Complex Computer Simulations, Numerical Artifacts, and Numerical Phenomena

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Abstract: The study of some typical complex computer simulations, presenting one or more Complexity features, as the: a) symmetry breaking, b) nonlinear properties, c) dissipative processes, d) high-logical depth, e) self-organizing processes, etc allows to point out some several numerical artifacts, namely the: (i) distortions, (ii) scattering, (iii) pseudo-convergence, (iv) instability, (v) mis-leading (false) symmetry-breaking simulations and others. The detailed analysis of these artifacts allowed clarifying the numerical mechanisms of some such artifacts, which can be named in following numerical phenomena, because their basic features can be exactly predicted.

Keywords: Computer Simulations, Numerical Artifacts, Numerical Phenomena, Self-organizing Processes.

1 Introduction

We live in a computerized world, our civilization being a "civilization of Computers". Taking into account that computers control the work of all-present complex installations and devices, the appearance (due to some numerical phenomena) of some important distortions of the simulated processes lead usually to major failures of the technical installations. Particularly, the events referring to the erroneous computer (numerical) simulation and design of the flight of the Patriot Missile which failed (with disastrous results) - during the Gulf War in 1991 - to stop a Scud Missile [1] and the self-destruction of the European Space Agency's Ariane 5 rocket, at 37 seconds after its launch [2], were both assigned to computer errors [3] and to their associated numerical artifacts/artefacts/phenomena.

Given being the computer simulations are considerably cheaper than the experimental studies and they allow the prediction of the physical systems behavior even in inaccessible conditions, the computer simulations are widely used in technical studies. Because the modern (optimized) technical systems are complex [4], the computer simulations are also complex, and - for this reason - they generate specific numerical artifacts. In fact, there is a huge number of publications reporting such phenomena (usually related to some complex numerical simulations), as it can be easily found consulting some search systems, e.g. the Google system. As it results from Table 1, even eliminating by the use of quotation marks (") the "parasitic" published works entitled as numerical simulations of... boiling *phenomena*, etc, there remain very large numbers of published works in these fields.

This work deals with the study of possibilities to discover the mechanisms of the artifacts intervening in some complex simulations and to predict quantitatively the basic parameters of

Topics	No quotation marks	With quotation marks, e.g. "Numerical Artifacts"
Numerical Artifacts	1,180,000	9,370
Numerical Artefacts	126,000	2,440
Numerical Phenomena	4,160,000	1,340
Complex Simulations		3,000

Table 1: Numbers of published papers found by the Google search system (beginning of 2009)

the computer generating errors, transforming so the observed numerical artifacts/artefacts in the so-called numerical phenomena. We have to underline from beginning that the discovery of these mechanisms belong to the field of Numbers Theory and that many problems in the field of Numbers Theory are extremely difficult. E.g., the statement of the (Pierre de) Fermat's last (greatest) theorem was published (after his death, by his eldest son - Clément Samuel Fermat) in 1670 [4], but its solution was found only in 1995 [5] by the professor Andrew Wiles [6].

We will focus mainly to the study of the main features of the classical [7], [8] and of the newly found [9], [10] numerical phenomena associated to the Finite Differences (FD) simulations [11] of the pulses propagation through media with sharp interfaces and attenuative character, as well as of other numerical methods (as the random walk method, the gradient one, etc), applied to the study of different physical processes, as diffusion [12], [13], solitary wave propagation, applications to the evaluation of the parameters of some physical systems, etc.

2   Symmetry breaking in some computing programs

2.1   Symmetry breaking of the wave equation in ideal media

The Finite Differences (FD) discretization of the wave equation in ideal media:

$$\frac{\partial^2 w}{\partial \tilde{t}^2} = V_\Phi^2 \frac{\partial^2 w}{\partial x^2} \rightarrow \frac{w_{t+1} + w_{t-1} - 2w}{\tau^2} = V_\Phi^2 \frac{w_{i+1} + w_{i-1} - 2w}{\epsilon^2} \tag{1}$$

which is symmetrical relative to the space steps $i-1$, i, $i+1$ and the time steps $t-1$, t, $t+1$, if the FD velocity and the wave propagation one are equal:

$$V_{FD} = \frac{\epsilon}{\tau} = V_\Phi \tag{2}$$

Defining the Courant's number [7] by means of the relation:

$$C = \frac{V_\Phi}{V_{FD}} \tag{3}$$

one finds easily that if: (i) $C > 1$, there will intervene *instabilities*, because the FD schema does not use all information received at the observation point ($V_\Phi > V_{FD}$), (ii) $C < 1$, there will intervene *distortions*, because for $V_\Phi < V_{FD}$, the FD schema uses more information than it receives, and this additional information acts as a jamming, (iii) $C = 1$, we have an ideal FD schema (stable and convergent), because this schema has all necessary physical information and nothing more! One finds that *the symmetry breaking for values different than 1 of the Courant number leads to the "classical" numerical phenomena.*

2.2 Symmetry breaking of the smoothing model of a sharp interface

Consider a sharp interface between 2 homogeneous elastic media. If the method of Finite Differences (FD) is used, then - in order to avoid the use of Dirac function - a certain smoothing of the sharp interface is necessary, spreading it over 2 or 3 FD nodes, whose indices i are denoted as $I-1$, I and $I+1$ (see Figure 1).
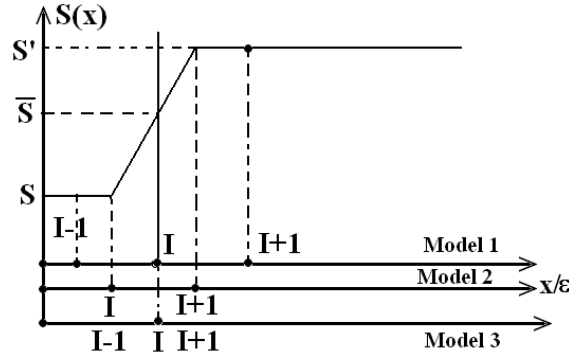

Figure 1: Smoothing models of the sharp 1-D interfaces (see also [14]-a).

Then the differential equation $\rho(x)\frac{\partial^2 w}{\partial t^2} = \frac{\partial}{\partial x}\left[S(x)\frac{\partial w}{\partial x}\right]$ of the elastic pulses propagation through an in-homogeneous medium becomes:

$$\tilde{\rho}_i \frac{w_{t+1} + w_{t-1} - 2w}{\tau^2} = \left\langle \frac{\partial S}{\partial x}\right\rangle_i \frac{w_{i+1} + w_{i-1}}{2\epsilon} + \tilde{S}_i \frac{w_{i+1} + w_{i-1} - 2w}{\epsilon^2}. \tag{4}$$

where $\tilde{\rho}_i = \langle\rho\rangle_i$, $\tilde{S}_i = \langle S\rangle_i$ and $\left\langle\frac{\partial S}{\partial x}\right\rangle_i$ are the chosen average values around the FD node i. The chosen expressions of these average values (see Table 2) can succeed or not to remake the (apparent) symmetry of the propagation medium in the frame of the FD simulation; e.g., one finds from the examination of Table 2, that all required expressions are symmetrical around the sites $I-1$, I and $I+1$ for model 1, and around the sites I and $I+1$ for model 2a, while this general symmetry is not kept for all average expressions of models 2b, 3a and 3b.

That is why - while the smoothing models 1 and 2a ensure always stable and convergent numerical simulations - for the smoothing models 2b 3a and 3b, respectively, there appear the basic types of usual numerical artifacts [7, 8, 14]: a) the instability, b) the pseudo-convergence. The plots of these numerical artifacts for the above-indicated 5 types of studied Finite Differences (FD) smoothing schemes (models), intended to the simulation of certain elastic pulses propagation through complex materials are presented by Figures 2 and 3 below (see also [15]).

i	$\tilde{\rho}_i$			$\tilde{S}_i$			$\left\langle\frac{\partial S}{\partial x}\right\rangle_i$		
	$I-1$	I	$I+1$	$I-1$	I	$I+1$	$\left\langle\frac{\partial S}{\partial x}\right\rangle_{I-1}$	$\left\langle\frac{\partial S}{\partial x}\right\rangle_I$	$\left\langle\frac{\partial S}{\partial x}\right\rangle_{I+1}$
1	ρ	$\frac{\rho'+\rho}{2}$	ρ'	S	$\frac{S+S'}{2}$	S'	0	$\frac{S'-S}{\epsilon}$	0
2a	ρ	$\frac{3\rho'+\rho}{4}$	$\frac{3\rho'+\rho}{4}$	S	$\frac{3S+S'}{4}$	$\frac{S+3S'}{4}$	0	$\frac{S'-S}{2\epsilon}$	$\frac{S'-S}{2\epsilon}$
2b	ρ	ρ	ρ'	S	S	S'	0	$\frac{S'-S}{2\epsilon}$	$\frac{S'-S}{2\epsilon}$
3a	ρ	$\frac{\rho'+\rho}{2}$	ρ'	S	$\frac{S+S'}{2}$	S'	$\frac{S'-S}{4\epsilon}$	$\frac{S'-S}{\epsilon}$	$\frac{S'-S}{4\epsilon}$
3b	ρ	$\frac{\rho'+\rho}{2}$	ρ'	$\frac{7S+S'}{8}$	$\frac{S+S'}{2}$	$\frac{S+7S'}{8}$	$\frac{S'-S}{4\epsilon}$	$\frac{S'-S}{\epsilon}$	$\frac{S'-S}{4\epsilon}$

Table 2: Expressions of the average values of the main elastic parameters for the basic smoothing models of one-dimensional (1-D) interfaces (see also [14]-a)
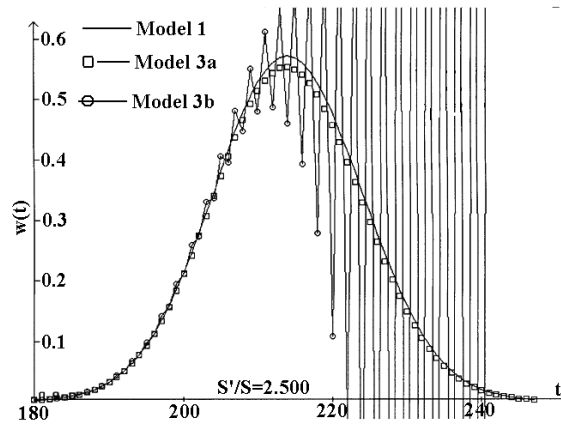
Figure 2: Plots of numerical simulations corresponding to different FD schemes (those of models 3a and 3b are pseudo-convergent, and unstable, respectively).
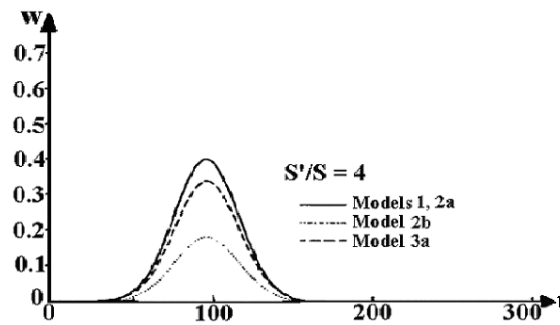

Figure 3: Convergent numerical simulations corresponding to models 1 and 2a, and pseudo-convergent ones for models 2b, 3a.

One finds that while the instabilities can be easily detected and eliminated, the pseudo-convergence is considerably more "dangerous", because: a) the pseudo-convergent simulations have a right shape, while: b) the corresponding wrong displacement values can be considerably more difficult observed, hence the pseudo-convergent simulations could be easily misleading.

3   Nonlinear properties of the propagation medium

It is well-known [7] that the computer rounding errors are amplified considerably in the frame of some non-linear equations, as those corresponding to certain solitary waves, leading due to some instability numerical artifacts (see Figure 4). Particularly, the Korteweg-de Vries equation:

$$\frac{\partial u}{\partial t} = -v_{00}u' - nuu' - d_1u''' \tag{5}$$

can be discretized as:

$$f(i) = p(i) - \gamma \cdot [a(i+1) - a(i-1)] + \alpha \cdot a(i) \cdot [a(i-1) - a(i+1)] + \beta \cdot [a(i-2) - a(i+2)] \tag{6}$$

There were studied the numerical artifacts corresponding to the 2 main types of nonlinear solitary waves (which can propagate keeping their shapes): the bell-shaped (or breathers) and
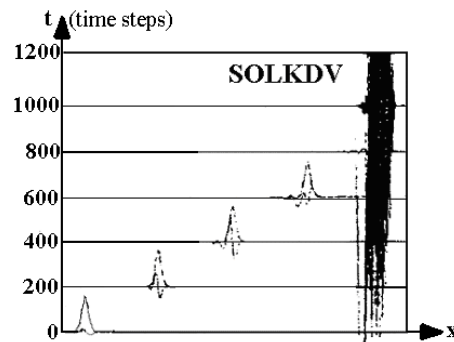
Figure 4: FD simulation of a Korteweg-de Vries (KdV) solitary wave breather propagation

the kink-shaped waves [16]. Figures 4 and 5 present the basic numerical artifacts intervening in the FD simulations of the breathers propagation (see also [17]).

While the artifacts intervening in the simulations of the KdV breathers propagation reduce to a monotonic increase of distortions up to the appearance of the instability (Figure 4), the use of the discrete version (DNLS) of the cubic nonlinear Schrödinger (NLS) equation to describe the wave-guide arrays with saturable nonlinearity leads in certain conditions to the artefact corresponding to the merging of two breathers with symmetry breaking (see Figure 5 and [17]).
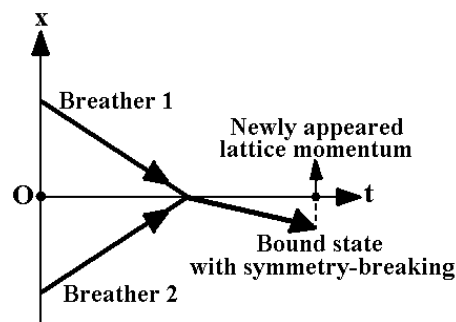

Figure 5: The symmetry breaking artefact intervening in the merging (bound state formation) of 2 symmetric SNLS breathers

4 Dissipative media

Because the modulus of the first solution of the attenuation-dispersion relation [15] is larger than 1: $|g_1| = e^{\epsilon E} > 1$, the FD schemes used for the simulation of the acoustic pulses propagation in dissipative media are always unstable. There were pointed out also: (i) the instability of the attenuated wave simulation, *even for absolutely exact initial conditions*, due to the generation of the amplified wave (mathematically possible, but without a physical meaning) by the stochastic local accumulation of some local "rounding" inaccuracies of the exact values corresponding to such waves, acting as a self-organising process in the computing program run, as well as: (ii) the extremely strong acceleration of the amplified wave generation when the complex wave-functions are used (stability and convergence radii of the magnitude order of 1 dB or even smaller). The introduction of some: (i) corrective measures (the use of some analytical expressions of some partial derivatives, particularly), (ii) properly chosen effective parameters, allows the weakening of these unpleasant numerical phenomena, ensuring stability and convergence radii of the magnitude order of 100 dB [13], which represent sufficiently high values for accurate descriptions, by

means of the finite difference method, of the cases of technical interest.

5   High Logical Depth

As it results from equation (1), the FD scheme of waves propagation in ideal media is not too intricate, even if the Courant's number is less than 1: $C < 1$. The repeated use [by a large number ($N > 10^5$) of successive iterations, e.g. for simulations of the ultrasonic non-destructive examinations of some industrial components] of this equation, leads however to the high logical depth Complexity feature of the used computer program, and consequently to several numerical artifacts indicated in the frame of Figure 6.

The expressions of the main limits are: $x_e = -Ct - 2\sqrt[3]{t}$, $x_p = 1 + C(t-1)$, $X_p = N + C(t-1)$, $x_n = Ct + N + 2\sqrt[3]{t}$, while for $C \approx 0.5$ and $N \approx 71$, the relative (to the incoming pulse one) amplitudes of the echo pulses have the magnitude orders: 0.1 for the rectangular pulse, 0.01 for the sine pulses, and 0.001 for the Gaussian pulses.
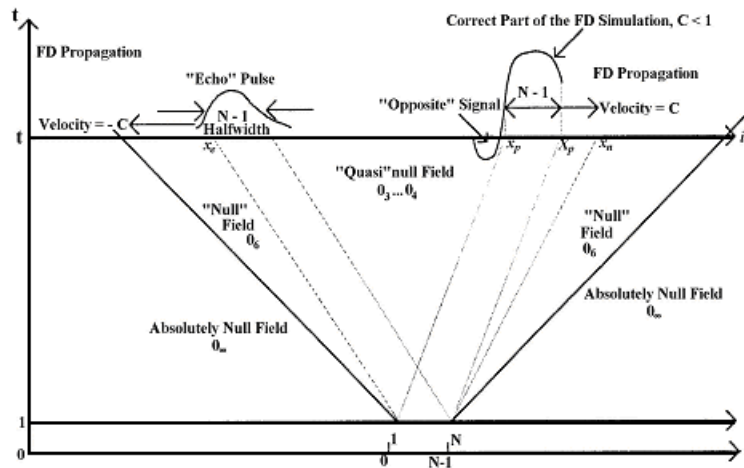

Figure 6: Structure of FD simulations of the propagation of pulses of different shapes

6   From the Numerical Artifacts to the Numerical Phenomena

6.1   Difficulties and main methods used to study the numerical artifact mechanisms

Because many problems in the field of Numbers Theory are extremely difficult, the aim of this study is to point out the main features of the mechanisms leading to some numerical artifacts intervening in the computer simulations of pulses propagation. The accomplished analysis pointed out that the main methods to study these numerical artifact mechanisms are the methods of the: a) FD transfer coefficients [18], b) Fourier's representation of the exact solutions of the discretized wave equation [19].

6.2   The method of transfer coefficients

In order to explain the results corresponding to the linear FD schemes, a partition of the incoming pulse in N components of amplitudes (in the order of their incoming on the studied

material) $s_1, s_2, \ldots, s_N$ is considered. The amplitudes of the same components in the previous time step are denoted by $s'_1, s'_2, \ldots, s'_N$.

The transfer coefficients k_{ti} are defined by means of the expressions (4) of the displacement w_{It} corresponding to the space site I at the moment (time step) t:

$$w_{It} = \sum_{j=1}^{N} k_{t,N+2+t-I-j} \cdot s_j - \sum_{j=1}^{N} k_{t,N+t-I-j} \cdot s'_j \tag{7}$$

A simplified definition of the transfer coefficients corresponds to the FD simulations with equal values of the real phase speed V_Φ and of the FD one: $V_{FD} = \frac{\epsilon}{\tau}$ (i.e. for the value 1 of the Courant number [7]: $C = \frac{V_\Phi}{V_{FD}}$), because then the pulse partition components at successive time steps coincide: $S'_i = s_i$ (for any $i = 1, 2, \ldots, N$). In the particular case of a sharp 1-D interface located in the site I, the transfer coefficients describing the transmitted wave are defined as [14]-a:

$$w_{I+1,t} = \sum_{j=1}^{t-2} k_j s_{t-j-1} \tag{8}$$

6.3   Fourier's representation method of the exact solutions of the discretized wave equation

The exact discrete solution of the wave equation is written by means of its Fourier expansion, as:

$$w_{j,t} = \sum_{k=-\infty}^{\infty} C_k \cdot [g(k)]^t \cdot e^{ik \cdot j\epsilon} \tag{9}$$

where $g(k)$ is named the amplification factor. Introducing this expression in the wave equation, one obtains the "attenuation-dispersion" relation:

$$g - 2 + \frac{1}{g} = F(k \cdot \epsilon, V_{FD}, w) \tag{10}$$

where $F(k \cdot \epsilon, V_{FD}, w)$ is a specific function of the considered wave.

According to von Neumann's theorem ([19]-a, p. 42), the considered FD scheme will be stable if both solutions of the algebraic equation (10) fulfil the requirement: $|g_{1,2}| \le 1$, else this scheme will be unstable.

6.4   Applications to the study of mechanisms of some numerical artifacts

The method of transfer coefficients. Appplying this method to the problem of sharp interfaces (see Section 2a and Figures 1 - 3), we will find that the above indicated numerical artifacts belong to the class of numerical phenomena, because they can be identified and described starting from the values of the roots of the characteristic equation [15]:

$$\xi^2 - (t\_t_1 + 2t\_t_2 + t_0 t_1)\xi - t\_t_2 = 0. \tag{11}$$

where: $t_i = a_{i-1} b_i - 1$, while a_i and b_i are the coefficients of the FD wave equation (4): $w_{i,t+1} = a_i w_{i+1,t} + b_i w_{i-1,t} - w_{i,t-1}$. One finds so that as $|\xi| > 1$ or $|\xi| < 1$, the used FD scheme is unstable, or it is stable.

The method of Fourier's representation. Using the above presented method of the Fourier's representation of the exact solutions to the problem of Korteweg-de Vries solitons

(Section 3), one obtains the following expression [19]-b,c of the upper threshold (for the numerical scheme stability) of the time step:

$$\tau_{max} = \frac{\epsilon}{\alpha A + \frac{4\beta}{\epsilon^2}} \tag{12}$$

Our study [15] pointed out both the validity of the Vliegenthart condition (13), as well as the monotonic improvement of the FD simulations accuracy as the representative point of the FD steps ϵ, τ tends to the Vliegenthart's boarder of the stability and instability regions.

One finds so that the stability field of the FD simulations of KdV solitons propagation is rather broad. Because the size and borders of the stability domain depend on the: a) strongly (e.g., in the case of some exponential dependencies) or weakly (as in the above studied case) character of the nonlinear dependence, b) number of interacting system components.

7   Stability and Convergence Radii of Different Numerical Schemes

The accomplished numerical studies [20], [21] have pointed out that, for given values of the wave frequency (or wavelength) and of the tangent of mechanical losses, beginning from a certain number of space (or time) steps x_{lim}, one finds usually the appearance of large oscillations of the simulated displacements, which lead quickly to instability. Because the instability is determined by the value of the factor e^{Ex} and: $E = k \tan \frac{\delta}{2}$, while the wave intensity is proportional to the square of displacement: $I \propto w^2$, one finds that the measure (in deci-Bells) of the intensity level corresponding to the stability field is:

$$\langle L_{I,stab} \rangle_{dB} = 2 \langle L_{w,stab} \rangle_{dB} = 20 E x_{lim} = 20 k x_{lim} \tan \frac{\delta}{2} = 40\pi \frac{x_{lim}}{\lambda} \tan \frac{\delta}{2}. \tag{13}$$

Of course, the decrease of the wave intensity corresponding to the stability field (limit) is:

$$\frac{I_{lim}}{I_0} = e^{-2Ex_{lim}} = e^{\frac{\langle L_{I,stab} \rangle}{10}} \tag{14}$$

Table 3 synthesizes the obtained numerical results.

Type of the wave equation	No. of numerical interactions	$\langle L_{I,stab} \rangle_{dB}$	t_{lim} (stability, life, steps)
Complex stiffness equation	12	0.0321	102
Complex stress relaxation time	10	4	12732
Complex wave-vector equation	8	20	63622
Space evolution Equation	6	40.476	128839
Real wave, equation	5	80.130	255062

Table 3: Stability radii and mean life of different numerical simulations [15].

8   Analysis of the Obtained Results for Different Studied Numerical Schemes and Physical Processes

The obtained results (Tables 1 and 2) concerning the stability and convergence radii of different numerical schemes intended to the computer simulation of certain physical processes

(acoustic pulse propagation, diffusion with drift, absorption, etc) indicate the "accessible" logical depths [22] of the specific studied physical problems, for each of the used numerical schemes. These results present also a considerable importance for the choice and optimization of the numerical schemes [23]. Certain numerical schemes, e.g. that corresponding to the complex stiffness $\bar{S}$ symmetric wave equation of the propagation in dissipative media:

$$\rho \frac{\partial^2 \bar{w}}{\partial t'^2} = \bar{S} \frac{\partial^2 \bar{w}}{\partial x^2} \qquad (15)$$

allow multiple solutions; using the FD descriptions: $t' = t\tau$ and: $x = I\epsilon$ (in terms of the time τ and space ϵ steps) of the real time t and space coordinate x, these solutions can be written as:

$$\bar{w}_{I,t} = A \cdot e^{\pm i\omega t\tau} \cdot e^{\pm(E+ik)I\epsilon} \qquad (16)$$

Even if the initial conditions launch only the "direct" wave:

$$\bar{w}_{I,t}^{\text{dir.}} = A \cdot e^{-EI\epsilon} \cdot e^{i(\omega t\tau + kI\epsilon)} \qquad (17)$$

some random accumulations of the rounding errors intervening in the evaluation of the partial derivatives produce a local ("spontaneous") generation of the inverse wave:

$$\bar{w}_{I,t}^{\text{inv.}} = A' \cdot e^{EI\epsilon} \cdot e^{i(\omega t\tau + kI\epsilon)} \qquad (18)$$

leading to the sudden apparition of instabilities.

One finds so that the numerical simulations of the waves propagation through dissipative media lead to a typical problem of self-organizing systems, with a spontaneous symmetry breaking. This symmetry breaking corresponds to the "spontaneous" local generation of the inverse wave, launched by the random accumulation of the "garbage" rounding errors and followed by the transition between the attenuated wave and the apparently amplified wave, corresponding to the "inverse" wave. The accomplished study (see Tables 1 and 2) points out that the "speed" of this self-organization process crucially depends on the number and intensity of the numerical "interactions" between the components (the values $w_{I,t}$ of the displacement in different sites I, t of the FD grid) of the simulation process.

Because such numerical "interactions" are achieved mainly by the FD approximate expressions of the partial derivatives, the "spontaneous" breaking of the symmetry appears quicker for (in the decreasing order of importance):

- a) large numbers of displacement components involved in the expressions of partial derivatives, e.g. when their expressions with 2 previous time steps (instead of those using an only one previous time step) are used[1]:
  $\dot{f}(0) = -f(2\tau) + 8f(\tau) - 8f(-\tau) + f(-2\tau)/12\tau$,
  $\ddot{f}(0) = -f(2\tau) + 16f(\tau) - 30f(\tau) + 16f(-\tau) - (-2\tau)/12\tau^2$ when the instabilities appear after only few tens of iterations,

- presence and repeated "mixture" of the values of both real and pure imaginary parts of the complex wave function (displacement) $\bar{w}$,

- more parasitic solutions,

- more partial derivatives involved in the expression of the differential equation of the acoustic pulse propagation.

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[1]The formulae in more points are considerably more accurate for rather small numbers of iterations, but they give rise later to spurious solutions and instability (see Table 1).

For these reasons, the highest "accessible" logical depth [22] is reached (for the simulations of the acoustic pulse propagation through attenuative media) for the numerical scheme using the real wave function equation (see table reftab02), with the usual FD approximations of the first 2 order derivatives:

$$\dot{f}(0) = \frac{f(\tau) - f(-\tau)}{2\tau}, \ddot{f}(0) = \frac{f(\tau) - 2f(0) + f(-\tau)}{\tau^2}. \tag{19}$$

9   Conclusions and Future Works

The obtained results concerning the different numerical phenomena associated to the complex computer simulations present a considerable importance for the choice and optimization of these numerical schemes [23]. It was also found that some numerical simulations (e.g, those of the acoustic pulse propagation through attenuative media) allow the study of some features of the self-organizing systems (the "spontaneous" symmetry breaking, the influence of the interactions between the system components on the "accessible" logical depth, etc).

Acknowledgments

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