# STUDY OF THE CONVERGENCE AND STABILITY RADII OF SOME PHYSICAL PROCESSES NUMERICAL SIMULATIONS*

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Starting from the definitions of the stability and convergence radii of the numerical simulations, their values are evaluated for different numerical methods and schemes. The obtained results are compared and analyzed. Besides the possibilities of best choice and optimization of the studied numerical schemes, the obtained results allow also the study of some basic features of the self-organizing systems.

*Key words:* Computer simulations, numerical phenomena, stability and convergence radii, acoustic pulse propagation, complexity theory, logical depth, self-organizing systems.

## 1. INTRODUCTION

According to the Murray Gell-Mann definitions of the effective and apparent complexity [1]: "We believe if you put these two (quantum electrodynamics and quantum chromodynamics) together you will get a description of atomic nuclei in great detail, including the positions of all their energy levels. But the computations are extremely long and difficult … So here is a case where we are looking at something *apparently complex* that has in fact low *effective complexity*, but a lot of *logical depth*". Taking into account that this high "apparent" complexity (in fact, the real one in practical problems) is met in many present scientific and technical topics [*e.g.* in the non-destructive examination of the eventual defects (of sizes of the magnitude order ~ 1 μm) in the wings (of sizes ~ 1 m) of an airplane, requiring so a high number ($10^5$…$10^6$) of successive iterations], the first goal of this work is to evaluate the accessible logical depth corresponding to different Finite Difference (FD) schemes.

Because the computers are complex systems, the computer programs are expected to exhibit the main Complexity features indicated by Philip Anderson [2]:

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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 the 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 [3–6].

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 [7]: for a given space of uniqueness parameters, it is defined the vector $\overline{t}$ of the test parameters and 2 zones: of acceptance $Z_a$, and its complementary $Z_c$. The probability $q = P\left(\overline{t} \in Z_c \middle| H = true\right)$ 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 $\chi^2$ (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 [8–9].

## 2. DEFINITION OF THE STABILITY AND CONVERGENCE RADII

The main features of the classification of some numerical schemes corresponding to different computer simulations, from the numerical phenomena point of view [5], are examined in the 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:

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

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, the dependence of the square mean deviation $s$ on the number $I$ of accomplished iterations has the shape from Fig. 1, presenting the form of: a) a certain relaxation, or of: b) some oscillations, finished by an abrupt exponential increase.

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

### 2.1. 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:

$$\ln s = I \cdot \ln|\xi| + const., \tag{2}$$

where $\xi$ is the ratio of the successive transfer coefficients [5] and $\ln|\xi| > 0$, 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 (2) of the abrupt part of the same dependence (see Fig. 2). We mention that relation (2) and the parts corresponding to instability from Figs. 1 and 2 point out the appearance of some auto-catalytic growths [2c], [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).

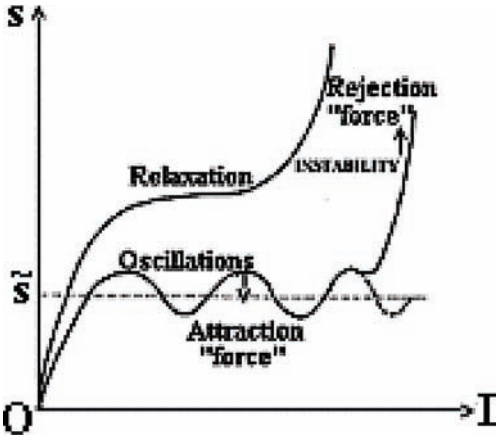


Fig. 1 – Different types of square mean deviation(s) *versus* iterations number ($I$) dependencies.

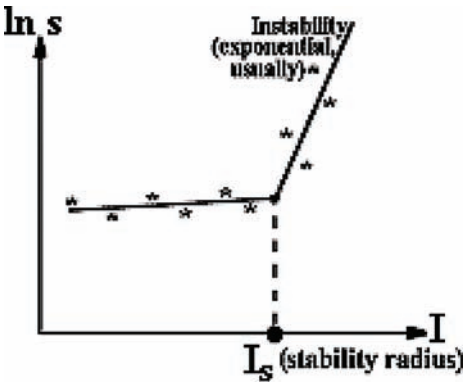


Fig. 2 – Graphical definition of the stability radius for relaxation & auto-catalytic growth type of the $s = f(I)$ dependence.

### 2.2. THE OSCILLATION TYPE $s = f(I)$ DEPENDENCE

Starting from the definition of a *pseudo-force constant* [describing the oscillations around the average value $\tilde{s}$ (for a sufficiently large number of iterations) of $s$, see Fig. 1:

$$k = -\frac{\ddot{s}}{s - \tilde{s}}, \qquad \text{where:} \quad \ddot{s} = \frac{\partial^2 s}{\partial I^2}, \tag{3}$$

one studies the dependence of this pseudo-force constant on the number $I$ of iterations (see Fig. 3).

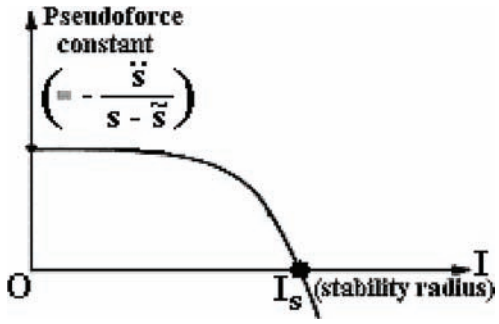


Fig. 3 – Definition of the stability radius by means of the pseudo-force constant.

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

$$k\left(I_s\right) = 0, \tag{4}$$

$I_s$ being so the number of iterations corresponding to the character change of pseudo-forces, from the: a) "attractive" character, describing the square mean relative oscillations, to the: b) "rejection" character, corresponding to the instability initiation.

### 2.3. DEFINITION OF THE CONVERGENCE RADIUS

Let $s_{\text{exp.}}$ be the square mean relative error corresponding to the averaged experimental errors:

$$s_{\text{exp.}} = \sqrt{\sum_{i=1}^{N} W_i \left(p_{i,\text{exp.}} - p_{i,analyt.}\right)^2}. \tag{5}$$

The convergence radius $I_{conv.}$ can be defined by means of the conditions:
(i) $s\left(I_{conv.}\right) = s_{\text{exp.}}$, where the function $s(I)$ is defined by relation (1) for:

$$p_{i,sim.} = p_{i,sim.}^{(I)}, \tag{6}$$

(ii) the representative points of the numerically simulated values of the studied parameter $p$ have to belong to all corresponding experimental 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 $I$ (see Fig. 4). Because the rejection of the compatibility of 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 $10^{-3}$, the convergence radius is defined in terms of this error risk threshold (see Fig. 5).

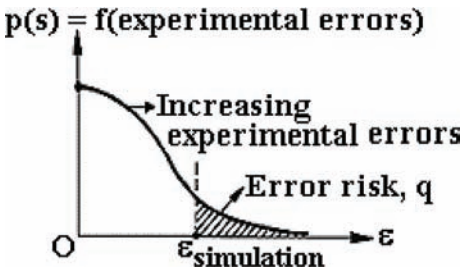


Fig. 4 – Evaluation of the error risk, starting from the errors distribution $p = f(\varepsilon)$.

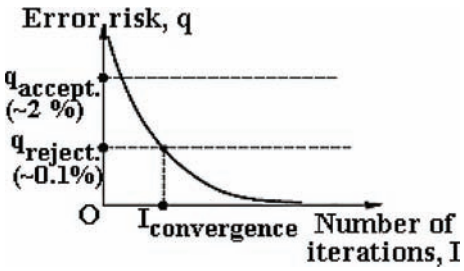


Fig. 5 – Definition of the convergence radius by means of the error risk value.

### 2.4. THE DEFINITION OF THE CONVERGENCE RADIUS CORRESPONDING TO 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 Section 2.3), it is more convenient to use an alternative definition of the stability radius in these cases, by means of the expression:

$$s\left(I_{conv.}\right) = 2\, s_{\exp.} \tag{7}$$

## 3. STABILITY AND CONVERGENCE RADII OF DIFFERENT NUMERICAL SCHEMES

The accomplished numerical studies [11, 12] 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:

$$\left\langle L_{I,stab.}\right\rangle_{dB} = 2\left\langle L_{w,stab.}\right\rangle_{dB} = 20E \cdot x_{\lim} = 20k \cdot x_{\lim} \cdot \tan\frac{\delta}{2} = 40\pi\frac{x_{\lim}}{\lambda}\tan\frac{\delta}{2}. \quad (8)$$

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

$$I_{\lim.}\Big/ I_o = \exp\left(-2E \cdot x_{\lim}\right) = \exp\left(-\left\langle L_{I,stab.}\right\rangle\Big/10\right). \quad (9)$$

Table 2 synthesizes the obtained numerical results.

## 4. 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 [1] 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 [13].

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

$$\rho\frac{\partial^2\overline{w}}{\partial t'^2} = \overline{S}\cdot\frac{\partial^2\overline{w}}{\partial x^2}, \quad (10)$$

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

$$\overline{w}_{I,t} = A\cdot e^{\pm i\omega t\tau}\cdot e^{\pm(E+ik)I\cdot\varepsilon}. \quad (11)$$

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

$$\overline{w}^{dir.}_{I,t} = A\cdot e^{-EI\cdot\varepsilon}\cdot\exp i(\omega t\tau - kI\cdot\varepsilon), \quad (12)$$

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

$$\overline{w}^{inv.}_{I,t} = A'\cdot e^{EI\cdot\varepsilon}\cdot\exp i(\omega t\tau + kI\cdot\varepsilon), \quad (13)$$

leading to the sudden apparition of instabilities.

*Table 1*

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

| **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 pulse propagation in dispersive media:** Without the transplant procedure [3] |
| | **Medium instability** | Medium stability radius (~ $10^2$…$10^3$ iterations) | **FD schemes intended to simulations of harmonic pulse propagation in dispersive media**: With several independent computation parameters |
| | **Slowly divergent** | Long stability radius (> $10^4$ iterations) | **FD schemes intended to simulations of harmonic pulse 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 pulse propagation through sharp interfaces:** (*e.g.* the smoothing model 2a [3]) 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 pulse propagation through sharp interfaces:** (*e.g.* the smoothing models 2b and 3a [3]) |
| | Dispersive *Note*: They can become non-convergent for rather large number of iterations | a) Generally Stable; b) Convergence radii of $10^3$…$10^5$ 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 pulse propagation through attenuative media

| The Differential Wave Equation | The Behavior at Sharp Interfaces | Is there a mixture of real and imaginary components in the FD equation? | Number of | | | FD Stability Radii for: $\tan\delta$ =0.01 and $\frac{\Delta w}{w}=0.1$ | | Observations |
|---|---|---|---|---|---|---|---|---|
| | | | Parasitic solutions | Noncompensated derivatives | Partial derivatives | $\langle L_I \rangle_{dB}$ | $\left(\frac{I_{stab.}}{I_o}\right)$, % | |
| $\rho\frac{\partial^2\overline{w}}{\partial t'^2}=\overline{S}\cdot\frac{\partial^2\overline{w}}{\partial x^2}$ (complex stiffness symmetric wave equation) | Suitable expressions of boundary conditions | YES | 3 | 1 | 2 | 0.0321 | 59.3 % | Very unstable FD scheme! |
| $\ddot{\overline{w}}-\omega^2\tau_\varepsilon\dot{\overline{w}}=\frac{M_R}{\rho}\left(1+j\omega\tau_\sigma\right)\overline{w}''$ (complex stress relaxation time wave equation) | IDEM | YES | 1 | 1 | 3 | ≈ 4 | ≈ 30 % | Good for direct FD descriptions of displacement in multi-layers |
| | | | | | | Necessary a $c<1$ optimization in order to reach the best performances | | |
| $\frac{\partial^2\overline{w}}{\partial t'^2}=\frac{S}{\rho}\left[\overline{w}''+(k-jE)\cdot\tan\delta\cdot\overline{w}'\right]$ (complex wave-vector wave equation) | IDEM | YES | 1 | – | 3 | ≈ 20 | ≈ 1 % | |
| $\overline{S}\frac{\partial^2\overline{w}}{\partial x^2}=-\rho\omega^2\overline{w}$ (space evolution wave equation) | IDEM | YES | 1 | 1 | 1 | 40.476 | $8.9\times10^{-3}$ % | |
| | | | | | | Conversion space → time evolution eliminates direct descriptions of multi-layers | | |
| $\rho\frac{\partial^2 w}{\partial t',^2}+R\frac{\partial w}{\partial t'}=S_o\frac{\partial^2 w}{\partial x^2}$ (real wave equation) | Difficult expressions of boundary conditions | NO | 1 | 1 | 3 | 80.13 | $< 10^{-4}$ % | Not suitable for FD simulations of interface phenomena |

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]:

$$\dot{f}(0) = \frac{-f(2\tau) + 8f(\tau) - 8f(-\tau) + f(-2\tau)}{12\tau}, \tag{14}$$

$$\ddot{f}(0) = \frac{-f(2\tau) + 16f(\tau) - 30f(\tau) + 16f(-\tau) - f(-2\tau)}{12\tau^2}, \tag{15}$$

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 pulse propagation.

For these reasons, the highest "accessible" logical depth [1] 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 2), with the usual FD approximations of the first 2 order derivatives:

$$\dot{f}(0) = \frac{f(\tau) - f(-\tau)}{2\tau}, \qquad \ddot{f}(0) = \frac{f(\tau) - 2f(0) + f(-\tau)}{\tau^2}. \tag{16}$$

## 5. CONCLUSIONS

The obtained results concerning the stability and convergence radii of some different numerical schemes intended to the computer simulation of the acoustic

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

pulse propagation through different media present a considerable importance for the choice and optimization of these numerical schemes [13].

It was also found that the numerical simulations of the acoustic pulse 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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