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Numerical Modeling of Non–Linear Elastic Wave Phenomena

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ABSTRACT

Non–linear elastic wave response in geological materials is a classical result, but due to its enormous complexity in theory and experiments, its linear elastic approximation has been mostly assumed and applied in geophysical sciences. However, realistic studies in terms of processing, migration, modeling, and inversion require a full solution of a general non–linear elastic wave theory. We present the first results of the development of a finite–difference (FD) approach that allows to account for non–linear elastic wave effects. This algorithm is based on a new velocity–displacement gradient formulation of the non–linear elastic plane wave equation, since common approaches such as the well–known velocity–stress method that are used for linear elastic wave problems do not work correctly here. We also make attendent problems evident such as numerical non–linear instability and handling related shock wave fronts, and present probable solutions.

INTRODUCTION

The description of linear seismic wave propagation within the earth has been successfully applied to seismology and exploration geophysics during the last decades. Assuming linear response, recorded spectra from seismic waves are used to estimate the magnitude, characterize high frequency roll–off and model source parameters. Based on the related principle of superposition, most of the seismic processing techniques (such as stacking) and interpretation algorithms (i.e. modeling, inversion, migration) could been developed. A necessary condition for this description is the assumption of infinitesimal deformations and a linear stress–strain relation of the geological materials. However, non–linear elastic behavior of rocks have been widely observed in laboratory measurements. Such behavior in strongly influenced by the presence of mechanical defects contained in rock, such as cracks, microfractures, grain joints and prestress (e.g., Bourbié et al., 1987). The non–linear generation of elastic waves in

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rock have been generated by Johnson and Shankland (1989), Meegan et al. (1993), and Johnson and Rasolofosaon (1996). The importance of the source influence on the non–linear effects in seismic waves is given in Johnson and McCall (1994) and Meegan et al. (1993). Recently, new theoretical models that describe the elastic behavior of hysteretic non–linear geological media are developed by Guyer et al. (1995) and Guyer and Johnson (1999). Furthermore, the influence of finite displacement amplitudes on the effect on non–linear elastic wave propagation has been demonstrated by Meegan et al. (1993) and Johnson and McCall (1994).

The development of numerical methods that considers the wavefield in heterogeneous non–linear elastic media are very useful for comparisons with the laboratory measurements mentioned above and seismic field experiments, the exploration of a transition domain of linear/non–linear effects, the influence of static pre–stress, caused by gravimetric and/or tectonic forces, large permanent deformations at the source region, caused by earthquakes and nuclear explosions, and technical applications such as extension of source signal bandwidths. For these reasons, a thorough theoretical research is requested to describe the complete solution of non–linear wave propagation in arbitrarily complex geological materials. However, since for non–linear wave propagation the principle of superposition breaks down, analytical methods are not available in closed forms, not even for the most simple cases (McCall, 1994). In this paper, first results on numerical study and properties of a finite–difference (FD) algorithm that simulates non–linear elastic wave propagation are presented. We point out the analytical and numerical problems when extrapolating FD approaches from the linear to the non–linear wave equation and demonstrate possibilities how to overcome those.

BASICS OF NON–LINEAR ELASTICITY

Elastic theory and wave propagation is based on the analysis of stress and strain. Very generally, this analysis is concerned with the positions of each particle of a continous medium in the current state and the positions in the original state. The original, i.e. initial undeformed geometry is described by Langrangian coordinates as the independent variables. They refer to a coordinate system fixed in the solid/fluid and undergoing all the motion and distortion of the solid/fluid. In contrast, the current, i.e. deformed geometry is described by Eulerian coordinates as the independent variables, which refer to a coordinate system fixed in space and through which the solid/fluid is thought of as a moving. Both Lagrangian and Eulerian form of the equations are equivalent. However, the Lagrangian form is usually preferred in theory, since the original relative positions influence the internal forces throughout the body at later times, and in numerics, since this form is more accurate and stable than the Eulerian form (e.g., Bland, 1969; Ames, 1977). In the approximation of linear elasticity both forms are interchangeable, which is not valid for the general non–linear case.

In Lagrangian formulation, the Green finite strain/deformation tensor is given by (e.g., Landau and Lifshitz, 1959):

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right], \tag{1}$$

where u is the displacement. Conventional summation notation on repeated indices is used. In the case of infinitesimal displacements and/or displacement gradients the third term on the right side of equation (1) can be neglected leaving the classical linear relation between the strain and the displacement (Hooke's law). However, when dealing with finite deformations, relation (1) is non–linear. This type of non–linearity is called *geometrical* or *kinematic* and is related to the difference between the Lagrangian and Eulerian coordinate description.

The general equation of motion (Newton's second law) in Lagrangian formulation is given by (Landau and Lifshitz, 1959; Bland, 1969):

$$\varrho_0 \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2}$$

where ϱ_0 denotes the density of the undeformed solid/fluid.

The stress tensor is defined by (Polyakova, 1964; Kulikovskii and Sveshnikova, 1995):

$$\sigma_{ij} = \frac{\partial \mathcal{E}}{\partial \left(\frac{\partial u_i}{\partial x_j}\right)} \tag{3}$$

with $\mathcal{E}$ as internal energy density of a homogeneous elastic solid describing adiabatic deformations.

The relation between $\mathcal{E}$ and ε_{ij} may be described in the following way. We employ the three invariants of the strain tensor (e.g., Bland, 1969):

$$\begin{aligned} I_1 &= \varepsilon_{ii} \quad \sim O(\varepsilon), \\ I_2 &= \frac{1}{2}\left(\varepsilon_{ii}\varepsilon_{jj} - \varepsilon_{ij}\varepsilon_{ji}\right) \quad \sim O(\varepsilon^2), \\ I_3 &= \det\left(\varepsilon_{ij}\right) \quad \sim O(\varepsilon^3), \end{aligned} \tag{4}$$

so that I_1, I_2, and I_3 denote the trace, sum of the principal minors, and the determinant of the strain tensor, respectively. Now we may expand $\mathcal{E} = \mathcal{E}(I_1, I_2, I_3)$ as a power series to third order, which yields for isotropic media (Murnaghan, 1951):

$$\mathcal{E} = \frac{\lambda + 2\mu}{2} I_1^2 - 2\mu I_2 + \frac{l + 2m}{3} I_1^3 - 2m I_2 I_2 + n I_3, \tag{5}$$

where λ and μ are the well–known Lamé parameters (second order elastic constants) and l, m, n are the so–called Murnaghan coefficients (third order elastic constants).

Those latter coefficients describe *physical* non–linearity (cubic anharmonicity), not related to geometrical/kinematic non–linearity mentioned above, and account for the fact that stress is no longer a linear function of strain even for moderate to small strain levels, i.e. even if equation (1) becomes linear. This is the case in materials exhibiting strong non–linearity such as rock (Johnson and Shankland, 1989; Meegan et al., 1993; Johnson and Rasolofosaon, 1996; Guyer and Johnson, 1999). The existence of both geometrical and physical non–linearity makes Hooke's law also non–linear and its non–linearities are determined, generally speaking, by the geometrical and physical non–linearities simultaneously.

WAVE EQUATION AND ITS PROPERTIES

Combining equations (1)–(5) yields for the plane wave propagation in a homogeneous medium (x direction) (Gol'dberg, 1960; Polyakova, 1964; McCall, 1994):

$$\begin{aligned} \varrho_0 \frac{\partial^2 u_x}{\partial t^2} &= (\lambda + 2\mu)\frac{\partial^2 u_x}{\partial x^2} + \frac{1}{2}\left[3(\lambda+2\mu) + 2(l+2m)\right]\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x}\right)^2 \\ &\quad + \frac{1}{2}(\lambda + 2\mu + m)\frac{\partial}{\partial x}\left[\left(\frac{\partial u_y}{\partial x}\right)^2 + \left(\frac{\partial u_z}{\partial x}\right)^2\right], \end{aligned} \tag{6}$$

$$\varrho_0 \frac{\partial^2 u_y}{\partial t^2} = \mu\frac{\partial^2 u_y}{\partial x^2} + (\lambda + 2\mu + m)\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x}\frac{\partial u_y}{\partial x}\right), \tag{7}$$

$$\varrho_0 \frac{\partial^2 u_z}{\partial t^2} = \mu\frac{\partial^2 u_z}{\partial x^2} + (\lambda + 2\mu + m)\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x}\frac{\partial u_z}{\partial x}\right). \tag{8}$$

These equations describe a system having linear and nonlinear elasticity. The respective first terms on the right side of equations (6)–(8) describe the linear part, whereas the remaining terms describe the non–linear part. Those quadratic terms depend on all components of u_i, respectively, leading to interaction between longitudinal (u_x) and transversal waves (u_y, u_z), even in this 1–D homogeneous case. This is in contrast to linear elastic wave theory. The quadratic corrections can be seen as driving forces acting differently for the longitudinal and transverse waves. Furthermore, it is obvious that propagation of purely non–linear longitudinal waves is possible, whereas propagation of non–linear transverse waves is only possible at presence of a longitudinal component.

If we only consider pure longitudinal wave propagation, this yields:

$$\frac{\partial^2 u_x}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u_x}{\partial t^2} = -\beta\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x}\right)^2, \tag{9}$$

where $c = \sqrt{\frac{\lambda+2\mu}{\varrho_0}}$ is the compressional wave velocity and:

$$\beta \ = \ \frac{3}{2} + \frac{l+2m}{\lambda+2\mu} \tag{10}$$

is the non–linear coefficient describing the strength of cubic anharmonicity. The first term on the right side of equation (10) denotes the geometrical non–linearity, caused by finite deformations, whereas the second term denotes the physical non–linearity.

The non–linear term β of the wave equation describes the interaction of the displacement/wave with itself, causing a creation of sum and difference frequencies, which leads to a breakdown of the superposition principle. For this reason, the propagation of non–linear waves is dominated by anharmonic effects not allowing any periodic/harmonic solutions of the wave field (Landau and Lifshitz, 1959; Gol'dberg, 1960). Due to these serious problems, even for the most simple case, a monofrequent wave, the solution of equation (9) has no closed form but is to be solved semianalytically by an iterative Green's function technique (McCall, 1994). For a realistic multifrequent wavelet the solution becomes much more complex since all source frequencies interact with all other source frequencies.

An outstanding feature of finite–amplitude non–linear elastic wave behavior is that the wave velocities depend on the strain level. As a consequence, an initially sinusoidal waveform will not maintain its shape during its propagation, because the wave crests overtake the wave troughs due to the interaction processes. This yields a transfer of energy in the Fourier space from long to short wavelenghts, i.e. low to high frequencies, resulting in a wave profile steepening and finally producing a sawtooth shock wave (Gol'dberg, 1960; Zarembo and Krasil'nikov, 1971; Kulikovskii and Sveshnikova, 1995).

NUMERICAL MODELING

Numerical forward algorithms, such as FD approaches, describe approximately the complete solution of wave propagation problems, i.e. the respective partial differential equations in arbitrarily complex geological materials. In fact, FD methods are very popular and have been widely applied for linear seismic problems in the past (e.g., Alford et al., 1974; Kelly et al., 1976; Virieux, 1986). However, we found that extrapolating linear FD methods to non–linear problems is neither trivial nor straightforward, but leads to arising problems. Those problems are: (i) non–symmetric wave propagation, (ii) non–linear instability, and (iii) the way of handling shock wave fronts. We will explain these issues more explicitly.

A consistent FD approach of our 1–D non–linear wave propagation problem can be realized by a direct approximation of the second order partial differential equation

(9) by explicit difference operators of second order in both time and space:

$$\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\triangle x)^2} - \frac{1}{c^2}\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\triangle t)^2} = -2\beta\frac{u_{i+1}^n - u_{i-1}^n}{2\triangle x}\left(\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\triangle x)^2}\right), \qquad (11)$$

where $\triangle t$ is the time step, $\triangle x$ the spatial discretisation, and indices n and i denote time and space coordinates, respectively [$u_i^n = u(n\triangle t, i\triangle x)$ with $n, i = 0, 1, 2, \ldots$]. This approximation has been widely applied to its analogous linear problem (e.g., Alford et al., 1974; Kelly et al., 1976). A more advisable and efficient, in terms of numerical and computational properties, method for the linear wave equation lies within the velocity–stress approach (e.g., Virieux, 1986), which is for the non–linear case:

$$\begin{aligned}\frac{\partial v}{\partial t} &= \frac{1}{\varrho}\frac{\partial \sigma}{\partial x} \\ \frac{\partial \sigma}{\partial t} &= (\lambda + 2\mu)\frac{\partial v}{\partial x} + (\lambda + 2\mu)\beta\left(\frac{\partial v}{\partial x}\right)^2,\end{aligned} \qquad (12)$$

where v denotes the velocity ($\partial u/\partial t$). Approximating this system of partial differential equations by staggered–grid FD operators of second order in both time and space [cf. Virieux (1986)], this yields:

$$\begin{aligned}\frac{v_i^{n+1/2} - v_i^{n-1/2}}{\triangle t} &= \frac{1}{\varrho}\,\frac{\sigma_{i+1/2}^n - \sigma_{i-1/2}^n}{\triangle x} \\ \frac{\sigma_{i+1/2}^{n+1} - \sigma_{i+1/2}^n}{\triangle t} &= (\lambda + 2\mu)\left[\frac{v_{i+1}^{n+1/2} - v_i^{n+1/2}}{\triangle x} + \beta\left(\frac{v_{i+1}^{n+1/2} - v_i^{n+1/2}}{\triangle x}\right)^2\right].\end{aligned} \qquad (13)$$

For the linear case, these two approaches are the most common ones in geophysics for modeling wave propagation in heterogeneous media.

Although the above presented FD schemes are consistent and work in the linear case ($\beta = 0$), they are not applicable to non–linear problems since the quadratic non–linear terms lead to unsymmetrical wave propagation results, which is not valid. We also applied several other FD operators to approximate the non–linear wave equation (9) and/or its velocity–stress formulation (12), such as compact, leap–frog, Adams–Bashforth, Euler–Backward, Crank–Nicholson, and Lax–Wendroff (e.g., Richtmyer and Morton, 1967; Ames, 1977), on staggered and non–staggered grids. In fact, all those approaches led to unsymmetrical wave propagation, so conventional methods applicable for the linear wave problems do not work succesfully for respective non–linear situations.

We present a new formulation that leads to symmetrical wave propagation. This approach is to be called velocity–displacement gradient method. We introduce:

$$v = \frac{\partial u}{\partial t}, \qquad g = \frac{\partial u}{\partial x}, \tag{14}$$

where g denotes the displacement gradient. Now by substituting into equation (9), this yields:

$$\begin{aligned} \frac{\partial v}{\partial t} &= c^2 \frac{\partial g}{\partial x} + 2\beta c^2 \, g \frac{\partial g}{\partial x} \\ \frac{\partial g}{\partial t} &= \frac{\partial v}{\partial x}. \end{aligned} \tag{15}$$

Applying a staggered leap–frog FD scheme of second order in both time and space leads to:

$$\begin{aligned} \frac{v_{i+1/2}^{n+1} - v_{i+1/2}^{n}}{\triangle t} &= c^2 \, \frac{g_{i+1}^{n+1/2} - g_i^{n+1/2}}{\triangle x} \left[1 + 2\beta \, \frac{g_i^{n+1/2} + g_{i+1}^{n+1/2}}{2} \right] \\ \frac{g_i^{n+1/2} - g_i^{n-1/2}}{\triangle t} &= \frac{v_{i+1/2}^{n} - v_{i-1/2}^{n}}{\triangle x}. \end{aligned} \tag{16}$$

This FD method leads to symmetric non–linear wave propagation.

FD approximations should be constrained by certain numerical stability criteria so that discrepancies between the exact and numerical solutions remain bounded. For example, when applying the linear version of the wave equation [$\beta = 0$ in equation (9)], the para- meter $c\triangle t/\triangle x$ must be limited (Richtmyer and Morton, 1967; Alford et al., 1974; Kelly et al., 1976; Virieux, 1986). However, with non–linear equations the situation is totally different and one reaches the limits of what can be stated for very general classes of FD approaches. Thus, except in special cases, very little has yet been proved till now about difference schemes for approximating the discontinuous solutions that frequently arise for such equations (e.g., Richtmyer and Morton, 1967; Ames, 1977; Thomas 1999). For non–linear hyperbolic, i.e. wave propagation problems, respective FD equations mostly have solutions which *explode*, even if the stability condition for the linearised equation is satisfied. Stability depends not only on the form of the FD system but also upon the solution being obtained; and for a given solution, the system may be stable for some values of t and not for others. This may be explained as follows: as mentioned before, even an initially smooth wavelet does not keep its smooth shape, but starts to build a steep wave front with increasing time due to energy transfer to high frequencies (Figure 1a). At a certain time, the analytical/physical solution is multivalued, and a shock wave front appears. Now the numerical solution misrepresents this discontinuity as a steep gradient bounded by a series of large–amplitude short–wavelength perturbations. These perturbations are amplifying rapidly and the numerical energy is growing without bound (Figure 1b). This exponential growing is a numerical instability, since the norm of the wave energy of the analytical solution does not increase with time in that way (Richtmyer and Morton, 1967). For this reason, a *conservative* FD approximation has to be found to avoid such numerical non–linear instabilities. However, since each non–linear problem and its solutions are different, no general methods do exist for studying stability. It should be noted that non–linear instabilities are not restricted to non–linear physical problems that include shock formations, since such instabilities may also occur in numerical simulations of very smooth, but non–linear flow (Thomas, 1999).

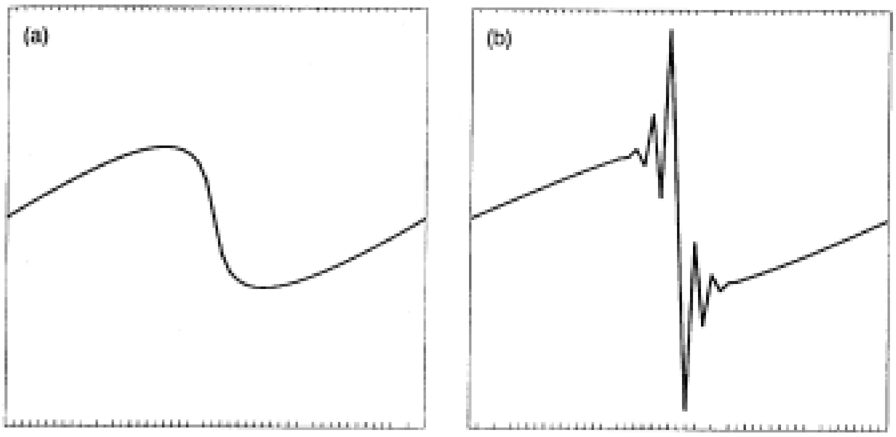

Figure 1: Schematic illustration of the numerically calculated development of a shock wave front for an initially smooth sinusoid function. (a) steepening of the wavelet after a certain time, shock front has not appeared yet; (b) at a later time: shock front is present now, leading to growing short–wavelength perturbation and numerical instability.

There might exist one or several FD approximations for our system (15). Those can eventually be realised by setting different weighting averages of the respective FD operators or by applying different FD techniques themselves that tend to be more conservative, such as Lax–Wendroff (e.g., Richtmyer and Morton, 1967). For the related problem presented here the derivation of such a stable/conservative FD scheme is, however, still an open question. Nevertheless, there are many numerical methods that have been developed for fluid dynamic processes for solving non–linear problems. Such methods might be extended to non–linear elastic wave problems.

The third aforementioned difference in FD modeling of non–linear in contrast to linear wave propagation problems is related to the physical appearence of shock wave fronts. Even when applying a conservative FD method, short–wavelength oscillations appear when approximating a shock front, though those do not continue to amplify (Figure 2). Those oscillations are non–physical and are not present in the correct analytical solution of the shock formation (e.g., Kulikovskii and Sveshnikova, 1995). This means that special numerical techniques must be used to control the development of those numerical over– and undershoots in the vicinity of a shock. One possible and useful solution to this problem might lie within the adding of artificial viscosity (e.g., Richtmyer and Morton, 1967; Ames, 1977; Thomas 1999). The application of viscosity to our otherwise non–viscous problem and scheme is in order to damp energy of the short–wavelength events. A modified version of our velocity–displacement gradient method [equation (15)] that includes viscosity is:

$$\frac{\partial}{\partial t}\begin{pmatrix} v \\ g \end{pmatrix} = \begin{pmatrix} 0 & c^2 + 2\beta c^2 g \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x}\begin{pmatrix} v \\ g \end{pmatrix} + \gamma \frac{\partial^2}{\partial x^2}\begin{pmatrix} v \\ g \end{pmatrix}, \qquad (17)$$

where γ is the viscosity coefficient that determines the strength of the smoothness. In fact, including viscosity in non–linear seismic wave propagation phenomena is a viable option, since attenuation of the wavefield is an omnipresent fact in earth materials.

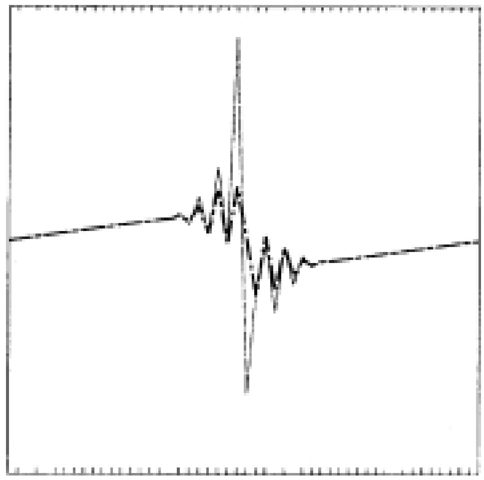

Figure 2: Schematic illustration of a numerically calculated shock wave front for an initially smooth sinus- oid function. Thin solid line: Conventional FD approach calculation that leads to numerical instabilities. Dash–dotted line: Conservative FD approach calculation leading to a numerically stable result.

It is still not clear in which way equation (17) has to be approximated by FD operators, and in literature there is no agreement about implementing numerically artificial viscosity in non–viscous schemes to smooth short–wavelength perturbations. For example, Ames (1977) suggested the combination of a high–order difference scheme that is accurate for smooth processes and therefore is to be applied on the dynamic parts of the wavefield [i.e. the first terms on the left and right side of equation (17)], whereas a low–order operator should be applied on the viscosity term [i.e. the second term on the right side of equation (17)] to limit the scale selectivity that has to be smoothed in the vicinity of shock fronts. In contrast, Richtmyer and Morton (1967) and Thomas (1999) favored an FD operator of higher order for the viscosity term to damp short wavelengths most rapidly, whereas long waves shall stay relatively unaffected. Therefore, a thorough analysis of these analytical and numerical phenomena is required.

CONCLUSIONS

We have presented the first results of the development of a finite–difference technique for modeling non–linear elastic wave propagation in earth materials. The finite–difference solution is based on a new velocity–displacement gradient formulation of the problem, since conventional approaches used for the respective linear wave equation do not account for the non–linear case and would lead to non–symmetrical wave propagation. Non–linear instability is an additional and serious phenomenon caused by the physical non–linear effect. We described this phenomenon and suggested possible solutions, i.e. the derivation of a conservative difference formulation to keep the numerical solutions bounded. Shock wave generations as a result of non–linear wave propagation in time and space cause steep waveform profiles analytically and yield short–wavelength oscillations numerically. We suggest to smooth such perturbations by adding of artifical viscosity. After developing a complete non–linear waveform difference algorithm, future work lies within the extension to heterogeneous and 2–D and 3–D media as well as the inclusion of realistic attenuation effects.

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