics.

In this paper some simulation models of wave propagation have been shown and analysed. The main features in computer modelling dynamical system evolution can be easily detected. Some theoretical prediction can be simulated only by using a computer algebra system. This arises some new possibilities and questions about computer modelling such as whether the theoretical model is strengthened by the computer modelling or the mathematical theory should be simplified in order to permit real physical experiments.

**REFERENCES**

FIGURES

FIGURE 1
INITIAL PULSE AS MEXICAN HAT

FIGURE 2
INITIAL EVOLUTION FOR $t << 1$

FIGURE 3
WAVE PROPAGATION AT TIME $t = 2 \times 10^4$
FIGURE 4
Wave Profile of the First Approximation for Large Time and Space Coordinates

FIGURE 5
Wave Profile of the Second Approximation for Large Time and Space Coordinates

FIGURE 6
Wave Profile of Both First and Second Approximation for Large Time and Space Coordinates