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Short Communication

About the Impact the Difference Schemes Produce on a Fictive Particle on the Grid

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Abstract: Fictive Forces Factor (3F) is introduced as the measure of an impact of the fictive forces always arising and producing non-physical effects when a boundary-value (or Cauchy) problem is being solved with the use of a difference scheme. 3F is a mean derivative of total energy of the fictive particle travelling along the function codomain grid, on coordinate. To demonstrate the approach, a well-known one-dimensional pseudo-curl transfer problem is considered with employment of two difference schemes, the central and the upwind scheme. Should the problem be solved analytically, the total energy is an invariant, whereas a numerical solution produces some quadratic deviation. In particular, it is demonstrated with the use of 3F that (and in which extent) the upwind scheme brings out a smaller impact of the fictive forces than the central does. The fictive particle total energy serves also as an indicator if the non-physical effects arose, resulting in the loss of the difference scheme stability.

Keywords: finite differences, stability, convergence, boundary-value problem, freedom

1. Introduction

The conservation property of a finite difference scheme is most frequently a preferrable feature when judging about rational choice of appropriate difference equations. The reason is that when these yield the conservation laws on the grid as the corresponding differential equations do, the computational results are expected to be usually perceived more viable as free of possible disbalances with respect to some physical values (measurables) [1]. However, this is known not to necessarily mean either a higher accuracy whose basic characteristic is the approximation order related to residue O of the grid step-sizes or their combinations, or a stability condition, if any. To study and ensure stability, estimates are typically accomplished which are based on energy or/and entropy inequalities [2]-[7]. Such estimates are to meet fully-discreet or, depending on possibilities, have to meet semi-discreet or continuum conditions. Noticeable is that they inherit the energy-related structure of original equations, frequently leading to cumbersome and tricky expressions to deal with. Pseudo-sources and -sinks themselves influencing numerical computations have purely discreet computational nature and are inherent to difference schemes. In the computational intercourse, no characteristics of their "fictitiousness power" are to meet. It would not be bad to have a trigger indicating an onset of effects due to the grid topology among whose are, e.g., those oscillations because of computational instabilities or even wrong boundary conditions, which are impertinent of the corresponding boundary-value (or Cauchy) problems in a continuous space.

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The aim of this short message is to consider preliminarily in the role of such a trigger the total energy of a Fictive Particle (hereinafter FP) having inhabited and then travelling along the function codomain grid (a discreet range of values), possessing its own mechanical energy and experiencing some impact produced by the grid. This impact affects FP mechanical energy. Properties of the grid the independent variables are defined on appear involved without saying to determine FP energy asset. In [8], the idea followed by some mathematical formalism was introduced to consider a particle freedom as a state without any influences brought into the particle ordinary environment. Then, the freedom of a particle freely travelling in the space, has to experience some harm should third-party forces arise and affect it. The harm factor is defined as the absolute value of power of such an impact and appears to be expressed through the expression $(T_0 + H_0)/(T_0 + H_0 + W) \times [T + H > 0]$, where T stands for kinetic and H for potential energy, subscript "0" denotes the time moment when the impact first arose, W is the work of external forces, Iverson's bracket indicates that FP still possesses non-zero energy and therefore some freedom. If external forces have FP's mechanical energy $E = T + H$ to dissipate, FP can lose once its freedom, when $E = T_0 + H_0 - |W| = 0$. Further action of the forces means a fully slave behaviour of FP, whose prehistory appears to have been erased when its total energy first reached zero. If work W increases FP mechanical energy, then FP appears to be driven by an external force in a gradually increasing proportion, and its freedom asymptotically tends towards zero. Important is to keep in mind, that energy E does not have anything to do with the energy in the physical process modelled by both differential and difference equations. It is the feature through that the approach presented in this paper, is to distinguish from the aforementioned energy or entropy inequalities. E can have a dimension other that the usual mechanical energy if the function codomain has a dimension other than a spatial coordinate. This represents the core difference between the approach proposed in this paper and those traditional which are energy- or entropy-based.

As a platform for the present consideration, I employ a well-known case of difference schemes for a quasi-curl transfer, analysed in detail at a purely computational angle in [9].

2. The model boundary-value problem and a fictive particle in motion

The one-dimensional model equation that has been extensively used to study particular aspects of computational approaches to solving spatial problems [9] is a linearised equation in dimensionless conservative form, with convection and diffusion terms, to be considered here under stationary conditions sufficient for our discussion:

$$-(u\zeta)_x + \alpha\zeta_{xx} = 0 \tag{1}$$

where ζ is a variable representing either a curl, coloured spot, a soliton, etc., α is the quasi-diffusion coefficient, and u is the constant linearised velocity of convection. Should Eq. (1) describe some curl, the coefficient α would correspond to the inverse Reynolds number in the curl transfer equation; however, since Eq. (1) is a one-dimensional equation, it cannot really represent a curl transfer. As we do not need u and α explicitly in further analysis, we transform Eq. (1) with $\beta = \alpha/u$ into:

$$\zeta_x = \beta\zeta_{xx} \tag{2}$$

Let the boundary conditions be $\zeta(0) = 0$, $\zeta(1) = 1$.

For the discretisation of this boundary-value problem, we consider the two schemes with a three-point stencil, namely the central and the upwind, which differ in the representation of the convective term as $\frac{\zeta_{i+1} - \zeta_{i-1}}{2\Delta x}$ for the former vs. $\frac{\zeta_i - \zeta_{i-1}}{\Delta x}$ for the latter, where Δx is the constant step-size on the grid. As the central schemes are known to be unable to suppress odd-even decoupling of the solution, artificial dissipation has generally to be added somehow to stabilise computations [10] to benefit from approximation order $O(\Delta x^2)$.

However, our purpose is the monitoring and "measurement" of instabilities rather than stabilisation. For this purpose, we introduce FP travelling along the ζ-axis and experiencing an impact of a conservative force $\mathbf{F} = m\ddot{\zeta}$ where m is FP mass, so that (the process different from that in Eq. (2))

$$m\ddot{\zeta} = -U_{\zeta} \tag{3}$$

where U is FP potential energy. Note that if ζ had a dimension other than that of a spatial coordinate, U would have a dimension other than energy and should rather be called pseudo-energy. For the sake of simplicity, we will address here U and related functions as energy. The second derivative in the left part can be represented as

$$\ddot{\zeta} = \zeta_{xx}\dot{x}^2 + \zeta_x\ddot{x} = \ldots$$

Our choice is that FP is travelling along the ζ-axis so that $\dot{x}$ = const. Therefore, we arrive at:

$$\ldots = C^2\zeta_{xx}$$

where C is the constant velocity of motion along x. By substituting this result into Eq. (3), we obtain

$$mC^2\zeta_{xx} = -U_{\zeta}$$

or

$$U = -mC^2\int\zeta_{xx}(x(\zeta))d\zeta \tag{4}$$

For FP kinetic energy T, we can write:

$$T = \frac{m\dot{\zeta}^2}{2} = \frac{mC^2}{2}\zeta_x^2 \tag{5}$$

Hence, combining Eqs. (4) and (5) gives the total mechanical energy E of the FP:

$$E = \frac{mC^2}{2}\left[\zeta_x^2 - 2\int\zeta_{xx}d\zeta\right]. \tag{6}$$

Eq. (6) has no reference to Eq. (2). Generally speaking, E is analytically expected to be an invariant E_{inv}, what we will have the opportunity to test hereinafter.

3. Results

By introducing the substitution $\rho(x) = \zeta_x(x)$ and then restoring original variables, we easily reproduce the analytical solution of Eq. (2) with the boundary conditions, given in [9]:

$$\zeta = (e^{x/\beta} - 1)/(e^{1/\beta} - 1) \tag{7}$$

It is easy to obtain:

$$\zeta_x = \frac{1}{\beta}\left[\frac{1}{\left(e^{1/\beta} - 1\right)} + \zeta\right] \tag{8}$$

i.e., the derivative ζ_x appears as a linear function of ζ, and, according to Eq. (2), so does ζ_{xx}. By substituting Eq. (7) into Eq. (6), one can make sure that all ζ-dependant terms cancel out, thereby yielding an arbitrary constant of the following composition:

$$E_{inv} = \frac{mC^2}{2} \frac{1}{\beta^2 \left(e^{1/\beta} - 1\right)^2} + E_0$$

where E_0 is an integration constant.

Our task now is to determine the value of E under discretisation. Since the fictitious forces produce some impact and, consequently, do work on the moving FP, the numerically computed FP energy E does not have to be invariant. With a forward and a successive backward sweep, we have for the intermediate coefficients: $\alpha_{1/2} = 0$, $\alpha_{i+1/2} = -\frac{c}{a\alpha_{i-1/2} + b}$ for $i = \overline{1, N}$, $\beta_{i+1/2} = 0$ for all is, and for the sought function $\zeta_0 = 0$, $\zeta_N = 1$, and $\zeta_i = a_{i+1/2}\zeta_{i+1}$ for other is, where $N + 1$ is the number of grid nodes (taken $N = 10$ in our computations like in [9]). The constants of the difference equation $a\zeta_{i-1} + b\zeta_i + c\zeta_{i+1} = 0$ corresponding to the differential equation (2), appeared to be $a = -(0.5 + \beta/\Delta x)/\Delta x$, $b = 2\beta/\Delta x^2$, $c = (0.5 - \beta/\Delta x)/\Delta x$, for the central scheme and $a = -(1 + \beta/\Delta x)/\Delta x$, $b = (2\beta/\Delta x + 1)/\Delta x$, $c = -\beta/\Delta x^2$ for the upwind scheme. We performed computations for $\beta = 0.03$ and 0.07. The central scheme is known to generate non-physical oscillations for $\beta < 0.05$ [9] (Figure 1). The computations yielded pretty good linear dependencies (as in Eq. (8)) for both $\zeta_x(\zeta)$ and $\zeta_{xx}(\zeta)$, with parameters presented in Table 1.

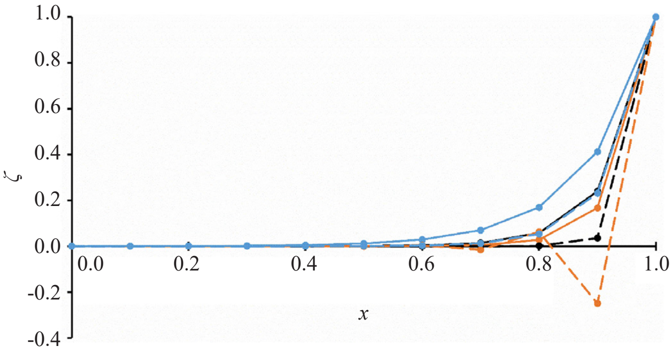

Figure 1. The pseudo-curl profile. Black: analytical solution (7); orange: the central scheme; blue: the upwind scheme. Solid: $\beta = 0.07$; dashed: $\beta = 0.03$

Table 1. Parameters♣ of computed linear dependencies $\zeta_{x,\,xx}(\zeta) = a\zeta + b$

Scheme	$\beta = 0.07$				$\beta = 0.07$			
	ζ_x♠		ζ_{xx}		ζ_x♠		ζ_{xx}	
	a	b	a	b	a	b	a	b
Central	29.2	4.82×10^{-7}	417	6.89×10^{-6}	-18.8	-1.79×10^{-5}	-625	-5.96×10^{-4}
Upwind	10.1	1.41×10^{-3}	84.0	1.18×10^{-2}	20.5	8.79×10^{-6}	256	1.10×10^{-4}

♣Floating point computations were performed with double precision (15 significant digits)
♠Computed with approximation order $O(\Delta x^2)$ for both schemes upon ζs were computed with the schemes-inherent approximation orders

FP total energy E was calculated numerically with the potential energy in the definite integral form (compared with Eq. (6))

$$E = \frac{mC^2}{2}\left[\zeta_x^2 - 2\int_{\zeta_{\min}}^{\zeta} \zeta_{xx}(x(\vartheta))\,d\vartheta\right]. \tag{9}$$

4. Discussion

Unlike the analytical case, the ζ-dependant terms originating from Table 1 do not cancel out after integration, and the quadratic dependencies on ζ arise (Figure 2). In terms of FP freedom, the upwind scheme produces a smaller impact on FP, so that its freedom degrades less than that with the central scheme. For the latter, and with the parameter value $\beta = 0.03$ (actually, with any parameter value less than 0.05), freedom has to go to zero (and further into the negative-value region, which is physically meaningless), implying that the FP completely loses its freedom and is driven by forces external to the physical process being modelled. These fictitious forces appear to be generated by the difference scheme. The extent to which the FP's freedom is affected can be conveniently characterised by the mean derivative E_ζ over the domain. This is termed a "mean derivative" for the following reason. $E(\zeta)$ is computed as a quadratic function. $E_\zeta(\zeta)$ appears then to be a linear function whose mean value is equal to E's derivative value in the middle point ζ_{mid} of the domain. With $E_\zeta(\zeta = 0.5) = \frac{mC^2}{2} \times 17.7$, the upwind scheme with $\beta = 0.07$ proves to be the closest (out of those considered here) to the theoretical invariant E_{inv}. Although we do not know the true value of E_{inv}, our judgement is based on the understanding that the less the dependence $E(\zeta)$ varies within the domain, the less it diverges from E_{inv}. With $\beta = 0.03$, the upwind scheme produces $E_\zeta(\zeta = 5) = \frac{mC^2}{2} \times 164$, whereas the central scheme with $\beta =$ 0.07 brings out $E_\zeta(\zeta = 5) = \frac{mC^2}{2} \times 543$. The true value of E_{inv} is thereby expected between the lowest and the greatest values produced by the upwind scheme, in the case $\beta = 0.07$ within $\frac{mC^2}{2} \times \left[2.00 \times 10^{-6},\ 17.7\right]$ and for $\beta = 0.03$ within $\frac{mC^2}{2} \times \left[7.72 \times 10^{-11},\ 165\right]$.

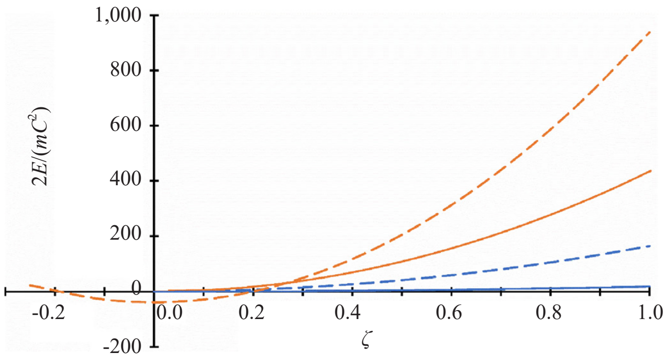

Figure 2. Computational dependence of FP total mechanical energy on ζ. Orange: the central scheme; blue: the upwind scheme. Solid lines: $\beta = 0.07$; dashed lines: $\beta = 0.03$

The analysis in terms of the numerical measure L^p leads, of course, to the same qualitative representation of divergences from the true E_{inv}. Having chosen the upwind scheme with $\beta = 0.07$ as the referential configuration and defined the respective norms as $\|E(\zeta) - E_r(\zeta)\|$ for the array $\{\zeta_j\}$ in the sense of L^1, L^2 and L^∞, where $E_r(\zeta_j)$ would be the referential value at $\zeta = \zeta_j$ and $E(\zeta_j)$ the energy value of evaluated configuration, we can present Table 2 as follows (compare with Figure 2).

The behaviour of the 3F measure is related to the grid resolution through the grid Reynolds number $Re_{\text{cell}} = \Delta x/\beta$. The domain grid step-size affects the stability oppositely, compared to β. In general, the larger Re_{cell} is, the greater work the fictive forces produce. This appears to be to key to the understanding of the relation between FP energy on the one part and numerical errors and consequently stability characteristics of the difference scheme on the other part. In the solution of the differential equation (2), term ζ_x at the boundary $x = 1$ is known [9] to unlimitedly grow with the growth of $1/\beta$ to balance the convective and diffusive terms of Eq. (2). However, in the solution of the corresponding difference equation $\delta\zeta/\delta x = \beta\delta^2\zeta/\delta x^2$, term $\delta\zeta/\delta x$ is limited. Therefore, with $Re_{\text{cell}} > 2$, $\delta^2\zeta/\delta x^2$ has to grow on account of decrease of ζ_{N-1} down to negative magnitudes (see Figure 1), in order to further balance the terms in the difference equation. If $\zeta_{N-1} < 1$, the magnitude of $(\delta^2\zeta/\delta x^2)|_{N-2}$ a bit decreases what is being transmitted along axis x, thereby enforcing the saw-shaped oscillations. Enforced changes in $\delta^2\zeta/\delta x^2$ originate its deviation from ζ_{xx}. However, the diffusive term is a part of Eq. (9) to be calculated numerically. Thus, a disbalance between $\delta\zeta/\delta x$ and $\delta^2\zeta/\delta x^2$ results in the magnitudes of E other than E_{inv}.

Table 2. L^p norms (p = 1, 2 and ∞) for all configurations of difference schemes (the upwind scheme with β = 0.07 is referential)

Configuration	Norm × 10^{-3}		
	L^1	L^2	L^∞
Central diff., β = 0.03	2.71	1.32	0.920
Central diff., β = 0.07	1.33	0.609	0.416
Upwind, β = 0.03	0.468	0.215	0.147

It makes sense to say a few words about the method suggested above to monitor and control stability, in the context of traditional methods. The von Neumann method considers discrete harmonics with the requirement of spectrum boundedness. The Hurt method uses the Courant-Friedrichs-Lewy (CFL) criterion, which is often used for the analysis of hyperbolic systems. The Eddy method directly considers the properties of the transition factor for finite-difference equations. Stability criteria in many methods are based on the boundedness of the solution. These criteria are not identical, and their quantitative comparison is predominantly conditional and based on experimental computations that indicate the types of problems for which particular criteria are more suitable. The approach proposed in this article differs from the above methods in its nature. Its essence lies in the fact that, simultaneously with the calculations, the behaviour of the energy of a fictitious particle with certain properties is being monitored. The case of zeroing the energy of a fictitious particle indicates the emergence of instability, which, on the other hand, indicates the loss of freedom of this fictitious particle within the framework of the corresponding concept [8].

The implementation of the proposed method remains valid in the case of multi-dimensional problems. The sequence of the equations analogous to Eqs. (4)-(6) arises in the following way. Starting with the Newton's second law (3), we are to express the second time derivative of as

$$\ddot{\zeta} = \zeta_{xx}C_x^2 + \zeta_{yy}C_y^2 + \zeta_{zz}C_z^2 \tag{10}$$

keeping in mind that the other terms turned out to be zero because FP velocity is constant, as are its projections C_x, C_y, and C_z onto axes x, y, and z (in the case of Cartesian coordinate system) are. As we ourselves define the FP motion, we may impose an additional condition such as $C_x = C_y = C_z \equiv C$ (the constant possibly other than that in section 2). Substituting Eq. (10) into Eq. (3), we obtain

$$mC^2(\zeta_{xx} + \zeta_{yy} + \zeta_{zz}) = -U_\zeta$$

and from this equation, we derive the following expression for the potential energy:

$$U = -mC^2\int[\zeta_{xx}(x(\zeta)) + \zeta_{yy}(y(\zeta)) + \zeta_{zz}(z(\zeta))]\, d\zeta. \tag{11}$$

The kinetic energy reads

$$T = \frac{m\dot{\zeta}^2}{2} = \frac{m}{2}\left(\nabla\zeta,\, \dot{\mathbf{r}}\right)^2 = \frac{mC^2}{2}\left(\zeta_x + \zeta_y + \zeta_z\right)^2. \tag{12}$$

Equations (11) and (12) are direct analogues of Eqs. (4) and (5), and their sum yields the analogue of Eq. (6).

Should the step sizes along different axes not be equal, the resulting fictitious forces will depend on their ratios in addition to the factors acting in the one-dimensional case.

5. Conclusions

In this short communication, I have presented an effect found in relation to difference schemes with respect to the physical notion freedom introduced earlier and attributed to a material point [8]. The difference schemes are known to produce fictive sequels which are non-physical phenomena in the context of a physical process under consideration, and influence both convergence and stability [9], [10]. Our idea to apply a fictive particle travelling along the function codomain grid, experiencing impact originating from the discreet nature of the grid and enabling us to monitor possible (and inevitable) degradation of its own freedom in the context of the difference scheme stability, is expressed in this study. While a travelling fictive particle remains under the impact of external forces, its total mechanical energy (possibly pseudo-energy, depending on the function codomain dimension) is changing, thereby indicating the particle's freedom gradual loss. The fictive particle energy definition found its final expression in Eq. (6) and enabled us to both analytically calculate and compute by means of Eq. (9) the running value of the fictive particle energy. As far as it must be invariant from the theoretical point of view, it varies when computed on the grid. Its deviation from a constant value characterised by its mean derivative indicates the harm [8] the difference scheme fictive forces cause. With the two difference schemes, one of whose (the central scheme) is known for saw-shaped oscillations in the region of instability in the model one-dimensional pseudo-curl transfer problem and another one (the upwind) is unconditionally stable, I showed that the fictive particle freedom is quite telltale in the sense of computational stability. Thus, in the parametric (in terms of β) region of instability, it appears to be fully lost, whereas in other regions, the deviation of its mean derivative $\frac{2E_{\zeta}\left(\zeta_{\text{mid}}\right)}{mC^2}$ from zero characterises the impact the difference scheme introduces. I name this mean derivative Fictive Forces Factor (3F). It gives rise to a quantitative comparison of the effects of different difference schemes on a grid covering the same region. Thus, compared to the central scheme, the upwind one proves to be more modest since it has a smaller 3F.

Typically, when given a novel problem in the framework of a trial approach with several proper difference schemes, one studies scrupulously the issues of stability and convergence by numerical experiment or/and analytically. Verification of numerical results has to be especially exigent when no analytical solution of the problem is possible. In such situations, a 3F-based analysis could hopefully find its place and contribute.

The results obtained here can be obviously extrapolated from one- to two- and three-dimensional problems as well as from scalar to vector functions. The fictitious particle is always tied to the grid, and computations of its energy simply accompany the computations on the grid. Therefore, analysis within the framework of a multidimensional problem does not differ from analysis within the framework of a one-dimensional problem. As promising in this sense, for example, look the equations describing wave propagation in convecting fluids, in flexo- and piezoelectric structures and in biosystems. As the analysis of the fictive particle freedom in connection to other popular finite difference implementations as well as to finite element applications in problems related to vibrational responses in engineering constructions requires time, I believe this justifies publication of this short communication.

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Statements and declarations

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Conflict of interest

The author has no competing interests.

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