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COULD BE ACTIVE IN NATURE SCIENCES – THE COMPLEXITY THEORY

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Rezumat. *Pornind de la caracteristicile de bază ale sistemelor complexe, lucrarea de faţă studiază posibilităţile de utilizare a acestor noţiuni pentru elucidarea unor probleme încă nerezolvate privind: a) procesele de creştere/acomodare din: (i) biofizică, (ii) cosmologie etc., b) teoria simulărilor numerice ale unor procese fizice diferite. Au fost definite şi evaluate razele de stabilitate şi – respectiv – convergenţă ale unor diferite scheme numerice, ceea ce a permis estimarea adâncimii logice accesibile a unor simulări numerice de diferite tipuri, considerate ele înşişi drept sisteme complexe.*

Abstract. *Starting from the basic features of the complex systems, this work studies the possibilities to use these basic notions in order to elucidate some still unsolved problems referring to the: a) growth/accommodation processes from: (i) biophysics, (ii) cosmology, etc., b) theory of numerical simulations of different physical processes. There were defined and evaluated the stability and convergence radii of different numerical schemes, which allowed to estimate the accessible logical depth of various numerical simulations, considered themselves as complex systems.*

Keywords: Complexity theory, Growth/accommodation processes, Inflation stage, Stability and Convergence Radii, Accessible Logical Depth

1. Introduction

Despite of the fact that the theory of Complexity was elaborated and supported by many illustrious scientists, as Ettore Majorana [1], the mathematicians Warren Weaver [2] and Claude Shannon [3], the Physics Nobel prize laureates Murray Gell-Mann [4], Philip Warren Anderson [5], Kenneth Geddes Wilson [6], Pierre-Gilles de Gennes [7], as well as by the Chemistry Nobel prize laureate Ilya Prigogine (1977) [8], some specialists still consider that "the very young science of complexity has promised much but delivered little so far" [9]. The accomplished study [10] pointed out that the basic features of the complex systems are: a) the preferential use of physical numbers (due to the Universality of the complex systems laws) and: b) the similitude theory, as well as of the: c) power laws in the Complexity theory, d) logical depth of each Physics problem,

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e) self-organizing processes, etc. Taking into account also the appreciation of the Physics laureates Russell Hulse (1993): "Physics continues to face a big challenge in terms of what it defines itself to be, and this will determine its fate as a field. If physics grows by integrating a broader interdisciplinary definition of itself, it will remain a pivotal science.

If it defines itself narrowly only in terms of what it has been in the past, its role and impact will diminish" and Nicholas Bloembergen (1981): "There are many unsolved problems, especially in biophysics and astrophysics", this work tries to find the possibility to use the basic Complexity notions in order to elucidate some still unsolved problems referring to the: a) growth processes from: (i) biophysics, (ii) cosmology, and of the: b) theory of the numerical simulations of different physical processes.

2. Complexity theory applications in description of the growth/accommodation processes

The use of the complexity theory to describe the growth/evolution processes of the: a) human body, b) Universe, was studied in detail by the work [11]. We have to underline: (i) the use of the physical numbers, e.g. of the variable $z = \ln y$, where y is the usual (dimensional) physical quantity (e.g. the human body weight or height, the Universe size, etc), (ii) the use of the similitude models and criteria in order to test the compatibility of a certain theoretical model relative to the experimental data, (iii) the use of the "phases space" $(\dot{z}, z)$ in order to describe the growth processes, (iv) the compatibility of the power law: $\dot{z} = C \cdot z^n$ [where: $n \in (0, 1)$ and: $C > 0$] both with the inflation stages corresponding to the human body growth and with that of the Universe evolution, (v) the capacity of the Universality classes U_0, U_1 and U_2 to describe also [12] the other types of growth stages by means of the equations:

a) $\dot{z} = s\ (constant)$, and: $z = \ln y = m + s.t$ (auto-catalytic growth, class U_0), (1)

b) $\dot{z} = a_o + \alpha_1(z - z_o)$, with: $a_o = \dot{z}_o$, $z_o = \ln y_o$ (Gompertz growth, class U_1), (2)

c) $\dot{z} = \left(1 + \dfrac{\beta}{\gamma \cdot a_o}\right) \cdot e^{\gamma z} - \dfrac{\beta}{\gamma}$, with: $\beta > 0, \gamma < 0$ (West type growth, class U_2), (3)

(vi) the possibility of appearance of some inflation phases also in the accommodation processes of different (e.g. complex magnetic) materials, as it is shown by Figure 1 for the time dependence of the magnetization process for an alnico rod [13], (vii) the use of the phase transitions of some industrial complex materials in order to optimize their technological performances, e.g. in order to ensure a certain stabilization of their basic parameters (for example of the permeability) at the usual temperatures (see Figure 2).

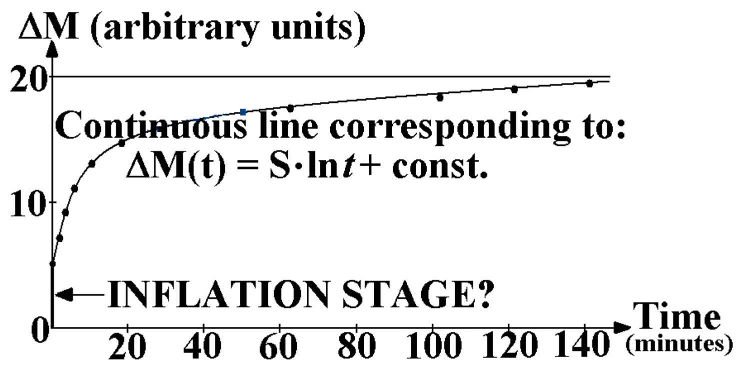

Fig. 1. The time dependence of the magnetization of an alnico rod [13]

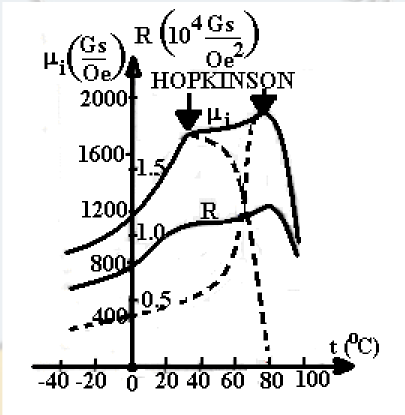

Fig. 2. Temperature dependencies of the initial magnetic permeability μ_i, and of the Rayleigh's coefficient R, for the industrial complex material $Fe_{2.0}Mn_{0.58}Zn_{0.42}O_4$ [14], [10] (p. 249).

We have to underline also finally the existence of some connections between different features of the complex systems. For example, consider 2 correlated physical parameters p and q. Let $\ln p$ and $\ln q$ be their *numerical (i.e. complexity) equivalents* and let assume the most elementary (basic) correlation – the linear one: $\ln p = \ln p_1 + s \cdot \ln q$, between them (where the intercept $\ln p_1$ and the slope s are constant). It results that: $p = p_1 \cdot q^s$, (4)
i.e. *the power law*, which is a basic feature of complex systems. If q corresponds to the sample size, then relation (4) represents a typical *fractal scaling law* describing the so-called *size effects* met for the complex systems.

Taking into account the definitions of Murray Gell-Mann of *the effective complexity* as "the length of a highly compressed (without redundancies) of the regularities of the entity under consideration" and of the *apparent* (but more interesting for applications) *complexity* as "*the logical depth* associated with the computation time" [4], this work will study *the accessible logical depth* corresponding to some numerical simulations of certain physical processes.

3. Evaluation of the Accessible Logical Depth of the Numerical Simulations of different physical processes

It is well-known that while the effective complexity is measured by the length of a highly compressed (without redundancies) description of the regularities of the studied entity, the apparent complexity (though the most important one from the point of view of applications) refers to the logical depth of the studied problem, i.e. to the necessary (often very long) computation time [4].

Taking into account that the accessible (by means of some numerical simulations) logical depth corresponds to the radii of stability and convergence of the used theoretical algorithms and numerical schemes, this work will study these elements for the computer simulations of different physical processes.

a) *Statistical Tests of Compatibility*

Because the computers are complex systems, the computer programs are expected to exhibit the main Complexity features indicated by Philip Anderson [5]: spontaneous symmetry breaking, power laws, auto-catalytic growth, some kind of self-organizing processes, etc. For this reason, this work aims to identify also these Complexity features in frame of a study intended to define, determine and interpret the results concerning the stability and convergence radii corresponding to different numerical simulations. Due to their advantages to be: a) considerably cheaper than the experimental determinations, b) possible even in *inaccessible experimental conditions*, the numerical simulations are frequently used in different scientific and technical studies. Unfortunately, the existing numerical phenomena (as those corresponding to instabilities, pseudo-convergence, distortions, etc) strongly limit the use possibilities of the numerical simulations [15]-[18].

Our study of the compatibility of some computer simulations, relative to some existing experimental data, begun from the classical test procedure of any statistical hypothesis [19]: for a given space of uniqueness parameters, it is defined the vector $\bar{t}$ of the test parameters and 2 zones: of acceptance Z_a, and its complementary Z_c. The probability $q = P(\bar{t} \in Z_c | H = true)$ to reject the statistical hypothesis *H*, when it is however true gives the criterion of acceptance/rejection of the studied statistical hypothesis: as the error risk $q < 0.001$ or $q > 0.02$, the statistical hypothesis is rejected, or it is accepted. The classical statistical tests χ^2 (Pearson), Kolmogorov, Massey, Sarkady etc. intended to the study of the compatibility of some theoretical distributions with the experimental ones are used sometimes also for the evaluation of the overall (general) compatibility of some theoretical relations and of some computer simulations relative to the existing experimental data [20], [21].

b) *Definitions of the stability radii*

The main features of the classification of some numerical schemes corresponding to different computer simulations, from the numerical phenomena point of view [17], are examined in frame of Table 1.

Let $p_{i,sim.}$ and $p_{i,analyt.}$ be the simulated and the "exact" (analytical) value of the test parameter *p* corresponding to the physical state *i*.

The deviation of the numerical description of the parameter *p* relative to the analytical description can be evaluated by means of the square mean relative deviation, defined as:

$$s = \sqrt{\sum_{i=1}^{N} W_i \left(p_{i,sim.} - p_{i,analyt.}\right)^2} \text{, where: } W_i = \frac{1}{N} p_{i,analyt.}^{-2} \qquad (5)$$

are the weights corresponding to the different analytical values $p_{i,analyt.}$ ($i = 1,N$).

For the strongly unstable and the medium instability numerical schemes (see Table 1), the dependence of the square mean deviation *s* on the number *I* of accomplished iterations has the shape from Fig. 3, presenting the form of: a) a certain relaxation, or of: b) some oscillations, finished by an abrupt exponential increase.

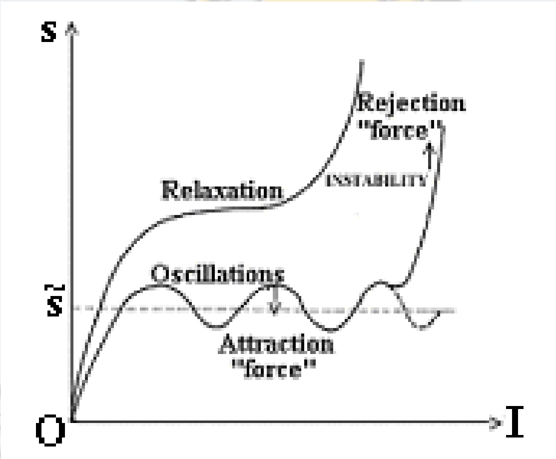

Fig. 3. Different types of square mean deviation (s) vs iterations number (I) dependencies

Depending on the shape of the *s* = *f*(*I*) dependence, the stability radius of the studied numerical simulation can be defined as below.

(i) *The s = f(I) dependence of relaxation type, followed by an auto-catalytic growth*

Taking into account that the abrupt (exponential) part of the *s* = *f*(*I*) dependence can be described by means of the power-law type relation:

$$\ln s = I \cdot \ln|\xi| + const. \; , \tag{6}$$

where $\ln|\xi| > 0$ and ξ could be the ratio of the successive transfer coefficients [17] [we mention that relation (6) and the parts corresponding to instability from figures 3 and 4 point out the appearance of some auto-catalytic growths [22], [10] during the transition from the ordered to the disordered phase of a numerical simulation; in this manner, the computer simulations behave exactly as complex systems: different phases, auto-catalytic growths, etc].

It results that the stability radius can be defined for this $s = f(I)$ dependence as the abscissa of the cross-point of the: (i) regression line corresponding to the relaxation part of the $\ln s = f(I)$ dependence, and of the: (ii) corresponding regression line (6) of the abrupt part of the same dependence (see Fig. 3).

(ii) *The oscillation type s = f(I) dependence*

Starting from the definition of a *pseudo-force constant* (describing the oscillations from fig. 4):

$$k = -\frac{\ddot{s}}{s - \tilde{s}}, \quad \text{where:} \quad \ddot{s} = \frac{\partial^2 s}{\partial I^2}, \tag{7}$$

one studies the dependence of this pseudo-force constant on the number I of iterations (see fig. 5).

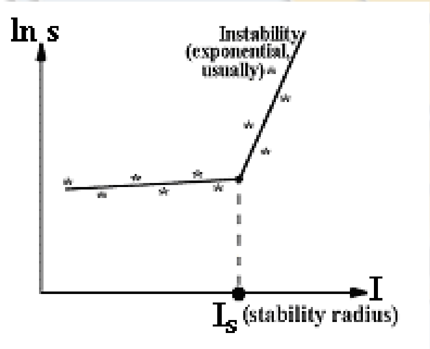

Fig. 4. Oscillation type s = f(I) dependence

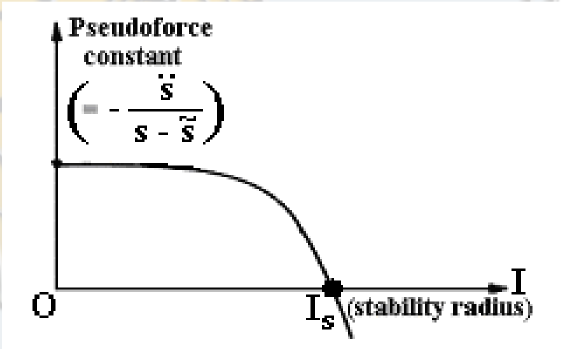

Fig. 5. Definition of the stability radius by means of the pseudo-force constant

c) *The definition of the convergence radius*

In this case, it is possible to define the stability radius I_S by the condition:

$$k(I_S) = 0, \tag{8}$$

being so the number of iterations corresponding to the character change of pseudo-forces, from the: (i) “attractive” character, describing the square mean relative oscillations, to the: (ii) “rejection” character, corresponding to the instability initiation.

Let $s_{exp.}$ be the square mean relative error corresponding to the averaged experimental errors: $s_{exp.} = \sqrt{\sum_{i=1}^{N} W_i \left(p_{i,exp.} - p_{i,analyt}\right)^2}$. (9)

The convergence radius $I_{conv.}$ can be defined as:

(i) $s(I_{conv.}) = s_{exp.}$, where the function $s(I)$ is defined by relation (5) for:

$$p_{i,sim.} = p_{i,sim.}^{(I)}, \tag{10}$$

(ii) of belonging of the representative points of the numerically simulated values of the studied parameter *p* to all corresponding confidence domains. In this aim, the error risks q_k corresponding to the rejection of the compatibility of the simulated values with the experimental ones for the physical state *k* are calculated for successive iterations *I*; as it is well known, the rejection of the compatibility a statistical hypothesis relative to the existing experimental data is decided if the error risk *q* accepted (assumed) to rejection is less than a certain threshold $q_{reject.}$, usually chosen between $2 \cdot 10^{-2}$ and 10^{-3} (see also figs. 6 and 7).

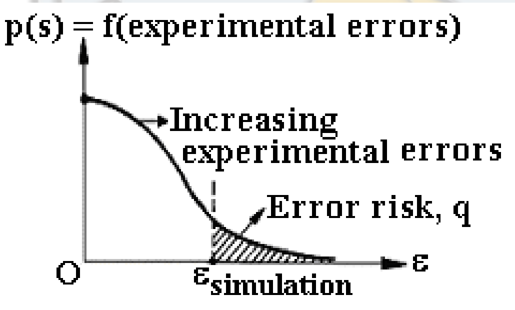

Fig. 6. Evaluation of the error risk, starting from the errors distribution p = f(ε)

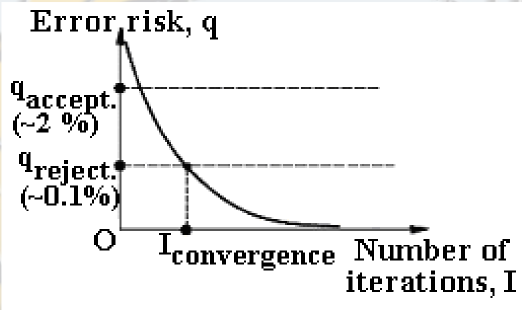

Fig. 7. Definition of the convergence radius by means of the error risk value

(iii) *The definition of the convergence radius for the slowly divergent numerical simulations*

To avoid the excessive time-consuming numerical calculations corresponding to the evaluation of the stability radius of slowly divergent numerical simulations (see Table 1) by means of the usual definitions (see above), it is more convenient to use an alternative definition of the stability radius in these cases, by means of the expression: $s(I_{conv.}) = 2\, s_{exp.}$ (11)

Table 1

Classification of the main numerical schemes of some computer simulations, from the numerical phenomena point of view

Stability Type	Specific features	Magnitude order of stability/convergence radii	Particular Examples
UNSTABLE	Strongly unstable ("explosive") numerical schemes	Short stability radius (< 10 iterations)	1) Gradient method: for bad choices of the zero-order approximations of the uniqueness parameters; 2) FD schemes intended to simulations of harmonic pulses propagation in dispersive media: Without the transplant procedure [17]
	Medium instability	Medium stability radius ($\sim 10^2 \ldots 10^3$ iterations)	FD schemes intended to simulations of harmonic pulses propagation in dispersive media: With several independent computation parameters
Generally STABLE or stable in rather large fields	Slowly divergent	Long stability radius ($> 10^4$ iterations)	FD schemes intended to simulations of harmonic pulses propagation in dispersive media: With few independent parameters
	Convergent (in the limits of experimental errors) numerical schemes	a) Generally Stable b) The convergence radius depends on the features of the numerical scheme	1) Well-directed gradient method applications (< 10 iterations, usually) 2) Some FD schemes intended to simulations of harmonic pulses propagation through sharp interfaces (e.g. the smoothing model 2a [17]) 3) Random walk simulations of some physical processes (diffusion with drift, absorption etc.)
	Pseudo-convergent (outside of the limits of physical errors) *Note:* These are the most misleading and "dangerous" numerical simulations!	a) Rather large stability fields b) The pseudo-convergence radius depends on the features of the numerical scheme	Some FD schemes intended to simulations of harmonic pulses propagation through sharp interfaces: (e.g. the smoothing models 2b and 3a [17])
	Dispersive *Note:* They can become non-convergent for rather large number of iterations	a) Generally Stable; b) Convergence radii of $10^3 \ldots 10^5$ iterations, depending on pulse shape	FD schemes intended to simulations of propagation of pulses with different shapes, using less than 1 values of the Courant's number

Table 2

Main features of the Finite Differences Schemes Used to Simulate the Ultrasonic Pulses Propagation through Attenuative Media

Stability Type	Specific features	Magnitude order of stability/convergence radii	Particular Examples
UNSTABLE	Strongly unstable ("explosive") numerical schemes	Short stability radius (< 10 iterations)	1) Gradient method: for bad choices of the zero-order approximations of the uniqueness parameters; 2) FD schemes intended to simulations of harmonic pulses propagation in dispersive media: Without the transplant procedure [17]
	Medium instability	Medium stability radius ($\sim 10^2 \ldots 10^3$ iterations)	FD schemes intended to simulations of harmonic pulses propagation in dispersive media: With several independent computation parameters
	Slowly divergent	Long stability radius ($> 10^4$ iterations)	FD schemes intended to simulations of harmonic pulses propagation in dispersive media: With few independent parameters
Generally STABLE or stable in rather large fields	Convergent (in the limits of experimental errors) numerical schemes	a) Generally Stable b) The convergence radius depends on the features of the numerical scheme	1) Well-directed gradient method applications (< 10 iterations, usually) 2) Some FD schemes intended to simulations of harmonic pulses propagation through sharp interfaces (e.g. the smoothing model 2a [17]) 3) Random walk simulations of some physical processes (diffusion with drift, absorption etc.)
	Pseudo-convergent (outside of the limits of physical errors) *Note*: These are the most misleading and "dangerous" numerical simulations!	a) Rather large stability fields b) The pseudo-convergence radius depends on the features of the numerical scheme	Some FD schemes intended to simulations of harmonic pulses propagation through sharp interfaces (e.g. the smoothing models 2b and 3a [17])
	Dispersive *Note:* They can become non-convergent for rather large number of iterations	a) Generally Stable; b) Convergence radii of $10^3 \ldots 10^5$ iterations, depending on pulse shape	FD schemes intended to simulations of propagation of pulses with different shapes, using less than 1 values of the Courant's number

d) *Stability and Convergence Radii of different numerical schemes*

The accomplished numerical studies [23], [24] 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:

$$\left\langle L_{I,stab.}\right\rangle_{dB} = 2\left\langle L_{w,stab.}\right\rangle_{dB} = 20E\cdot x_{\lim} = 20k\cdot x_{\lim}\cdot\tan\frac{\delta}{2} = 40\pi\frac{x_{\lim}}{\lambda}\tan\frac{\delta}{2}. \qquad (12)$$

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

$$I_{\lim.}/I_o = \exp\left(-2E\cdot x_{\lim}\right) = \exp\left(-\left\langle L_{I,stab.}\right\rangle/10\right) \qquad (13)$$

Table 2 synthesizes the obtained numerical results.

e) *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 pulses propagation, diffusion with drift, absorption, etc) indicate the “accessible” logical depths [4] 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 [25].

Certain numerical schemes, e.g. that corresponding to the complex stiffness $\bar{S}$ symmetric wave equation of the propagation in dissipative media:

$$\rho\frac{\partial^2\overline{w}}{\partial t'^2} = \bar{S}\cdot\frac{\partial^2\overline{w}}{\partial x^2}\ , \qquad (14)$$

allow multiple solutions, i.e.: $\overline{w}_{I,t} = A \cdot e^{\pm i\omega t\tau} \cdot e^{\pm(E+ik)I\cdot\varepsilon}$. (15)

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

$$\overline{w}_{I,t}^{dir.} = A \cdot e^{-EI\cdot\varepsilon} \cdot \exp i(\omega t\tau - kI \cdot \varepsilon), \tag{16}$$

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

$$\overline{w}_{I,t}^{inv.} = A' \cdot e^{EI\cdot\varepsilon} \cdot \exp i(\omega t\tau + kI \cdot \varepsilon), \tag{17}$$

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 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:

$$\dot{f}(0) = \frac{-f(2\tau) + 8f(\tau) - 8f(-\tau) + f(-2\tau)}{12\tau}, \tag{18}$$

$$\ddot{f}(0) = \frac{-f(2\tau) + 16f(\tau) - 30f(\tau) + 16f(-\tau) - f(-2\tau)}{12\tau^2}, \tag{19}$$

when the instabilities appear after only few tens of iterations,

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

c) more parasitic solutions,

d) more partial derivatives involved in the expression of the differential equation of the acoustic pulses propagation.

For these reasons, the highest "accessible" logical depth [4] is reached (for the simulations of the acoustic pulses propagation through attenuative media) for the numerical scheme using the real wave function equation (see table 2), with the usual FD approximations of the first 2 order derivatives:

$$\dot{f}(0) = \frac{f(\tau) - f(-\tau)}{2\tau}, \quad \ddot{f}(0) = \frac{f(\tau) - 2f(0) + f(\tau)}{\tau^2}. \tag{20}$$

Conclusions

The obtained results concerning the stability and convergence radii of some different numerical schemes intended to the computer simulation of the acoustic pulses propagation through different media present a considerable importance for the choice and optimization of these numerical schemes [25].

It was found also that the numerical simulations of the acoustic pulses propagation through attenuative media allow to study 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).

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