Parallel Computing in the Acoustic and Elastic Wave Propagation in Periodic Media

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Abstract

In this paper we present calculations for acoustic and elastic waves propagating in periodic composites consisting of spheres in a host material. Our aim is to examine whether stop bands appear in these composites and under what conditions. To perform these calculations our methods were associated with a simple parallelization procedure which is also presented.

1 Introduction

In recent years considerable attention from the condensed matter physicists has been given to the study of the classical wave[1] propagation in periodic composite systems. The attention is focused on the question of the existence or not of spectral gaps (stop bands - frequency regions of forbidden propagation) in these periodic systems in analogy with the gaps in the electron wave propagation in solids. The similarities between the classical wave equation and the Schrodinger equation (which governs the electron wave propagation) gave the idea that we can observe in classical waves (CW) the same phenomena which have been observed in electrons and have constituted the heart of the condensed matter physics over the last 70 years.

One reason for the interest about stop bands in the CW propagation stems from the possible applications mainly in filter technology. Another reason is related with what is called localization: It has been found that if we randomize a periodic medium which exhibits a stop band (gap) this stop band finally becomes a region of localized states (states which do not correspond to propagating waves but to waves trapped in a region within the composite and attenuated exponentially) [1, 2]. Thus, by studying periodic composites (something easier due to the symmetry) we can locate spectral regions where localized states may appear as we randomize the composite. This is not surprising as both gaps and localization are due to the same mechanisms: scattering and the destructive interference of the multiple scattered waves.

Electromagnetic waves were the first to attract attention. Both theoretical results and experimental data showed that, although the existence of a gap is not something a priori guaranteed, one can construct structures (photonic crystals) which exhibit wide gaps; one can also control the frequency of these gaps. Up to now structures have been fabricated with gaps up to 10^{14} Hz.

Acoustic and elastic waves on the other hand only recently attracted some attention, especially for experimental investigation [3, 4, 5, 6] stimulated by theoretical studies [7, 8, 9, 10, 11].

In this paper we present calculations for acoustic and elastic waves propagating in periodic composites consisting of *spheres in a host material*. Our interested is concentrated on the question of possible appearance of stop bands in these composites. This question is examined by calculating the dispersion relation, $\omega = f(\mathbf{k})$, of waves in the composites. For these calculations we have employed two methods which are associated with a simple parallelization procedure. In what follows we present first our main equations, then the methods and the parallelization procedure and finally we present and discuss our main results.

2 Wave Equations

The starting point for our calculations is the elastic and acoustic wave equations in isotropic media. The elastic wave equation can be written in the form

$$\frac{1}{\rho}\{\frac{\partial}{\partial x_i}(\lambda\frac{\partial u^\ell}{\partial x_\ell}) + \frac{\partial}{\partial x_\ell}[\mu(\frac{\partial u^i}{\partial x_\ell} + \frac{\partial u^\ell}{\partial x_i})]\} + \omega^2 u^i = 0. \quad (1)$$

In the above equation u^i are the cartesian components of the displacement vector, $\mathbf{u}$, $\rho(\mathbf{r})$ is the mass density and $\lambda(\mathbf{r})$ and $\mu(\mathbf{r})$ the Lamé coefficients of the medium.

For fluids the coefficient μ is equal to zero and, by introducing the pressure $p = -\lambda\nabla\mathbf{u}$, Equation (1) can be written as

$$\nabla[\frac{1}{\rho(\mathbf{r})}\nabla p(\mathbf{r})] + \frac{\omega^2}{\lambda(\mathbf{r})}p(\mathbf{r}) = 0. \quad (2)$$

For periodic systems the coefficients $\rho(\mathbf{r})$, $\lambda(\mathbf{r})$ and $\mu(\mathbf{r})$ are periodic functions with the periodicity of the structure. Moreover, the fields, $\mathbf{u}$ and p, obey the so called Bloch's theorem. Bloch's theorem states that $\mathbf{u}$ or p can be written as a plane wave but with an amplitude which is periodic function with the periodicity of the system: $\mathbf{u}(\mathbf{r}) = \mathbf{u}_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$, $p(\mathbf{r}) = p_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$.

3 Methods of Calculation

3.1 Plane Wave Method (PW)

The Plane Wave (PW) method is based on the expansion of the periodic coefficients in the wave equation in Fourier sums [8, 11]:

$$f(\mathbf{r}) = \sum_{\mathbf{G}} f_{\mathbf{G}}e^{i\mathbf{G}\mathbf{r}}, \qquad f: \lambda\,(\text{or}\,\lambda^{-1}), \mu, \rho^{-1}. \quad (3)$$

[1]Waves obeying a second order equation in the time domain (electromagnetic, acoustic, elastic) - in contrast to electrons which obey Schrödinger's equation (a first order in the time domain equation).

Applying Bloch's condition to the fields and expanding the coefficients λ (or λ^{-1}), μ, ρ^{-1}, $\mathbf{u_k}$ and $p_\mathbf{k}$ according to Equation (3), both the acoustic and the elastic wave equation are transformed to matrix eigenvalue equations.

From Equation (1) (for periodic solid composite systems) one obtains

$$\begin{aligned}\omega^2 u^i_{\mathbf{k}+\mathbf{G}} = \sum_{\mathbf{G}'} \quad & \{\sum_{\ell,\mathbf{G}''} \rho^{-1}_{\mathbf{G}-\mathbf{G}''} \\ & [\lambda_{\mathbf{G}''-\mathbf{G}'}(\mathbf{k}+\mathbf{G}')_\ell(\mathbf{k}+\mathbf{G}'')_i \\ & +\mu_{\mathbf{G}''-\mathbf{G}'}(\mathbf{k}+\mathbf{G}')_i(\mathbf{k}+\mathbf{G}'')_\ell]u^\ell_{\mathbf{k}+\mathbf{G}'} \\ & +\sum_{\mathbf{G}''}[\rho^{-1}_{\mathbf{G}-\mathbf{G}''}\mu_{\mathbf{G}''-\mathbf{G}'} \qquad (4) \\ & \sum_j(\mathbf{k}+\mathbf{G}')_j(\mathbf{k}+\mathbf{G}'')_j]u^i_{\mathbf{k}+\mathbf{G}'}\}.\end{aligned}$$

For N terms in the Fourier sums, Equation (4) is a 3N×3N matrix eigenvalue equation of the form $A\mathbf{X} = \omega^2\mathbf{X}$. Its solution gives the 3N permitted frequencies ω for a periodic solid composite. For achieving convergence N usually has to be of the order of 400-500. It means that Equation (4) will be a system of the order of 1500×1500.

For fluid systems (starting from Equation (2)) the corresponding to Equation (4) result is

$$\begin{aligned}&\sum_{\mathbf{G}'} \rho^{-1}_{\mathbf{G}-\mathbf{G}'}(\mathbf{k}+\mathbf{G})(\mathbf{k}+\mathbf{G}')p_{\mathbf{k}+\mathbf{G}'} \\ &\qquad = \omega^2 \sum_{\mathbf{G}''} \lambda^{-1}_{\mathbf{G}-\mathbf{G}''} p_{\mathbf{k}+\mathbf{G}''}. \qquad (5)\end{aligned}$$

For N terms in the Fourier sums Equation (5) is a N×N matrix equation of the form $A\mathbf{X} = \omega^2 B\mathbf{X}$.

3.2 Multiple Scattering Method

Although PW is a very direct and easy to apply method, it is unable to give accurate results for *mixed* composites consisting of *solid scatterers in a fluid host*. To cover this case we employed a Multiple Scattering (MS) method based on a theory known, from the electronic band structure calculations, as the Korringa-Kohn-Rostoker's (KKR) theory [12, 13].

The main idea of the method is that the incident wave at each scatterer has to be equal with the scattered waves from all the other scatterers (in the absence of an external incident field). This idea can be expressed mathematically as

$$p^{inc}_n(\mathbf{r}) = \sum_{p\neq n} p^{sc}_p(\mathbf{r}), \qquad (6)$$

where the subscript n denotes the scatterer at the lattice position $\mathbf{R}_n$. We can write the incident and the scattered wave at each lattice position as a sum of elementary spherical waves:

$$\begin{aligned}p^{inc}_n(\mathbf{r}) &= p^{inc}(\mathbf{r}-\mathbf{R}_n) \\ &= \sum_{lm} a^n_{lm} j_l(k_o|\mathbf{r}-\mathbf{R}_n|)Y_{lm}(\mathbf{r}-\mathbf{R}_n), \qquad (7)\end{aligned}$$

$$\begin{aligned}p^{sc}_p(\mathbf{r}) &= p^{sc}(\mathbf{r}-\mathbf{R}_p) \\ &= \sum_{lm} b^p_{lm} h_l(k_o|\mathbf{r}-\mathbf{R}_p|)Y_{lm}(\mathbf{r}-\mathbf{R}_p). \qquad (8)\end{aligned}$$

(In the above equations j_l and h_l are the first kind spherical Bessel function and the first kind spherical Hankel function respectively [14].) Relating the scattered wave by each scatterer with the incident wave at the same scatterer (by solving a simple single scattering problem) one can relate the coefficients b^p_{lm} with the a^p_{lm}:

$$b^p_{lm} = t_l a^p_{lm}. \qquad (9)$$

(The scattering coefficients t_l [15] for the case of identical scatterers are independent on the lattice position.)

Using Bloch's condition one can relate also the coefficients a_{lm} of the different lattice sites:

$$a^p_{lm} = e^{i\mathbf{k}(\mathbf{R}_p-\mathbf{R}_n)} a^n_{lm}. \qquad (10)$$

Substituting all the above in Equation (6) and using the expansions of the elementary spherical functions $h_l(k_o|\mathbf{r}-\mathbf{R}_p|)Y_{lm}(\mathbf{r}-\mathbf{R}_p)$ in terms of the functions centered at $\mathbf{R}_n$ (see Equation (A1)), Equation (6) takes the form

$$\begin{aligned}\sum_{l'm'} \quad [& \sum_{p\neq n} e^{i\mathbf{k}(\mathbf{R}_p-\mathbf{R}_n)} g_{lml'm'}(\mathbf{R}_p-\mathbf{R}_n) \\ & -(t^{-1}_{l'})\delta_{ll'}\delta_{mm'} \ ] \ a^n_{l'm'} = 0 \\ \Leftrightarrow \qquad & \sum_{L} \Lambda_{LL'} a_{L'} = 0, \quad L \equiv (l,m), \qquad (11)\end{aligned}$$

which corresponds to a homogeneous algebraic system. The condition for this system to have non vanishing solutions (det($\Lambda = 0$) gives the eigenmodes of a periodic composite in the framework the MS method.

The coefficients $g_{lml'm'}$, which are given in the Appendix, are dependent only on the elastic parameters of the host material and on the characteristics of the lattice. The scattering material affects the above equation only through the scattering coefficients t_l. t_l can be calculated very easily for both solid and fluid scatterers [15].

3.3 Parallelization Procedure

In order to examine if a full stop band (forbidden frequency region for all directions) exists in a periodic system we have to solve Equation (4) or (5) or (11) for a lot of values of the parameter (wave vector) $\mathbf{k}$. Taking into account that the typical running time for 1 $\mathbf{k}$ is of the order of 1/2 CPU hour, one can see that the total calculation can be extremely time consuming.

There is, however, the advantage that the calculation for each $\mathbf{k}$ is independent. The only restriction is that in order to obtain a picture of the dispersion relation the results ($\omega_\mathbf{k}(j)$) have to be printed in the correct sequence of $\mathbf{k}$s.

The independence of the different $\mathbf{k}$ calculations helped us to apply a simple parallelization procedure (see Figure

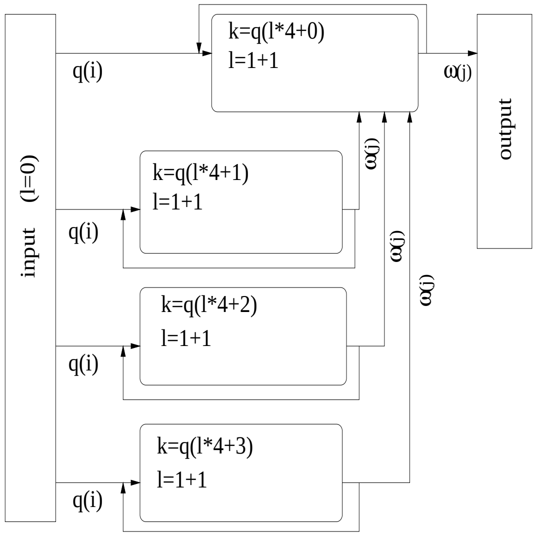

Figure 1: Parallelization procedure for a network of 4 processors. The processors are denote with the parallelograms. The corresponding to each processor values of **k** are written inside the parallelograms.

1) which reduced the time of our calculation by a factor almost equal to the number of the processors used. This parallelization procedure has been applied to both PW and MS method. The input values of **k** are stored in an array, $q(i)$, (in fact three arrays, one for each cartesian component of the vector **k**) and they are sorted in the special way which we require for the results. The $q(i)$s are distributed over the different processors (by using cycling distribution - see Figure 1). Each processor performs the eigenvalue calculation for each own $\mathbf{k} = q(i)$, sends the resulting eigenfrequencies, $\omega_{\mathbf{k}}(j)$, to the master processor (with blocking communication) and continues with its next input **k** value. The master processor receives the results from the others in a way which retains the **k**s in the same order as in the array $q(i)$ and prints them.

The above way of parallelization has the important advantage that there is balancing of the work over the different processors (all the processors have almost the same work to perform). Moreover, the communications over the different processors take place only at the end of the calculation for each **k**, which means minimum number of communications. These two characteristics have as a result the maximum reduction of the running time relatively to the sequential running time. Another advantage of the above procedure is that in order to apply it one needs minor changes in the structure of the sequential program. Thus the program can be easily understood and used by people not familiar with parallel programming.

For the implementation of the above parallelization procedure we have used Message Passing Interface (MPI) in a distributed memory parallel machine.

4 Results

As it has been already mentioned, our interest is focused on the question of gap formation in acoustic and elastic periodic composites and on the optimal conditions for the existence of these gaps. To examine the above question we calculated the dispersion relation for a variety of composites and we examined how the dispersion relation depends on the parameters of the system.

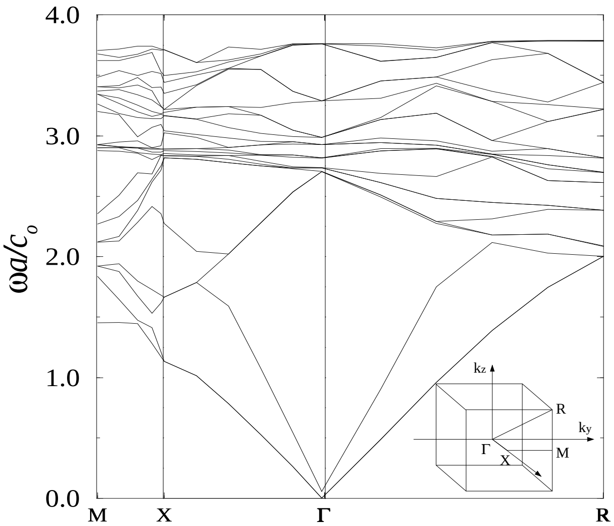

Figure 2: Dispersion relation along the directions MXΓR for a sc periodic composite consisting of epoxy spheres of volume fraction $f = 30\%$ in Cu. c_o is the longitudinal wave velocity in the Cu and a the lattice constant.

In Figure 2 we show a typical form of the dispersion relation. It concerns a composite consisting of epoxy spheres in copper. The epoxy spheres are arranged in a simple cubic structure, of volume fraction $f = 0.3$. The horizontal axis in Figure 2 is the **k** axis and the perpendicular axis is dimensionless frequency axis. **k** moves along certain directions in the so called first Brillouin zone. (First Brillouin zone is the primitive cell of the fourier transformed lattice and it is shown in the inset graph.) The letters on the **k**-axis denote certain points in the first Brillouin zone (see the inset graph). As can be seen in Figure 2, for each frequency, ω, there is at least one wave vector **k** which can be a possible channel for propagation. Thus there is no stop bands. Usually this is the case for most of the periodic material combinations which we have examined.

Examination of a variety of composites showed that gaps can exist only under rather extreme conditions. To determine these conditions we examined the role of each of the parameters of the problem.

We examined first the role of the density contrast ρ_o/ρ_i, where ρ_o is the mass density of the host material and ρ_i the mass density of the scatterers. In Figure 3 we show the inverse periodic arrangement of Figure 2, where copper spheres are periodically placed in epoxy (copper volume fraction $f = 0.3$). The characteristic of this composite is the very low ρ_o/ρ_i ratio. As one can see in Figure 3 there is a relatively wide gap with midgap frequency at $\omega a/c_o \approx 2.75$. In contrast, in the opposite case (of high ρ_o/ρ_i - see Figure 2) no gaps exist. In general, we found that for solid composites (solid scatterers in solid host) gap formation is favored by high density scatterers in low density host. And the higher this density contrast is, the wider the gap.

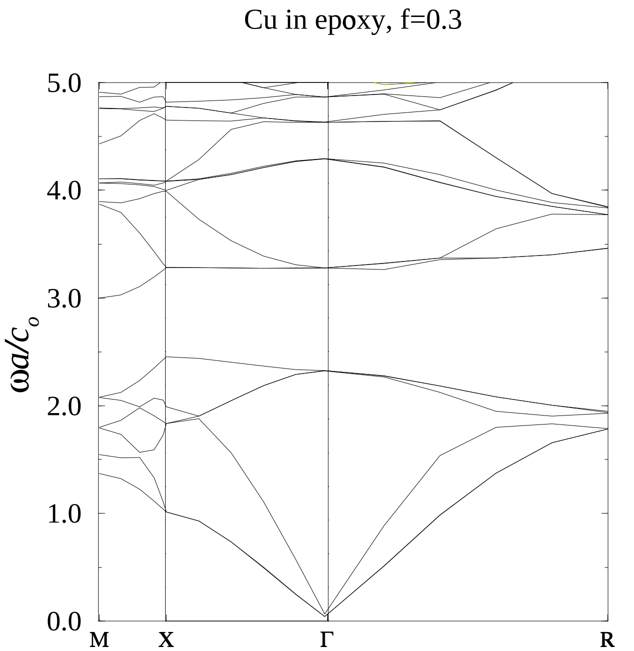

Figure 3: Dispersion relation along the directions MXΓR for a sc periodic composite consisting of Cu spheres in epoxy in volume fraction $f = 30\%$. c_o is the longitudinal wave velocity in the epoxy and a the lattice constant.

The opposite is true for fluid composites (fluid scatterers in fluid host). There, gap formation is favored by low density scatterers in high density host. A composite with this characteristic is shown in Figure 4. Figure 4 shows the dispersion relation for air bubbles in water in air volume fraction $f = 0.3$. The bubbles are arranged in fcc structure [16]. Here one can see a succession of very wide gaps alternating with some extremely narrow bands (these bands correspond to resonance frequencies in the scattering cross section by a single air sphere in water). In contrast, the inverse arrangement (water spheres in air) does not exhibit any gap.

The difference between solid and fluid composites regarding the dependence of the gap on the density contrast can be understood if one considers the single scattering cross section: For fluids, it is the isotropic term in the single scattering which is responsible for the strong scattering and thus for the gap. This term is almost absent in solids. This isotropic scattering term becomes very strong when the ratio ρ_i/ρ_o is very low, because the low density sphere can be easily compressed by the surrounding fluid medium.

Another parameter which affects the appearance of gaps is the velocity contrast between scatterers and host. In the absence of density contrast we have found that gap formation is favored by low velocity scatterers in high velocity host. In the presence of density contrast, however, the role

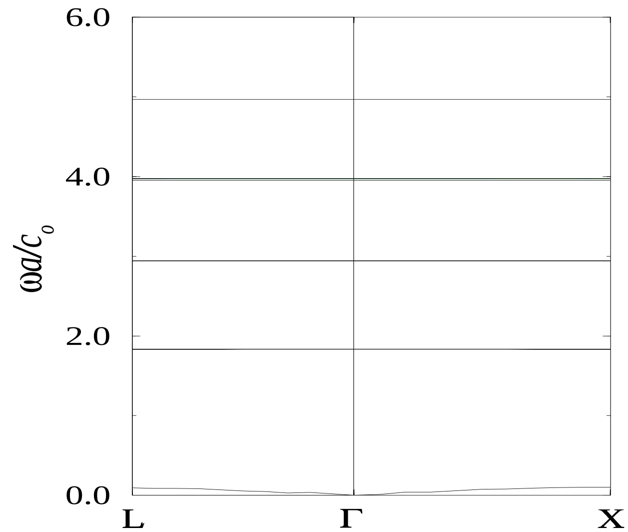

Figure 4: Dispersion relation along the directions LΓX for a fcc periodic composite consisting of air bubbles in water. Air volume fraction $f = 30\%$. c_o is the wave velocity in the water and a the lattice constant.

of the velocity contrast is more complicated. For large density contrast it is preferable for the velocity contrast to be small. Again it can be understood by studying the single scattering cross-section [17].

Concerning the rigidity of the scatterers: the rigidity of the scatterers seems to affect the dispersion relation only when both density and velocity contrasts between scatterers and host are very low. If one of these parameters starts to become important, then solid scatterers give almost the same dispersion relation with fluid scatterers of the same density and velocity.

Finally we examined the dependence of the gap on the scatterers volume fraction. In Figure 5 we show the width of the gap over the midgap frequency versus the volume fraction of the scatterers for a composite consisting of lead spheres in epoxy in various periodic arrangements. From Figure 5 and analogous figures one can see that the optimum for gap volume fraction is between 10% and 50%.

5 Conclusions

We studied the propagation of acoustic and elastic waves in periodic composites consisting of spherical scatterers in a host material. Our aim was to examine if and under what conditions one can observe stop bands in these composites. This was done through dispersion relation calculations. To calculate the dispersion relation we have employed two methods and a simple parallelization procedure. We found that gaps can exist under rather extreme conditions, which concern mainly the density and velocity contrast of the components of the composites and the volume fraction of one of the two components. For solid systems (or for solid host systems) gap formation is favored by high density scatterers in low density host, while for fluids by low density scatterers in low density host. Also gap forma-

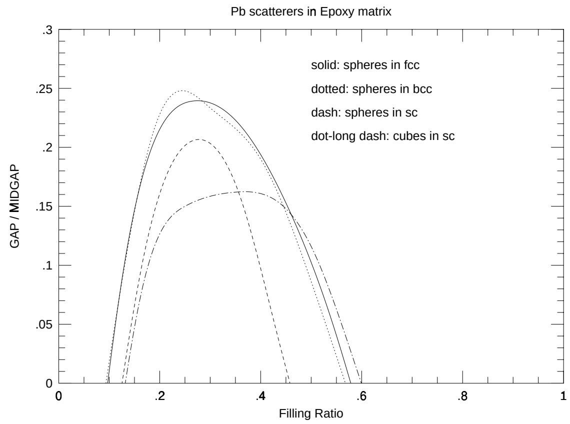

Figure 5: The width of the gap over the midgap frequency versus the volume fraction of the scatterers for a periodic composites consisting of lead spheres in epoxy.

tion is favored by scatterers with velocity lower than that of the host and scatterers volume fraction between 10% and 50%.

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APPENDIX: Transformations of elementary spherical functions.

$$h_l(k_o|\mathbf{r}-\mathbf{D}|)Y_{lm}(\mathbf{r}-\mathbf{D}) = \sum_{l'm'} j_{l'}(k_o r)Y_{l'm'}(\mathbf{r})g_{l'm'lm}(\mathbf{D}) \quad \text{for } |\mathbf{r}| < |\mathbf{D}|, \tag{A.1}$$

where

$$g_{l'm'lm}(\mathbf{D}) = \sum_{LM} (-1)^{(l'-l-L)/2} 4\pi C_{l'm'lmLM} h_L(kD)Y_{LM}(\mathbf{D}). \tag{A.2}$$

$C_{l'm'lmLM}$ are the Gaunt numbers [19]:

$$C_{l'm'lmLM} = \int Y_{l'm'}(\mathbf{r})Y^*_{lm}(\mathbf{r})Y_{LM}(\mathbf{r})d\Omega_{\mathbf{r}}. \tag{A.3}$$

For given l, m, l', m' the only value of M that gives non zero $C_{l'm'lmLM}$ is $M = m - m'$. Thus, the double sum in (A.2) is in fact a sum only over L, with $M = m - m'$.

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