AN ALGORITHM FOR COMPUTING FUNDAMENTAL SOLUTIONS OF DIFFERENCE OPERATORS

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Abstract. We propose an FFT-based algorithm for computing fundamental solutions of difference operators with constant coefficients. Our main contribution is to handle cases where the symbol has zeros.

Key words. Discrete fundamental solutions, fast Fourier transform

AMS subject classifications. Primary 65T50, 39A70; Secondary 65N22, 65F10

1. Background.

Fundamental solutions play an important role in the theory of linear partial differential equations. Among other things, fundamental solutions can be used to prove existence and investigate regularity of solutions, see for example the work by Hörmander, in particular [10].

Fundamental solutions have the potential of playing an equally important role in the theory of difference equations, although this area of research has not achieved the same amount of attention. One important result however, is due to de Boor, Höllig, and Riemenschneider. In 1989, they proved that every partial difference operator with constant coefficients has a fundamental solution that grows no faster than a polynomial [6].

But fundamental solutions are not only of theoretical interest. If a fundamental solution is explicitly known it provides a large amount of information about the solution of the differential or difference equation. The boundary element method [3] [11] utilises this fact, and so does the method of fundamental solutions [5] [12]. Our interest stems from the area of iterative solvers for systems of equations arising when discretising partial differential equations on structured grids. In [2] we introduced a convergence acceleration technique that uses fundamental solutions for constructing an efficient preconditioner.

In this paper we show that fundamental solutions of difference operators with constant coefficients can be computed using the fast Fourier transform. This is almost trivial as long as the symbol is invertible everywhere, and our main contribution is to propose a possible remedy for the problem that occurs when the symbol has zeros.

The paper is organised as follows. In Sections 2 and 3, the concept of fundamental solutions and the discrete Fourier transform is introduced. Section 4 focuses on the division problem and how to deal with symbols that have zeros. Several examples are given in Section 5. Section 6 relates discrete fundamental solutions to theory for Toeplitz matrices and the paper is ended with a summary in Section 7.

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2. Introduction. Let u be a vector function defined on the integer lattice $\mathbb{Z}^d$, and let P denote a partial difference operator with constant matrix coefficients B_k. Then,

$$(Pu)_j = \sum_{k\in\mathbb{Z}^d} B_k\, u_{j-k}, \quad j \in \mathbb{Z}^d.$$

We assume P to have finite order, thus requiring the matrix function B to have compact support. For simplicity, we use the notation

$$Pu = B * u.$$

In the scalar case "$*$" denotes the usual convolution, while its generalisation to the non-scalar case is a non-commutative operation.

A fundamental solution of P is a matrix function E that satisfies

$$B * E = \delta I, \tag{2.1}$$

where I is the identity matrix, $\delta_0 = 1$, and $\delta_j = 0$, $j \neq 0$. The theoretical interest in fundamental solutions is due to the relation

$$P(E * u) = B * (E * u) = (B * E) * u = \delta I * u = u.$$

Thus, E can be used to construct a right inverse of P. In fact, convolving with E also yields a left inverse of P, which can be proved by Fourier technique.

In this paper we show that (2.1) can be solved using fast Fourier transform. We cannot compute a solution in all of $\mathbb{Z}^d$, and require (2.1) to be fulfilled only in a box

$$\Omega_m = \{ j \in \mathbb{Z}^d \,|\, j_\nu = -m_\nu, -m_\nu + 1, \ldots, m_\nu - 1 \}.$$

We assume the support of B to be contained in this box, and consider the problem:
Problem. Find a matrix function E that satisfies (2.1) for every $j \in \Omega_m$.

Note that there are many solutions to (2.1). If E is a fundamental solution and U satisfies $B * U = 0$, then $E + U$ is also fundamental solution. To determine E uniquely, we need to specify boundary conditions. One possibility is to use periodic boundary conditions, which are implicitly imposed by the Fourier transform.

3. The discrete Fourier transform. The discrete Fourier transform $\widehat{u}$ of a $2m$-periodic function u is given by

$$\widehat{u}_k = \sum_{j\in\Omega_m} u_j\, e^{-\pi i\left(\frac{j_1 k_1}{m_1} + \cdots + \frac{j_d k_d}{m_d}\right)}, \quad k \in \Omega_m,$$

where

$$u_j = \frac{1}{2^d m_1 \cdots m_d} \sum_{k\in\Omega_m} \widehat{u}_k\, e^{\pi i\left(\frac{j_1 k_1}{m_1} + \cdots + \frac{j_d k_d}{m_d}\right)}.$$

Both the transform and its inverse can be computed by the fast Fourier transform algorithm in $\mathcal{O}(m_1 \cdots m_d \log(m_1 \cdots m_d))$ arithmetic operations.

The formula

$$\widehat{u * v} = \widehat{u}\,\widehat{v},$$

where u and v are scalar functions, is widely used for computing convolutions. It holds also more generally, and

$$\widehat{Pu} = \widehat{B * u} = \widehat{B}\,\widehat{u}, \tag{3.1}$$

where $\widehat{B}$ is known as the symbol of P.

4. The division problem. If the symbol of P is nonsingular for every $k \in \Omega_m$, E can easily be computed using Fourier technique. To see how, consider the transform of (2.1), that is

$$\widehat{B}\widehat{E} = \widehat{\delta} I. \tag{4.1}$$

Solving this matrix problem for every $k \in \Omega_m$ gives $\widehat{E}$, and the inverse Fourier transform yields the result.

However, if the symbol of P is singular at some point k', it is no longer possible to invert the matrix $\widehat{B}_{k'}$ which is needed to compute $\widehat{E}_{k'}$.

Looking for solutions of (4.1) is a problem known as the division problem. It was originally posed by Schwarz [13], who studied partial differential equations using Fourier technique. Given scalar distributions φ and ψ, he asked if it is possible to find another distribution u that satisfies

$$\varphi\, u = \psi. \tag{4.2}$$

In 1958, Hörmander proved the existence of a tempered distribution that solves (4.2) when φ is a polynomial, and as a direct consequence, the existence of a tempered fundamental solution [9]. The result by de Boor, Höllig, and Riemenschneider on the existence of a well behaved fundamental solution for difference operators with constant coefficients occurred thirty years later [6].

Unfortunately, none of this theory is constructive and it does not give any directions on how to actually compute a fundamental solution. The following theorem is more relevant in our context.

THEOREM 4.1. *Equation (2.1) with periodic boundary conditions has a unique solution if and only if the symbol is nonsingular for every $k \in \Omega_m$.*

Proof. It follows from (3.1) that every $2m$-periodic solution to $B * E = \delta I$ has a transform $\widehat{E}$ that satisfies $\widehat{B}\widehat{E} = \widehat{\delta} I$, $\forall k \in \Omega_m$. Conversely, every $\widehat{E}$ that satisfies $\widehat{B}\widehat{E} = \widehat{\delta} I$, $\forall k \in \Omega_m$, has an $2m$-periodic inverse transform E that solves $B * E = \delta I$. Therefore, if one of the problems has a unique solution, so does the other. □

Thus, the division problem indicates that the difference equation (2.1) is ill posed with periodic boundary conditions. As a consequence, it is natural to propose the following remedy.

Remedy. Replace the periodic boundary conditions in one of the dimensions by another set of boundary conditions.

The goal is to construct a problem with a unique solution. To achieve this, it may be sufficient to alter the boundary conditions in one dimension only, which still allows for E to be computed in a fast way. The modified algorithm uses a $(d-1)$-dimensional discrete Fourier transform. Without restriction, we may assume that the transform is performed in all dimensions but the first. Applying the transform to both sides of (2.1) yields

$$\sum_{l} \tilde{B}_{l,k_2,\dots,k_d}\, \tilde{E}_{j_1-l,k_2,\dots,k_d} = \delta_{j_1} I, \quad j_1 = -m_1, \dots, m_1 - 1. \tag{4.3}$$

For every $\tilde{k} = (k_2, \dots, k_d)$, this is an ordinary difference equation with constant coefficients. As long as we are able to provide boundary conditions such that all of the difference equations (4.3) have unique solutions, the corresponding coefficient matrices are nonsingular band matrices. Hence, by using a direct band solver, it is possible to compute the solution of each system in $\mathcal{O}(q^2\, m_1)$ arithmetic operations, where q is the bandwidth. Once $\tilde{E}$ has been computed, E is given by a $(d-1)$-dimensional inverse discrete Fourier transform.

The following is an analogue of Theorem 4.1. The proof is similar and is left out.

THEOREM 4.2. *Assume that a set of boundary conditions is imposed on (4.3). The resulting difference equation has a unique solution for every $\tilde{k}$ if and only if there exists a unique fundamental solution to P that is periodic in $d-1$ dimensions and satisfies the given set of boundary conditions in the remaining dimension.*
The importance of Theorem 4.2 is that we instead of proving that the partial difference equation (2.1) has a unique solution when a certain set of boundary conditions is provided, we may study an ordinary difference equation with constant coefficients. For the latter problem there is a well developed theory, see for example [1].

One potential set of boundary conditions is initial conditions. They are attractive since $\tilde{E}$ then can be computed by explicit time-stepping. Also, from the theory of ordinary difference equations we know that an initial value problem

$$\begin{aligned} B_0 u_j + \cdots + B_n u_{j+n} &= f_j, \quad j = 0, 1, \dots \\ u_0 &= c_0, \\ &\vdots \\ u_{n-1} &= c_{n-1}, \end{aligned}$$

has a unique solution if $\det(B_n) \neq 0$, which is a condition far less restrictive then requiring the symbol $\widehat{B}$ to be nonsingular everywhere.

For some applications, it may be preferable to put boundary conditions at both sides of the interval. Proving uniqueness is then slightly more difficult, but a sparse solver still provides a fast method of solution.

In many applications, it is not only of interest to prove that the algorithm suggested in this section succeeds in finding a fundamental solution, that is, the existence of a fundamental solution satisfying a certain set of boundary conditions. It may also be of interest to study a sequence of operators, and the norm of the corresponding fundamental solutions. For two of the examples in the next section we perform such a study.

5. Examples. In this section, we give two examples where we avoid the division problem by using the remedy proposed in Section 4. We also give an example that shows that it is not always possible to find boundary conditions such that (4.3) has a unique solution.

5.1. A convection operator. Let $m_1 = m_2 \equiv m$ and define $h = 1/m$. The scalar difference operator P given by

$$(Pu)_j = \frac{u_{j_1,j_2} - u_{j_1-1,j_2}}{h} + \frac{u_{j_1,j_2} - u_{j_1,j_2-1}}{h}$$

is a finite difference approximation of the differential operator $\partial/\partial x_1 + \partial/\partial x_2$.

The symbol

$$\widehat{B}_k = (2 - e^{-\pi i k_1/m} - e^{-\pi i k_2/m})/h$$

has a zero at $k = 0$ and cannot be inverted at that point. Note that every constant function u satisfies both $Pu = 0$ and the periodic boundary conditions imposed by the discrete Fourier transform. Thus, neither does the difference equation have a unique solution, nor is the symbol invertible everywhere, a result consistent with Theorem 4.1.

Following the ideas of Section 4, we replace the periodic boundary conditions in the first dimension by another set of boundary conditions and consider

$$\begin{array}{lcll} (PE)_{j_1,j_2} & = & \delta_{j_1,j_2}, & j_1, j_2 = -m, \ldots, m-1, \\ E_{-m-1,j_2} & = & 0, & j_2 = -m, \ldots, m-1, \\ E_{j_1,-m-1} & = & E_{j_1,m-1}, & j_1 = -m, \ldots, m-1. \end{array} \tag{5.1}$$

To see that this problem has a unique solution, we apply the discrete Fourier transform in the second dimension. The result,

$$\begin{array}{rcl} (2 - e^{-\pi i k_2/m})\widetilde{E}_{j_1} - \widetilde{E}_{j_1-1} & = & h\,\delta_{j_1}, \quad j_1 = -m, \ldots, m-1, \\ \widetilde{E}_{-m-1} & = & 0, \end{array}$$

is a set of initial value problems. Since $2 - e^{-\pi i k_2/m}$ is different from zero for every $k_2 = -m, \ldots, m-1$, all problems can be solved by explicit time-stepping and we conclude that they have unique solutions. Using Theorem 4.2, we find that so does Equation (5.1), and the division problem has been avoided.

This example can be examined even further, and the following theorem shows that the particular fundamental solution generated by our algorithm is well behaved as $h^{-1} = m \to \infty$.

THEOREM 5.1. *The solution E of (5.1) satisfies $||E||_1 = 1$.* The proof is based on the following two lemmas.

LEMMA 5.2. *Let $f \geq 0$. The function u is non-negative if it satisfies*

$$\begin{array}{rcll} u_j - \frac{1}{2}u_{j-1} & = & f_j, & j = -m, \dots, m-1, \\ u_{-m-1} & = & u_{m-1}. & \end{array} \tag{5.2}$$

Proof. Extend f periodically with period $2m$. The sum $u_j = \sum_{k=0}^{\infty} 2^{-k} f_{j-k}$ is convergent, solves (5.2), and is non-negative if f is. □

LEMMA 5.3. *The solution E of (5.1) is non-negative.*

Proof. Using the boundary conditions in (5.1) we see that E_{-m,j_2} satisfies (5.2) with $f \equiv 0$. Thus, according to Lemma 5.2, $E_{-m,j_2} \geq 0$. Assume $E_{j_1,j_2} \geq 0$. Then, E_{j_1+1,j_2} satisfies (5.2) with $f_{j_2} = (h\,\delta_{j_1+1,j_2} + E_{j_1,j_2})/2 \geq 0$, and according to Lemma 5.2, $E_{j_1+1,j_2} \geq 0$. The proof follows by induction. □

We are now prepared to prove Theorem 5.1.

Proof. According to Lemma 5.3, E is non-negative. Therefore,

$$||E||_1 \equiv \sum_{j_1=-m}^{m-1} \sum_{j_2=-m}^{m-1} |E_{j_1,j_2}| = \sum_{j_1=-m}^{m-1} \sum_{j_2=-m}^{m-1} E_{j_1,j_2}.$$

From (5.1), basic properties of the δ-function, and the periodicity of E follows that

$$\begin{aligned} 2\sum_{j_2=-m}^{m-1} E_{j_1,j_2} &= \sum_{j_2=-m}^{m-1} (h\,\delta_{j_1,j_2} + E_{j_1-1,j_2} + E_{j_1,j_2-1}) \\ &= h\,\delta_{j_1} + \sum_{j_2=-m}^{m-1} E_{j_1-1,j_2} + \sum_{j_2=-m}^{m-1} E_{j_1,j_2}, \end{aligned}$$

or equivalently,

$$\sum_{j_2=-m}^{m-1} E_{j_1,j_2} = h\,\delta_{j_2} + \sum_{j_2=-m}^{m-1} E_{j_1-1,j_2}.$$

Since $E_{-m-1,j_2} = 0$, this implies that

$$\sum_{j_2=-m}^{m-1} E_{j_1,j_2} = \begin{cases} 0, & j_1 = -m, \dots, -1 \\ h, & j_1 = 0, \dots, m-1 \end{cases},$$

and we conclude that $||E||_1 = mh = 1$. □ The numerical results in Table 5.1 show that Theorem 5.1 holds also for the fundamental solution of the d-dimensional difference operator

$$(Pu)_j = \sum_{\nu=1}^{d} \frac{u_{j_1,\cdots,j_\nu,\cdots,j_d} - u_{j_1,\cdots,j_\nu-1,\cdots,j_d}}{h}.$$

TABLE 5.1
The norm of E as a function of d, when $h = 1/8$.

d	2	3	4	5	6
$\|\|E\|\|_1$	1	1	1	1	1

5.2. The Euler equations. In two space dimensions, the steady state solution of the linearised Euler equations for compressible isentropic flow satisfies

$$A_{1,0}\frac{\partial u}{\partial x_1} + A_{0,1}\frac{\partial u}{\partial x_2} = 0, \tag{5.3}$$

where

$$A_{1,0} = \begin{pmatrix} v_1 & c & 0 \\ c & v_1 & 0 \\ 0 & 0 & v_1 \end{pmatrix} \quad \text{and} \quad A_{0,1} = \begin{pmatrix} v_2 & 0 & c \\ 0 & v_2 & 0 \\ c & 0 & v_2 \end{pmatrix}.$$

Here, $u = (\rho, u_1, u_2)^T$ is the departure from $v = (r, v_1, v_2)^T$, and c is the speed of sound.

Discretising the operator given by (5.3) using second order centred finite differences and second order artificial viscosity of strength γ yields

$$\begin{aligned}(Pu)_j =& \frac{1}{2h_1}(A_{1,0} - \gamma I)u_{j_1+1,j_2} - \frac{1}{2h_1}(A_{1,0} + \gamma I)u_{j_1-1,j_2} \\ &+ \frac{1}{2h_2}(A_{0,1} - \gamma I)u_{j_1,j_2+1} - \frac{1}{2h_2}(A_{0,1} + \gamma I)u_{j_1,j_2-1} \\ &+ (\frac{\gamma}{h_1} + \frac{\gamma}{h_2})u_{j_1,j_2},\end{aligned}$$

where $h_1 = 1/m_1$ and $h_2 = 1/m_2$. The symbol

$$\begin{aligned}\widehat{B}_k =& \frac{1}{2h_1}\Big((A_{1,0} - \gamma I)e^{\pi i k_1/m_1} + 2\gamma I - (A_{1,0} + \gamma I)e^{-\pi i k_1/m_1}\Big) \\ &+ \frac{1}{2h_2}\Big((A_{0,1} - \gamma I)e^{\pi i k_2/m_2} + 2\gamma I - (A_{0,1} + \gamma I)e^{-\pi i k_2/m_2}\Big)\end{aligned}$$

cannot be inverted at $k = 0$. Therefore, we proceed as suggested in Section 4 and apply the transform in the second dimension only,

$$\begin{aligned}&\frac{1}{2h_1}(A_{1,0} - \gamma I)\widetilde{E}_{j_1+1} \\ &+ \frac{1}{2h_2}\Big((A_{0,1} - \gamma I)e^{\pi i k_2/m_2} + 2\gamma(1 + h_2/h_1)I - (A_{0,1} + \gamma I)e^{-\pi i k_2/m_2}\Big)\widetilde{E}_{j_1} \\ &- \frac{1}{2h_1}(A_{1,0} + \gamma I)\widetilde{E}_{j_1-1} = \delta_{j_1}, \qquad j_1 = -m_1, \dots, m_1 - 1.\end{aligned} \tag{5.4}$$

For every $k_2 = -m_2, \dots, m_2 - 1$, this is a system of ordinary difference equations with constant coefficients. If $v_1 \neq \gamma$ and $v_1 - \gamma \neq \pm c$, then $\det(A_{1,0} - \gamma I) \neq 0$, and (5.4) with initial conditions

$$\widetilde{E}_{-m_1-2} = \widetilde{E}_{-m_1-1} = 0,$$

has a unique solution.

In Table 5.2, the l_1-norm

$$\|E\|_1 \equiv \sum_{j_1=-m_1}^{m_1-1} \sum_{j_2=-m_2}^{m_2-1} \|E_{j_1,j_2}\|_1$$

has been computed numerically for different grid sizes. Here, $v_1 = v_2 = 1$, $c = 2$, $\gamma = 1/32$, and $h_1 = h_2 = h$.

In contrast to the example in the previous section, the norm of the fundamental solution is now increasing exponentially when the grid is refined. On the other hand, numerical experiments show that if we instead use the boundary conditions

$$\widetilde{E}_{-m_1-1} = \widetilde{E}_{m_1} = 0,$$

the norm actually decreases as a function of $1/h$, see Table 5.2. Thus, the example in this section illustrates the importance of choosing boundary conditions not only in such a way that (2.1) has a unique solution, but also so that it depends continously of the data of the problem.

Table 5.2
The norm $||E||_1$ as a function of $1/h$.

$1/h$	8	16	32	64	128	256
initial conditions	$1.5 \cdot 10^{2}$	$7.3 \cdot 10^{4}$	$3.8 \cdot 10^{10}$	$2.2 \cdot 10^{22}$	$1.6 \cdot 10^{46}$	$1.5 \cdot 10^{94}$
boundary conditions	8.63	7.73	6.36	5.24	4.50	4.11

5.3. An unsolved case. The symbol

$$\widehat{B}_k = 1 - e^{\pi i k_1/m_1} - e^{\pi i k_2/m_2} + e^{\pi i (k_1/m_1 + k_2/m_2)}$$

of the operator

$$(Pu)_j = u_{j_1,j_2} - u_{j_1+1,j_2} - u_{j_1,j_2+1} + u_{j_1+1,j_2+1},$$

cannot be inverted at $k = 0$. Transforming only in the second dimension yields

$$(1 - e^{\pi i k_2/m_2})\widetilde{E}_{j_1} - (1 - e^{\pi i k_2/m_2})\widetilde{E}_{j_1+1} = \delta_{j_1}.$$

For $k_2 = 0$, this equation lacks solution no matter what boundary condition we choose, and due to symmetry of P the problem cannot by avoided by interchanging the two dimensions. Thus, there are cases where the proposed remedy fails.

6. Relation to Toeplitz matrices. A Toeplitz matrix T is a matrix with constant diagonals, i.e.

$$T = \begin{bmatrix} b_0 & b_{-1} & \cdots & b_{-n+1} \\ b_1 & b_0 & b_{-1} & \\ \vdots & \ddots & \ddots & b_{-1} \\ b_{n-1} & \cdots & b_1 & b_0 \end{bmatrix},$$

and can be considered as a finite section of the biinfinite matrix representing a one-dimensional scalar difference operator P. Then

$$(Pu)_j = \sum_{k\in\mathbb{Z}} b_k u_{j-k}.$$

For analysis and applications of Toeplitz systems, we refer to [7]. A function f is said to generate T if

$$b_j = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)e^{-ij\theta}d\theta.$$

The relation between f and the symbol of P, $\hat{b}$, can be specified if the latter is considered as a function of a continuous variable by letting $\theta = \pi k/m$. Integrating yields

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{b}(\theta)e^{-ij\theta}d\theta = \frac{1}{2\pi}\int_{-\pi}^{\pi}\sum_{k=-m}^{m-1} b_l e^{-ik\theta}e^{-ij\theta}d\theta$$

$$= \sum_{k=-m}^{m-1}\frac{1}{2\pi}b_k\int_{-\pi}^{\pi} e^{-i(k+j)\theta}d\theta = \begin{cases} b_{-j}, & j=-m,\ldots,m-1 \\ 0, & \text{otherwise}, \end{cases}$$

and we find that $\hat{b}(-\theta)$ generates T. In other words, we have found a function f that generates T and at the same time satisfies

$$f(\pi k/m)\hat{E}_k = 1, \quad k=-m,\ldots,m-1,$$

which, since $\hat{\delta} = 1$, is a scalar case of (4.1).

The function $1/f$ has been used to generate an approximate inverse of a given Toeplitz matrix. In [4] by R. Chan and Ng, $1/f$ is used explicitly, and $1/f(\theta_0)$ is replaced by zero when $f(\theta_0) = 0$. Our remedy to the problem with symbols with zeros is not applicable, since the systems considered have pure Toeplitz structure, corresponding to one-dimensional scalar difference operators.

In [8] by Hanke and Nagy, the relation to f is more implicit, but the division problem occurs also there, and it is treated in a similar way as in [4]. One important difference is that the method in [8] is applied to block Toeplitz matrices with Toeplitz blocks, corresponding to two-dimensional scalar difference operators. Hence, our method could be worth considering.

The relation between Toeplitz matrices and difference operators is easily generalised to several dimensions. A d-dimensional difference operator P with constant matrix coefficients corresponds to a $(d+1)$-level block matrix, where the d outer block levels have Toeplitz structure, and the innermost level have blocks which are identical to the matrix coefficients of P. A generalised lexicographical ordering of the lattice points is assumed.

7. Summary. We propose an FFT-based algorithm for computing fundamental solutions of difference operators with constant coefficients. This is easy as long as the symbol of the difference operator is invertible everywhere, and our main contribution is to introduce a remedy for cases where the symbol has zeros.

The discrete Fourier transform imposes periodic boundary conditions, and the idea in this paper is to replace these conditions in one of the dimensions by another set of boundary conditions. The fundamental solution can then still be computed by a fast algorithm. We show that it is sufficient to investigate an ordinary difference equation when deciding on the new set of boundary conditions.

We investigate the norm of the fundamental solution for two different model problems, and a grid refinement study shows that in both cases, fundamental solutions that are bounded with respect to the grid parameter are found.

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