# POSSIBILITIES AND LIMITS OF THE TRANSFER COEFFICIENTS METHOD*

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In order to describe the basic numerical phenomena (instabilities, divergence, distortions) intervening in the finite-differences (FD) simulations of the pulse propagation through different media, we introduced the method of transfer coefficients, relating the simulated pulse components to those of the true pulses. The accomplished study pointed out: a) the remarkable possibilities of this method to describe accurately (sometimes, even exactly) the stability and convergence of some schemes, for linear homogeneous media and equal physical and FD speeds, b) the existing, but limited (due to some computation difficulties) possibilities to describe also the distortions intervening for values $C < 1$ of the Courant number), c) the practical impossibility to use this method for nonlinear media. Some newly obtained results concerning certain power laws and auto-catalytic growth processes pointing out the Complexity of the studied algorithms were also reported.

## 1. INTRODUCTION

Despite of the fact that the main numerical phenomena (instability, divergence, distortions) specific to the Finite Difference (FD) simulations of the pulses propagation in *ideal* media were studied even since 1920's years, when Courant and his collaborators established [1] the condition for the appearance of instabilities and distortions: $C = \tau \cdot V_\Phi / \varepsilon > 1$ (instabilities), $C = \tau \cdot V_\Phi / \varepsilon < 1$ (distortions, resp.), (1) where $C$, $\tau$, and $\varepsilon$ are the Courant similitude criterion, and the FD time and space steps, respectively, and some additional such phenomena were pointed out later [2], the largest part of the numerical phenomena intervening for more complex propagation media remained non-explained.

Introducing the method of transfer coefficients [3, 4], we succeeded to explain some instability, divergence and distortions phenomena intervening in the numerical simulations of the pulses simulations: a) through sharp interfaces between homogeneous media, b) by means of FD schemes with less than 1 values of the Courant number, etc. The main goal of this work is to synthesize and complete these previously obtained results [5].

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## 2. DEFINITIONS OF TRANSFER COEFFICIENTS FOR INTERFACE PHENOMENA AND EXPLANATION OF INSTABILITY

In order to simulate the transmission-reflection processes of an elastic pulse through (on) a sharp interface by means of FD procedures, this pulse must be divided in the components $s_1$, $s_2$, … $s_N$ corresponding to the incoming (in this order, on the considered interface) displacements, distanced by the space step $\varepsilon$.

Starting from the discretized initial conditions:

$w_{i,0} = s_{I-1-i}$ for: $i \in \{I-N-1, I-N, ...I-2\}$ and: $w_{i,0} \equiv 0$ for all other values of $i$, $w_{i,1} = s_{I-i}$ for: $i \in \{I-N, I-N+1, ...I-1\}$, and: $w_{i,0} \equiv 0$ for all values of $i$, (where $I$ represents the value of $i$ corresponding to the considered sharp interface), it results that for the time steps $t \geq 3$, the displacements corresponding to the transmitted and reflected pulse, respectively, in the transition field are:

$$w_{I+1,t} = \sum_{j=1}^{t-2} k_j s_{t-j-1} \text{ and: } w_{I-1,t}^{refl.} = \sum_{j=1}^{t} h_j s_{t-j+1}\ , \tag{1}$$

where $k_j$ and $h_j$ are *the transfer coefficients* corresponding to the transmitted and reflected pulse, resp.

Let denote now by $j$ (= 1, 2, … $N$) and $p$ (= 1, 2, … $t-2$) the indices of the incoming pulse components $s_j$ and of the components $s'_p$ of the completely (for $t \geq N+2$) transmitted pulse, respectively. One finds that for all $t \geq N+2$, we have:

$$s'_p = \sum_{j=1}^{N} k_{p+1-j} s_j \quad (\text{for } p = 1, 2, \dots t-2), \tag{2}$$

where $k_n = 0$ for $n \leq 0$ (for $p > N$, the corresponding $s'_p$ ($\neq 0$) components represent the damage (garbage) of the simulated transmitted pulse).

If for all $p \in \{1, 2, \dots t-2\}$, we have $k_{p+1-j}^2 < M$ (where $M$ is a constant upper limit), because $w_{it} = 0$ for $i \geq I + t - 1$, it results that (for $t \geq N + 2$):

$$\sum_{i=I+1}^{\infty} |w_{it}|^2 = \sum_{p=1}^{t-2} |s'_p|^2 = \sum_{p=1}^{t-2} \left| \sum_{j=1}^{N} k_{p+1-j} s_j \right|^2 \leq N \sum_{p=1}^{t-2} \sum_{j=1}^{N} k_{p+1-j}^2 s_j^2 < N \cdot M \sum_{p=1}^{t-2} \sum_{j=1}^{N} s_j^2 =$$

$$= N \cdot M (t-2) \sum_{i=-\infty}^{\infty} |w_{i0}|^2\ , \tag{3}$$

where $w_{it}$ represents the wave displacement in the FD node $i$ at moment $t$.

In these conditions, it results that for very large $t$:

$$k_t \approx \xi^{\frac{t-1}{2}} \cdot k_1 ,$$

where:

$$\xi = \lim_{j \to \infty} \frac{k_{2j+1}}{k_{2j-1}} . \tag{4}$$

Therefore – in order to satisfy the stability condition [equivalent to (3)] corresponding to the FD schemes for second order differential equations [6, p. 158], the FD schemes have to fulfill the condition $|\xi| < 1$ [7]. One finds also that for $|\xi| > 1$, the transfer coefficients $k_t$ (and the corresponding displacements) present the power law, equivalent to the *auto-catalytic growth* certified by relation (4a), leading to instability (see also Fig. 1).

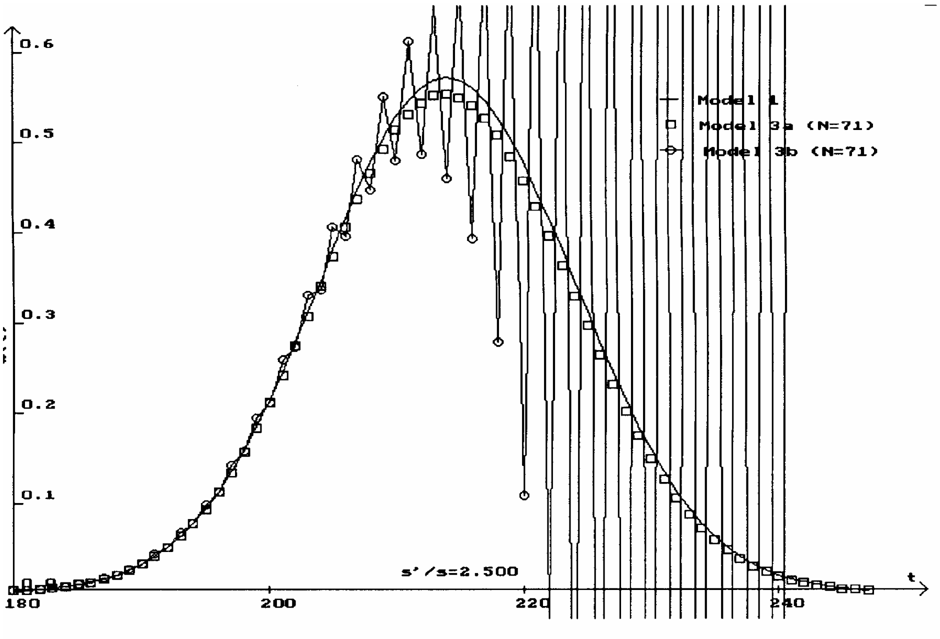


Fig. 1 – FD numerical simulations of a Gaussian pulse (with $N = 71$ components, described by the corresponding displacements $w(t)$) transmitted through a sharp interface between 2 homogeneous media, whose stiffness modules fulfil the ratio $S'/S = 2.5$.

### 3. EXPLANATION OF THE PSEUDO-CONVERGENCE OF SOME FD SCHEMES

In order to study the convergence of certain FD models of 1D interface phenomena, we will consider a discretization of the arbitrary incoming pulse in $N$ components $s_n$ ($n$ = 1, 2, … $N$) and a fixed fraction $f \in [\gamma, 1]$ (where $\gamma$ is not much less than 1) so that $f \cdot N$ = integer ($\in N^*$). Starting from the definitions of the transmission $T$ and reflection coefficients, respectively, *we will consider that a* *certain FD model* used to describe the 1D-interface phenomena (reflection, transmission) *is convergent* [3, p. 19] *if, and only if*: $\lim_{N\to\infty}\frac{1}{s_{fN}}\sum_{j=1}^{fN}k_j s_{fN+1-j}=T$ or:

$$\lim_{N\to\infty}\frac{1}{s_{fN-2}}\sum_{j=1}^{fN}h_j s_{fN+1-j}=R\,, \tag{5}$$

in conditions when: $\delta=\frac{\tau}{N}\to 0$.

If the limits defined by the relations (5) exist, but they are different than the true (physical) transmission $T$ and reflection $R$ coefficient (corresponding to the boundary conditions), respectively, we will say that the respective *FD schemes* are *pseudo-convergent*.

In order to exemplify the really misleading and sometimes even dangerous numerical phenomenon of pseudo-convergence, we will present in Fig. 2, the plots of the simulated pulses corresponding to the FD schemes built starting from the smoothing models (of the considered sharp interface) 1, 2a, 2b and 3a, the first 2 smoothing models ensuring convergent FD schemes, while the other 2 smoothing models lead to pseudo-convergent models.

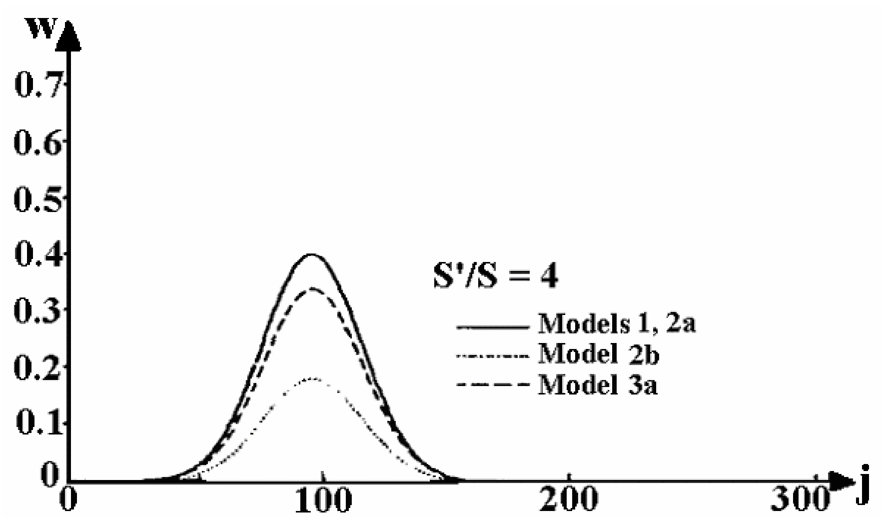


Fig. 2 – Transmitted pulse corresponding to the smoothing models 1, 2a, 2b and 3a for $S'/S = 4$.

## 4. CLASSIFICATION AND EXPLANATION OF PULSE DISTORTIONS

Starting from a certain partition (division) of the incoming signal (pulse) in $N$ components of amplitudes (in the order of their incoming on the studied material)

$s_1$, $s_2$, … $s_N$, and denoting the amplitudes of the same components in the previous time step by $s_1^{'}, s_2^{'}, ... s_N^{'}$, one obtains the expressions of the displacements (elongation and oscillations) corresponding to the different sites $I$ of the FD lattice, at various times $t$, by means of the expression [1]:

$$w_{It} = \sum_{i=1}^{I+t} k_{ti} s_{N+i-I-t} - \sum_{i=1}^{I+t} k_{t-1,i} s^{'}_{N+i-I-t} , \tag{6}$$

where $k_{ti}$ are *the transfer coefficients* relating the components of the simulated and incoming pulse.

Let be $j$ the "current" index of a pulse component and $i_1$, $i_2$ – the corresponding indices from the 2 sums of relation (6): $j = N + t - I - i_1 = N + t - I - i_2$; to do obvious the pulse components in the relation (6), this relation can be written in the following form:

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

Finally, in order to point out the expression of a certain ($j_s$ – th) component of the incoming pulse in the simulated one, we will observe that its position after $t$ time steps is: $I\left(j_s, t\right) = t\sqrt{c} + N + 1 - j_s$, therefore the relation (7) becomes:

$$s_{j_s}(t) \equiv w_{I(j_s,t),t} = \sum_{j=1}^{N} k_{t,t\left(1-\sqrt{c}\right)+1+j_s-j} \cdot s_j(0) - \sum_{j=1}^{N} k_{t-1,t\left(1-\sqrt{c}\right)-1+j_s-j} \cdot s_j(-1) , \tag{8}$$

where: $s_j(0) \equiv s_j$ and: $s_j(-1) \equiv s^{'}_j$ .

Taking into account that: $s^{'}_j = s\left(j + 1 - \sqrt{c}\right) \cong s(j) + \left(1 - \sqrt{c}\right)\dfrac{\partial s}{\partial j}$, it results that the relation (8) can be written in the approximate form:

$$s_{j_s}(t) \cong \sum_{j=1}^{N} \left[ k_{t,t\left(1-\sqrt{c}\right)+1+j_s-j} - k_{t-1,t\left(1-\sqrt{c}\right)-1+j_s-j} \right] \cdot s_j + \left(\sqrt{c} - 1\right) \sum_{j=1}^{N} \frac{\partial s}{\partial j} \cdot k_{t-1,t\left(1-\sqrt{c}\right)-1+j_s-j} . \tag{9}$$

Because:

$$\Delta k_{ti} = k_{t,i+1} - k_{t-1,i-1} \cong \left(2 - \sqrt{c}\right) \left.\frac{\partial k_{ti}}{\partial i}\right|_{t+i\frac{\sqrt{c}}{2}} , \tag{10}$$

the relation (9) can be written in its final (approximate) form:

$$s_{j_s}(t) \cong \left(2 - \sqrt{c}\right) \sum_{j=1}^{N} \left.\frac{\partial k_{ti}}{\partial i}\right|_{t,i+\frac{\sqrt{c}}{2}} \cdot s_j + \left(\sqrt{c} - 1\right) \sum_{j=1}^{N} \left.\frac{\partial s}{\partial j}\right|_{j+\frac{1-\sqrt{c}}{2}} \cdot k_{t-1,t\left(1-\sqrt{c}\right)-1+j_s-j} , \tag{11}$$

where: $i = t\left(1-\sqrt{c}\right) + j_s - j$ .

One obtains [5] the following *iteration* (*recurrence*) *equation between the transfer coefficients* $k_{ti}$ of the incoming pulse components in the expression (6) of the simulated pulse:

$$k_{ti} = c\left(k_{t-1,i} + k_{t-1,i-2}\right) + k \cdot k_{t-1,i-1} - k_{t-2,i-2} ,$$

where

$$k = 2\ (1 - c). \tag{12}$$

Introducing the position number $s = i - t - 1$, the recurrence relation (12) becomes:

$$k_{ts} = c\left(k_{t-1,s+1} + k_{t-1,s-1}\right) + k \cdot k_{t-1,s} - k_{t-2,s} , \tag{13}$$

which is equivalent to the recurrence (iteration) relation corresponding to a pulse ($k_{ts}$) propagation. The corresponding differential equation is:

$$\frac{\partial^2 k_{ts}}{\partial s^2} = \frac{1}{c} \cdot \frac{\partial^2 k_{ts}}{\partial t^2} . \tag{14}$$

It results that the successive generation of the transfer coefficients $k_{ts}$ is somewhat similar to the 1D-propagation (in the 2 opposite directions of the axis $s$ , with the FD speed $\sqrt{c}$ ) of the initial pulse $k_{00} = 1$ located initially in the origin ($s$ = 0) of the $s$ axis. In $t$ time steps, this "pulse" (corresponding to nonzero $k_{ts}$ coefficients) arrives to the $\pm t\sqrt{c}$ FD sites. It results that after $t$ time steps there are approximately $1 + 2t\sqrt{c}$ nonzero $k_{ts}$ coefficients. One finds that:

$$\sum_{-\infty}^{\infty} k_{ts} = t + 1 . \tag{15}$$

therefore the nonzero $k_{ts}$ coefficients will "oscillate" around a value approximately equal to:

$$\left\langle \left(k_{ts}\right)_{oscill.} \right\rangle \cong \frac{t+1}{2t\sqrt{c}+1} . \tag{16}$$

The above findings are confirmed by the numerical calculations of the $k_{ts}$ coefficients (Fig. 3).

Due to the dispersive character of the FD schemes with $c < 1$, the structure of the field inside which there can be found nonzero values of displacements is rather intricate; a general description of this dispersion field for pulses of different shapes (sine, gaussian, gaussian modulated multiple sine, rectangular) and even some quantitative characterizations are given in Fig. 4. The extensive numerical study performed [5], supports a description of the structure of the simulated propagated pulse with features independent from the initial pulse shape, the number of time steps and of the pulse components, as well as on the Courant number *C*, in good agreement with the theoretical predictions of this Section.

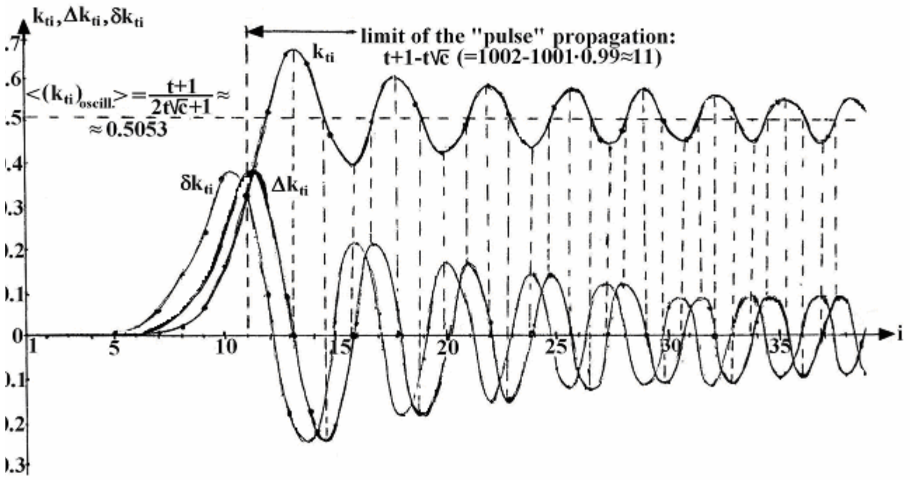


Fig. 3 – Typical dependence of the $k_{ti}$ transfer coefficients on *i*, for *c* = 0.9801.

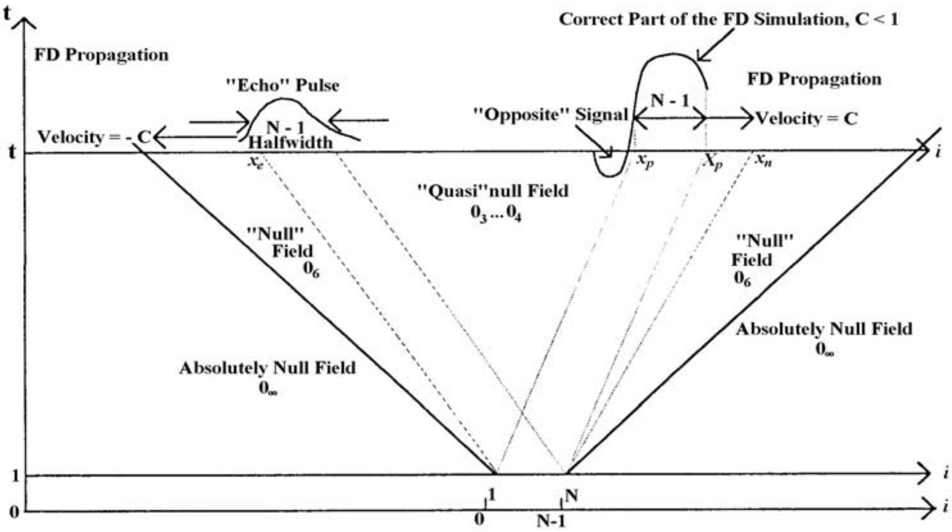


Fig. 4 – Structure of the FD simulation of the propagation of pulses of different shapes.

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.

The obtained results (Fig. 4) indicate that several pseudo-pulses add on to the source pulse during its FD simulated propagation. If the original pulse is initially located between $i = 2$ and $i = N$, after $t$ time steps of the FD numerical simulation, it will be located in the region $1 + C(t - 1) \le i \le N + C(t - 1)$. Outside this region, some pseudo-pulses appear and they may be classified according to Fig. 4.

For a rectangular pulse: $s(j) = 1$ (constant), therefore: $\frac{\partial s}{\partial j} = 0$, and the relation (11) leads to:

$$s_{j_s(t)} \approx \left(2-\sqrt{c}\right)\left(k_{t,t\left(1-\sqrt{c}\right)+j_s} - k_{t,t\left(1-\sqrt{c}\right)+j_s-N}\right). \tag{17}$$

While qualitative explanation of the "opposite" pulse appearance is given in Fig. 5, its quantitative description is given by the above relation (17).

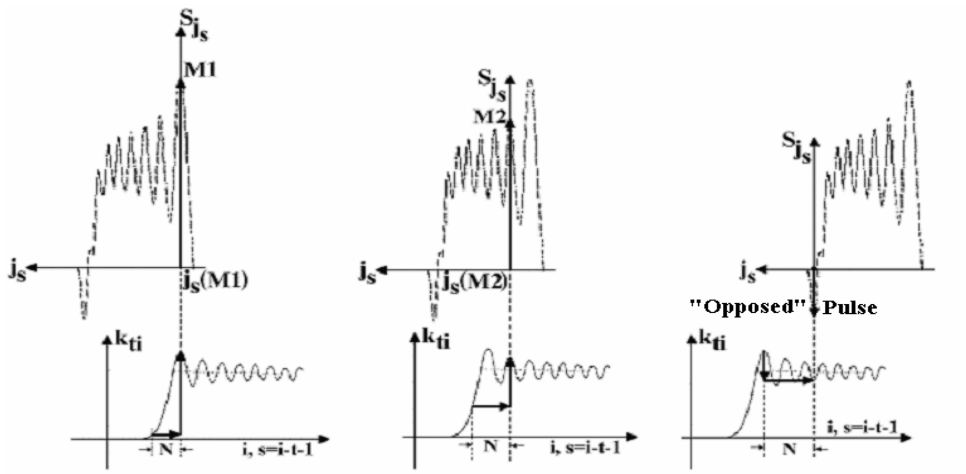


Fig. 5 – The explanation of the "opposite" pulse appearance by means of relation (17).

## 5. APPLICATION LIMITS OF THE TRANSFER COEFFICIENTS METHOD

While the transfer coefficients method proves itself as extremely efficient for the description of the numerical phenomena intervening in the numerical simulation of the linear propagation processes of arbitrary pulses, it cannot be used obviously for the description of the numerical simulations of pulses propagation in nonlinear media (KdV, etc), being even rather cumbersome (intricate) for the descriptions of the numerical simulations in dispersive media.

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