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To cite this version:
Naum Khutoryansky. Explicit Stencil Computation Schemes Generated by Poisson’s Formula for the 2D Wave Equation. 2019. hal-02091615v2

HAL Id: hal-02091615
https://hal.archives-ouvertes.fr/hal-02091615v2
Submitted on 2 May 2019

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Explicit Stencil Computation Schemes Generated by Poisson’s Formula for the 2D Wave Equation.

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Abstract

An approach to building explicit time-marching stencil computation schemes for the transient 2D acoustic wave equation without using finite-difference approximations is proposed and implemented. It is based on using the integral representation formula (Poisson’s formula) that provides the exact solution of the initial-value problem for the transient 2D scalar wave equation at any time point through the initial conditions. For the purpose of constructing a two-step time-marching algorithm, a modified integral representation formula involving three time levels is also employed. It is shown that integrals in the two representation formulas are exactly calculated if the initial conditions and the sought solution at each time level as functions of spatial coordinates are approximated by stencil interpolation polynomials in the neighborhood of any point in a 2D Cartesian grid. As a result, if a uniform time grid is chosen, the proposed time-marching algorithm consists of two numerical procedures: 1) the solution calculation at the first time-step through the initial conditions; 2) the solution calculation at the second and next time-steps using a generated two-step numerical scheme.

Three particular explicit stencil schemes (with five, nine and 13 space points) are built using the proposed approach. Their stability regions are presented. The obtained stencil expressions are compared with the corresponding finite-difference schemes available in the literature. Their novelty features are discussed. Simulation results with new and conventional schemes are presented for two benchmark problems that have exact solutions. It is demonstrated that using the new first time-step calculation procedure instead of the conventional one can provide a significant improvement of accuracy even for later time steps.

Keywords: Transient 2D acoustic wave equation, Initial-boundary value

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1. Introduction

Stencil computations are widely implemented in many numerical algorithms that involve structured grids, including finite-difference techniques in such diverse areas as acoustics, fluid dynamics, solid mechanics and electromagnetism. Classical methods to obtain finite-difference approximations of their governing partial differential equations are mostly based on Taylor expansions. However, for some stencils with multiple nodes, coefficients of these approximations cannot be uniquely determined without additional conditions (see, e.g., [8]) which creates competing finite-difference schemes for the same problem of interest and for the same set of stencil nodes.

In an explicit finite-difference scheme, a solution value at each point in a time-space grid is calculated using a linear combination of values at its spatial neighbors from previous time steps. Among the explicit schemes for the transient 2D wave equation the main attention in the literature has been given to two-step schemes (which operate over three time levels $t_{k+1} = (k + 1) \tau$, $t_k = k \tau$ and $t_{k-1} = (k - 1) \tau$ where $\tau$ is a fixed time increment). They have been intensively studied and reviewed in many articles and books (see, e.g., [4, 8, 2, 3, 13, 10]).

Due to the above mentioned uncertainties that building finite-difference schemes for the transient 2D wave equation can encounter, it is reasonable to consider building explicit stencil computation schemes for this equation based on principles different from the finite-difference approximation of differential operators. There are very few papers in this direction. An integral evolution formula that can be useful for building two-step schemes was derived in [1]. This formula was implemented in [11] for the 2D case using a least square piecewise polynomial approximation and quadrature algorithm but for the sake of simplicity ignoring the first time-step issues ("startup issues").

The two-step schemes pose some challenges when imposing the initial conditions. To calculate the value of a sought solution $u$ at the first time level $t_1$, one needs values of $u$ from time levels $t_0$ and $t_{-1}$. The initial condition for $u$ provides the required values at $t_0$. The needed information at the earlier time $t_{-1}$ must be inferred. The initial condition for $v = \partial u / \partial t$ can be used to do this in different ways [13]. The conventional approach described in many textbooks (see, e.g., [10]) uses the central difference for approximating that initial condition. For
any point \( x \) in \( \mathbb{R}^2 \), the value of \( u(x, t-1) \) is inferred as \( u(x, t_1) - 2\tau v(x, 0) \). Even though this add-hoc approach is attractive due to its simplicity, it is worthwhile to consider the numerical schemes for both the first time step and the other steps in the framework of a unified approach.

This paper focuses on building explicit time-stepping stencil computation schemes for the transient 2D acoustic (scalar) wave equation without using finite-difference methods. The approach implemented here is based on using a famous integral representation formula (Poisson’s formula) that provides the exact solution of the initial-value problem for the transient 2D scalar wave equation at any time point through the initial conditions. For the purpose of constructing a two-step time-marching numerical scheme, a modification of Poisson’s formula involving three time levels is also employed. A general form of the proposed time-stepping algorithm is presented in section 3 where separate integral expressions are given for the first time-step and for the further steps.

A main part of the paper deals with deriving explicit stencil computation schemes from these integral expressions using polynomial interpolation on stencils and exact integration which is described in sections 4 and 5. Particular numerical schemes for 5-, 9- and 13-point stencils presented as linear combinations of node values are obtained in section 6 where exact coefficients of the linear combinations are expressed through the Courant number. For each scheme, two separate expressions are derived: 1) a one-step expression for the first time-step through the stencil interpolated initial conditions; 2) a two-step expression for the second and next time-steps. All the obtained expressions for the first time-step have not been previously presented in the literature. A generated two-step expression for the 9-point stencil is also new. In contrast, the obtained two-step expressions for 5- and 13-point stencils coincide with the corresponding finite-difference stencil expressions. It is shown by simulation that the derived numerical schemes can significantly improve accuracy of stencil computations in comparison with conventional approaches.

2. Representation formulas

Consider a Cauchy problem for the transient 2D scalar wave equation

\[
\frac{\partial^2 u}{\partial t^2} - c^2 \left( \frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) = 0, \quad u = u(x, t), \quad x = (x_1, x_2) \text{ in } \mathbb{R}^2, \quad (1)
\]

\[
u(t=0) = u_0(x), \quad \frac{\partial u}{\partial t} |_{t=0} = v_0(x). \quad (2)
\]
Its solution is given by the representation formula which is often named Poisson’s formula for the 2D wave equation [5]:

\[ u(x,t) = \frac{1}{2\pi ct^2} \int_{|y-x|^2<ct^2} t u_0(y) + t \nabla u_0(y) \cdot (y-x) + t^2 v_0(y) \sqrt{c^2 t^2 - |y-x|^2} \, dy_1 dy_2 \tag{3} \]

where \( \nabla \) denotes the gradient operator and \( y = (y_1, y_2) \in \mathbb{R}^2 \) is a variable of integration.

Rewriting the previous integral on the unit disk, we get

\[ u(x,t) = \frac{1}{2\pi} \int_{|z|<1} u_0(x+ctz) + ct \nabla u_0(x+ctz) \cdot z \sqrt{1 - |z|^2} \, dz_1 dz_2 \tag{4} \]

where \( z = (z_1, z_2) \in \mathbb{R}^2 \) is a new variable of integration.

Formulas (3) and (4) are also valid for negative \( t \) which can be proved based on the time reversal property of the wave equation. By substituting \( -t \) for \( t \) in formula (4) and changing \( z \) to \( -z \) inside its integrals, we obtain the following analog of that formula for negative time:

\[ u(x, -t) = \frac{1}{2\pi} \int_{|z|<1} u_0(x+ctz) + ct \nabla u_0(x+ctz) \cdot z \sqrt{1 - |z|^2} \, dz_1 dz_2 \tag{5} \]

The only difference between the right-hand sides of (4) and (5) is the opposite signs of the second term. So, one can eliminate this term by summing (4) and (5). Shifting the initial moment in the resulting formula from \( t = 0 \) to \( t = t_* \), we obtain the following expression involving three time points with a time increment \( \tau \):

\[ u(x, t_* + \tau) + u(x, t_* - \tau) = \frac{1}{\pi} \int_{|z|<1} \frac{u(x+ctz, t_*) + ct \nabla u(x+ctz, t_*) \cdot z \sqrt{1 - |z|^2} \, dz_1 dz_2}{\sqrt{1 - |z|^2}} \tag{6} \]

where the right-hand side does not include the time derivative \( v \). A similar representation formula involving three time levels has been derived (in a different form) in [1].

Both formulas (4) and (6) will be used below to build a time-marching stencil computation algorithm for the wave equation.
3. The proposed time-stepping algorithm in the integral operator form

Consider a uniform time grid \( \{ t_0 = 0, t_1 = \tau, \ldots, t_k = k\tau, \ldots \} \) where \( \tau \) is a fixed time-step. Denote by \( u_k(x) \) the restriction of \( u(x,t) \) to a moment \( t = t_k \). Next, denote by \( A(x, \tau) \) and \( B(x, \tau) \) the following integral operators acting on continuous functions defined in \( \mathbb{R}^2 \):

\[
A(x, \tau)f(\cdot) = \frac{1}{2\pi} \int_{|z|<1} \frac{f(x+c\tau z)+c\tau \nabla f(x+c\tau z) \cdot z}{\sqrt{1-|z|^2}} \, dz_1 \, dz_2
\]

\[
B(x, \tau)f(\cdot) = \frac{\tau}{2\pi} \int_{|z|<1} \frac{f(x+c\tau z)}{\sqrt{1-|z|^2}} \, dz_1 \, dz_2
\]

The time-stepping algorithm proposed in this paper consists of two procedures based on the representation formulas (4) and (6):

1) The procedure for the first time-step which, according to (4), calculates \( u_1(x) \) as

\[
u_1(x) = A(x, \tau)u_0(\cdot) + B(x, \tau)v_0(\cdot), x \in \mathbb{R}^2
\]

2) The procedure for the second and next time-steps which, using (6) for \( t_\ast = t_k \), calculates \( u_{k+1}(x) \) as

\[
u_{k+1}(x) = 2A(x, \tau)u_k(\cdot) - u_{k-1}(x), x \in \mathbb{R}^2, k = 1, 2, \ldots
\]

While formula (10) involves three time levels (two time-steps), formula (9) for the first time-step incorporates only two time levels (one time-step) without any finite difference approximation of the time derivative.

4. Using polynomial interpolation on stencils

Consider a two-dimensional uniform Cartesian grid \( \{(i_1h, i_2h)\} \) where \( i_1 \) and \( i_2 \) are integers, and \( h \) is the grid spacing in both directions \( x_1 \) and \( x_2 \). Suppose that the evaluation point \( x \) in formulas (9) and (10) is a grid point \( x_{ij} = (ih, jh) \). Our intention is to choose a stencil in the Cartesian grid and reduce the integral formulas (9) and (10) to linear combinations of the stencil node values of \( u_k(x) (k = 0, 1, 2, \ldots) \) and \( v_0(x) \). Such a reduction will be done by using polynomial interpolation.

Assume that a particular stencil with \( m \) nodes is chosen for polynomial interpolation. The corresponding index set \( \{(q_1, q_2)\} \) is denoted by \( Q_m \). The stencil index components \( q_1 \) and \( q_2 \) are numbered relative to the referencing point located
at the evaluation point \( x_{ij} \). So, polynomial interpolation in a neighborhood of the evaluation point \( x_{ij} \) will be carried out using interpolation points

\[
x_{ij} + x_{q_1,q_2} = x_{i+q_1,j+q_2}, \quad (q_1,q_2) \in Q_m.
\]  

(11)

Following [12] we associate with \( Q_m \) a set of \( m \) distinct bivariate monomials

\[
M_m = \{ x_1^{\alpha(q_1)} x_2^{\alpha(q_2)}, (q_1,q_2) \in Q_m \}
\]  

(12)

where

\[
\alpha(q) = \begin{cases} 
2|q| - 1 & \text{if } q < 0 \\
2q & \text{if } q \geq 0.
\end{cases}
\]  

(13)

The above function has a unique inverse function

\[
q(\alpha) = (-1)^{\alpha} \left\lfloor \frac{\alpha + 1}{2} \right\rfloor
\]  

(14)

where \([\cdot]\) is the whole part function. So, for each index value \((q_1,q_2) \in Q_m\) there exists a unique monomial from \( M_m \) and vice versa.

Consider a polynomial space \( \mathcal{P}_m \) spanned by \( M_m \). We will use only those stencils for which the Lagrange interpolation problem is unisolvent in \( \mathcal{P}_m \) (see [6]). In this case, there exists a Lagrange basis for \( \mathcal{P}_m \) that can be built as described below.

Suppose that there is an ordering imposed on the monomials in \( M_m \)

\[
\{ \mu_1(x), \ldots, \mu_m(x) \}.
\]  

(15)

The corresponding stencil nodes are numbered accordingly using (12)-(14):

\[
\{ x_{(1)}, \ldots, x_{(m)} \}.
\]  

(16)

Thus, one can compute the following matrix:

\[
D = [ \mu_i(x_{(r)}) ]_{m \times m}
\]  

(17)

If this matrix is non-singular, i.e., \( \det(D) \neq 0 \), which means that the Lagrange basis exists, then the inverse matrix

\[
C = [c_{sr}]_{m \times m} = D^{-1}
\]  

(18)
can be calculated. Its components are instrumental in expressing the Lagrange basis functions through the chosen set of monomials:

\[ L_s(x) = \sum_{r=1}^{m} c_{sr} \mu_r(x), \quad s = 1, \ldots, m. \] (19)

Once the Lagrange basis is obtained, we again need two indexes to denote the Lagrange basis functions in accordance with the two index notation for grid points. The sequence (15) defines a relationship \( s = g(\alpha_1, \alpha_2) \) between the ordinal number \( s \) and monomial exponents \( (\alpha_1, \alpha_2) \). Then, the resulting relationship between an index pair \((q_1, q_2)\) and the corresponding ordinal number \( s \) is given by the following expression:

\[ s = \gamma(q_1, q_2) = g(\alpha(q_1), \alpha(q_2)). \] (20)

where \( \alpha(\cdot) \) is specified in (13). Therefore, by introducing a new (two index) notation for the Lagrange basis functions

\[ \phi_{q_1,q_2}(x) = L_{\gamma(q_1,q_2)}(x), \] (21)

we get the interpolation formula for a continuous function \( f(x) \) in the form

\[ \tilde{f}(x) = \sum_{(q_1,q_2) \in Q_m} f_{i+q_1,j+q_2} \phi_{q_1q_2}(x) \] (22)

Even though different sets of monomials and their sequences can be employed for building Lagrange bases, we will use a particular method of monomial ordering that is described below.

Denote by \( \mathcal{M} \) the set of all monomials \( x_{1}^{\alpha_1} x_{2}^{\alpha_2} \) where \( \alpha_1 \) and \( \alpha_2 \) are natural numbers including 0. For each monomial \( x_{1}^{\alpha_1} x_{2}^{\alpha_2} \), the corresponding ordinal number \( s \) will be assigned using the following function:

\[ s = g(\alpha_1, \alpha_2) = \frac{(\alpha_1 + \alpha_2)(\alpha_1 + \alpha_2 + 1)}{2} + \begin{cases} \alpha_1 - \alpha_2 & \text{if } \alpha_2 < \alpha_1, \\ \alpha_2 - \alpha_1 + 1 & \text{if } \alpha_2 \geq \alpha_1. \end{cases} \] (23)

It is easy to prove that the function (23) provides a one-to-one correspondence between \( \mathcal{M} \) and the set of all positive natural numbers with the usual ordering. The order induced by (23) uses the total degree as the first sorting parameter (similarly to the more common graded lexicographic order) while the difference
between individual degrees with the same total degree is used as the next sorting variable.

The set $\mathcal{M}$ endowed with the order induced by (23) will be denoted by $\mathcal{M}^*$. The initial segment of $\mathcal{M}^*$ with $m$ members is denoted below by $\mathcal{M}^*_{\leq m}$. It will be shown in section 6 that such ordered monomial sets play a useful role in building particular numerical schemes.

**Example 1.** Consider building the Lagrange basis for the space of complete second degree polynomials. In this case, the monomial basis sequence ordered according to (23) is as follows:

$$\mathcal{M}^*_{\leq 6} = \{1, x_1, x_2, x_1 x_2, x_1^2, x_2^2\} \quad (24)$$

The corresponding interpolation stencil node sequence will be written according to (14) as

$$\{(0, 0), (-h, 0), (0, -h), (-h, -h), (h, 0), (0, h)\}$$

The index set $Q_6$ for this stencil is shown in Figure 1.

![Figure 1: Index set for the 6-point interpolation stencil](image-url)
Calculating matrix $D$ we get

$$D = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
0 & -h & 0 & -h & h & 0 \\
0 & 0 & -h & -h & 0 & h \\
0 & 0 & 0 & h^2 & 0 & 0 \\
0 & h^2 & 0 & h^2 & h^2 & 0 \\
0 & 0 & h^2 & h^2 & 0 & h^2
\end{bmatrix}$$

This matrix is non-singular with $\det(D) = 4h^8$. As a result, we get the Lagrange basis as

$$\phi_{0,0} = L_1 = 1 + \frac{x_1 x_2}{h^2} - \frac{x_2^2}{h^2} - \frac{x_1^2}{h^2}, \quad \phi_{-1,0} = L_2 = -\frac{x_1}{2h} - \frac{x_1 x_2}{h^2} + \frac{x_1^2}{2h^2},$$

$$\phi_{0,-1} = L_3 = -\frac{x_2}{2h} - \frac{x_1 x_2}{h^2} + \frac{x_2^2}{2h^2}, \quad \phi_{-1,-1} = L_4 = \frac{x_1 x_2}{h^2},$$

$$\phi_{1,0} = L_5 = \frac{x_1}{2h} + \frac{x_1^2}{2h^2}, \quad \phi_{0,1} = L_6 = \frac{x_2}{2h} + \frac{x_2^2}{2h^2}. \quad (25)$$

One can see that the Lagrange basis (25) includes monomials in the scaled variables $x_1/h$ and $x_2/h$ with coefficients independent of $h$.

It is worth to mention here that node $(-h,h)$ will disappear in the corresponding numerical scheme (see section 6).

5. Calculating the integrals

Let $\mathbf{x} = \mathbf{x}_{ij}$ in the integral operators (7) and (8). Without loss of generality, assume that the origin of the 2D coordinate system is located at $\mathbf{x}_{ij}$ which can be achieved by a parallel translation of coordinates. Let $f(y)$ appearing in (7) and (8) be a monomial in variables $y_1/h$ and $y_2/h$

$$\mu(y) = \left(\frac{y_1}{h}\right)^{\alpha_1} \left(\frac{y_2}{h}\right)^{\alpha_2}, \quad (\alpha_1, \alpha_2) \in \mathbb{N}^2. \quad (26)$$

Then the integrals in (7) and (8) can be exactly calculated and expressed through the Courant number

$$\lambda = \frac{c\tau}{h} \quad (27)$$

Indeed, using the table of integrals of Gradshteyn & Ryzhik [7], expressions (7) and (8) are reduced to the following exact values:

$$A(\mathbf{x}_{ij}, \tau)\mu(\cdot) = 0, \quad B(\mathbf{x}_{ij}, \tau)\mu(\cdot) = 0 \quad \text{if } \alpha_1 \text{ or } \alpha_2 \text{ are non-negative odd integers}, \quad (28)$$
A(x_{ij}, \tau)\mu(\cdot) = \frac{(\alpha_1 - 1)!!(\alpha_2 - 1)!!}{(\alpha_1 + \alpha_2 - 1)!!} \lambda^{\alpha_1 + \alpha_2},

B(x_{ij}, \tau)\mu(\cdot) = \frac{\tau}{\alpha_1 + \alpha_2 + 1} A(x_{ij}, \tau)\mu(\cdot)

(29)

if \alpha_1 and \alpha_2 are both non-negative even integers

where (\cdot)!! is the double factorial. It is assumed that (-1)!! = 1, 0!! = 1.

The above formulas allow one to exactly calculate integrals (7) and (8) when \( f(\cdot) \) is a polynomial from the Lagrange basis (see section 4).

6. Particular explicit two-step schemes

Now we can start building some numerical schemes by transforming the procedures (9) and (10) into algebraic expressions. All the functions \( u_0(x), v_0(x) \) and \( u_k(x), k = 1, 2, \ldots \) included in these procedures will be interpolated in a stencil’s center neighborhood using the same stencil nodes. The following standard notations for grid values of the solution and initial conditions will be used in the computation schemes:

\[
  u^0_{ij} = u(x_{ij}, 0), v^0_{ij} = v(x_{ij}, 0),
\]

(30)

\[
  u^k_{ij} = u(x_{ij}, k\tau), k = 1, 2, \ldots
\]

(31)

6.1. The 5-point stencil

Consider the monomial basis (24) used in example 1 and the corresponding Lagrange basis (25). Using formulas from section 5 and notation (21) we get

\[
  \begin{align*}
  A(x_{ij}, \tau)\phi_{00}(\cdot) & = 1 - 2\lambda^2, & A(x_{ij}, \tau)\phi_{-1,-1}(\cdot) & = 0, \\
  A(x_{ij}, \tau)\phi_{\pm1,0}(\cdot) & = A(x_{ij}, \tau)\phi_{0,\pm1}(\cdot) = \frac{1}{2} \lambda^2,
  \end{align*}
\]

(32)

\[
  \begin{align*}
  B(x_{ij}, \tau)\phi_{0,0}(\cdot) & = \tau(1 - \frac{2}{3}\lambda^2), & B(x_{ij}, \tau)\phi_{-1,-1}(\cdot) & = 0, \\
  B(x_{ij}, \tau)\phi_{\pm1,0}(\cdot) & = B(x_{ij}, \tau)\phi_{0,\pm1}(\cdot) = \frac{\tau}{6} \lambda^2,
  \end{align*}
\]

(33)

So, all coefficients for node \((-h, -h)\) disappear and the corresponding computational scheme contains only 5 spatial points which is shown in Figure 2.
6.1.1. A new first time-step expression

As a result, the proposed 5-point numerical scheme is as follows:

1) for the first time-step

\[ u_{ij}^1 = u_{ij}^0 + \tau v_{ij}^0 + \frac{\lambda^2}{2} \left( u_{i-1,j}^0 + u_{i+1,j}^0 + u_{i,j-1}^0 + u_{i,j+1}^0 - 4u_{ij}^0 \right) + \frac{\tau \lambda^2}{6} \left( v_{i-1,j}^0 + v_{i+1,j}^0 + v_{i,j-1}^0 + v_{i,j+1}^0 - 4v_{ij}^0 \right); \]  \hspace{1cm} (34)

2) for the second and next time-steps

\[ u_{ij}^{k+1} = 2u_{ij}^k - u_{ij}^{k-1} + \lambda^2 \left( u_{i-1,j}^k + u_{i+1,j}^k + u_{i,j-1}^k + u_{i,j+1}^k - 4u_{ij}^k \right). \hspace{1cm} k = 1, 2, \ldots \]  \hspace{1cm} (35)

The conventional approach for the 5-point stencil (described in many textbooks) uses the same procedure (35) for the second and next time-steps. However, for the first time-step, the conventional approach uses another formula (rather than (34)) based on the central difference for approximating the initial condition for \( v \) combined with (35) for \( k = 0 \) (see, e.g., [10]):

\[ u_{ij}^1 = u_{ij}^0 + \tau v_{ij}^0 + \frac{\lambda^2}{2} \left( u_{i-1,j}^0 + u_{i+1,j}^0 + u_{i,j-1}^0 + u_{i,j+1}^0 - 4u_{ij}^0 \right). \hspace{1cm} \]  \hspace{1cm} (36)
Comparing (34) and (36) one can see that the first three terms of the right-hand parts of these equations coincide, but the forth term present in the right-hand side of (34) is absent in (36). Thus, the difference between these two first time-step expressions depends on properties of $v_0(x)$. If, for example, $v_0(x)$ is a linear function of spatial coordinate, then there is no difference between (34) and (36). However, for more general cases encountered in practice, the difference may exist and can be influential from the accuracy point of view which is shown in the two examples below (subsections 6.1.2 and 6.1.3).

The stability condition for both numerical schemes utilizing (35) is well known from von Neumann stability analysis [13]:

$$\lambda \leq \lambda_{\text{max}} = \frac{\sqrt{2}}{2}. \quad (37)$$

6.1.2. Standing wave simulation

To make a numerical comparison of both approaches, we use the initial and boundary conditions corresponding to a standing wave exact solution:

$$u_e(x_1,x_2,t) = \sin(2\pi x_1) \sin(2\pi x_2) \sin(2\sqrt{2}\pi ct). \quad (38)$$

This solution creates the following pair of initial conditions for the numerical simulation:

$$u_0(x_1,x_2) = 0, \quad v_0(x_1,x_2) = 2\sqrt{2}\pi c \sin(2\pi x_1) \sin(2\pi x_2). \quad (39)$$

We consider the unit square $\Omega = [0,1]^2$ as a space region for the numerical solution and apply boundary condition $u = 0$ on $\partial\Omega$ generated by (38). In addition, we assume that $c = 1$. Let $n_t$ be the number of time-steps and $n \geq 2$ be the space discretization number related to $h$ by equation $nh = 1$. The above numerical schemes have been employed over a spatial index set $\{(i,j), 0 < i,j < n\}$ using grid boundary conditions

$$u_{0,j}^k = u_{n,j}^k = u_{i,0}^k = u_{i,n}^k = 0, \quad 0 \leq i,j \leq n, \quad k \geq 0.$$  

The accuracy of both numerical schemes have been estimated using the relative $L^2$ error defined as

$$E(n,n_t) = \left( \frac{\sum_{k=1}^{n_t} \sum_{i=0}^{n} \sum_{j=0}^{n} (u_{i,j}^k - u_e(ih,jh,k\tau))^2}{\sum_{k=1}^{n_t} \sum_{i=0}^{n} \sum_{j=0}^{n} (u_e(ih,jh,k\tau))^2} \right)^{1/2}. \quad (40)$$
The relative $L^2$ errors for the proposed new 5-point scheme (34)&(35) (based on Poisson’s formula) and the conventional one (36)&(35) are denoted by $E_{P5}(n,n_t)$ and $E_{C5}(n,n_t)$, respectively. Calculated values of $E_{P5}(n,n_t)$, $E_{C5}(n,n_t)$ and their ratio for different combinations of $n$, $n_t$ and $\lambda = 0.707$ are presented in table 1 below. For every value of $n$ used, three values of $n_t$ are considered: $n_t = 1$ (to check errors after the first step), $n_t = n$ and $n_t = 2n$ (to demonstrate the error accumulation process).

| $n$ | $n_t$ | $\lambda$ | $E_{P5}$ | $E_{C5}$ | $E_{C5}/E_{P5}$ |
|-----|-------|------------|----------|----------|-----------------|
| 10  | 1     | 0.707      | 9.0843 · 10^{-4} | 6.8938 · 10^{-2} | 75.9 |
| 10  | 10    | 0.707      | 9.1540 · 10^{-4} | 6.8945 · 10^{-2} | 75.3 |
| 10  | 20    | 0.707      | 9.1604 · 10^{-4} | 6.8945 · 10^{-2} | 75.3 |
| 20  | 1     | 0.707      | 5.4767 · 10^{-5} | 1.6636 · 10^{-2} | 304 |
| 20  | 20    | 0.707      | 5.6800 · 10^{-5} | 1.6638 · 10^{-2} | 293 |
| 20  | 40    | 0.707      | 5.7372 · 10^{-5} | 1.6638 · 10^{-2} | 290 |
| 40  | 1     | 0.707      | 3.3924 · 10^{-6} | 4.1230 · 10^{-3} | 1215 |
| 40  | 40    | 0.707      | 4.0331 · 10^{-6} | 4.1234 · 10^{-3} | 1022 |
| 40  | 80    | 0.707      | 4.4928 · 10^{-6} | 4.1234 · 10^{-3} | 918 |
| 80  | 1     | 0.707      | 2.1158 · 10^{-7} | 1.0285 · 10^{-3} | 4861 |
| 80  | 80    | 0.707      | 4.3820 · 10^{-7} | 1.0286 · 10^{-3} | 2347 |
| 80  | 160   | 0.707      | 6.5824 · 10^{-7} | 1.0286 · 10^{-3} | 1563 |

Table 1 clearly shows that the demonstrated accuracy of the new scheme is much higher than that of the conventional one with the error ratio $E_{C5}(n,n)/E_{P5}(n,n)$ exceeding $10^3$ for more dense grids. So, using the new first time-step calculation procedure instead of the conventional one is able to provide a significant increase of accuracy even for later time-steps. Observed increases of the relative $L^2$ errors from $n_t = n$ to $n_t = 2n$ are negligible (less than $10^{-6}$).
6.1.3. Simulation of a trailing wave produced by a point impulse source

Another benchmark example that we have simulated in the same space region \( \Omega = [0,1]^2 \) is a trailing wave solution for \( t \geq 0 \) corresponding to a point impulse source wave excited from the center of region \( \Omega = [0,1]^2 \) at a negative moment \( t = -d \):

\[
u_e(x_1,x_2,t) = \frac{1}{2\pi c} \frac{H(c(t+d) - r)}{\sqrt{c^2(t+d)^2 - r^2}}, \quad r = \sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2},
\]

where \( H(\cdot) \) is the Heaviside function and \( d > 0 \) is large enough to allow the corresponding wavefront to move outside of the region \( \Omega \) before \( t = 0 \). This condition is satisfied if we assume that \( cd > 1 / \sqrt{2} \). For the numerical simulation, it is assumed that the solution (41) specifies boundary values of \( u(x,t) \) on \( \partial \Omega \) and the following pair of initial conditions (setting \( c = 1 \) for the simplicity sake):

\[
u(x_1,x_2,0) = \frac{-d}{2\pi(d^2 - r^2)^{3/2}} \quad \text{in } \Omega.
\]

The resulting relative \( L^2 \) errors (40) for \( d = 0.75 \) are presented in Table 2. They show that the accuracy of the new scheme is approximately 10 times higher than that of the standard one.

| \( n \) | \( n_t \) | \( d \) | \( \lambda \) | \( E_{P5} \) | \( E_{CS} \) | \( E_{CS} / E_{P5} \) |
|------|------|------|------|------|------|-------|
| 10   | 10   | 0.75 | 0.707| 1.1478 \cdot 10^{-3} | 1.1124 \cdot 10^{-2} | 9.69   |
| 20   | 20   | 0.75 | 0.707| 3.8221 \cdot 10^{-4} | 3.8228 \cdot 10^{-3} | 10.0   |
| 40   | 40   | 0.75 | 0.707| 1.0799 \cdot 10^{-4} | 1.1281 \cdot 10^{-3} | 10.4   |
| 80   | 80   | 0.75 | 0.707| 2.8379 \cdot 10^{-5} | 3.0000 \cdot 10^{-4} | 10.6   |

6.2. A 9-point square stencil

Consider the initial segment \( \mathcal{M}_{\leq 11}^* \) of \( \mathcal{M}^* \) with the last member equal to \( x_1^2 x_2^2 \):

\[
\{1,x_1,x_2,x_1 x_2,x_1^2,x_2^2,x_1^2 x_2,x_1 x_2^2,x_1^3,x_2^3,x_1^2 x_2^2\}
\]

This set includes all the monomials of total degree \( \leq 3 \) and one monomial of total degree \( = 4 \), and is the minimal initial segment of \( \mathcal{M}^* \) that includes the bivariate
tensor-product of the monomial bases for the second degree polynomials in each spatial coordinate. The corresponding index set $Q_{11}$ is shown in Figure 3 where both solid dots and empty circles denote interpolation points. The corresponding Lagrange basis can be easily calculated using matrix (17) and presented similar to (25). However, it is preferable to avoid presenting long expressions that include 11 monomials and display only terms that will be used later. Denote by $\phi_{e,q_1,q_2}$ a part of $\phi_{q_1,q_2}$ that includes all the monomial terms with even exponents in both coordinates. Then we get

$$\phi_{0,0}^e = 1 - \frac{x_1^2}{h^2} - \frac{x_2^2}{h^2} + \frac{x_1^2 x_2^2}{h^4}, \quad \phi_{2,0}^e = \phi_{0,-2}^e = 0,$$

$$\phi_{\pm 1,0}^e = \frac{1}{2} \left( \frac{x_1^2}{h^2} - \frac{x_1^2 x_2^2}{h^4} \right), \quad \phi_{0,\pm 1}^e = \frac{1}{2} \left( \frac{x_2^2}{h^2} - \frac{x_1^2 x_2^2}{h^4} \right), \quad \phi_{\pm 1,\pm 1}^e = \frac{1}{4} \frac{x_1^2 x_2^2}{h^4}. \quad (44)$$

6.2.1. A new 9-point time-stepping scheme

It follows from the results (28) and (29) of section 5 that functions $\phi_{e,q_1,q_2}$ rather than the complete Lagrange basis will be used in building numerical schemes. Therefore, two points (-2,0) and (0,-2) (presented by empty circles in Figure 3) will disappear in the corresponding numerical scheme. The remaining nodes (solid circles in Figure 3) create the 9-point square-shaped computational stencil. Using

![Figure 3: Index set for the 11-point interpolation stencil](image-url)
(28)-(29) we obtain:

\[ A(x_{ij}, \tau) \phi_{00} (\cdot) = 1 - 2 \lambda^2 + \frac{\lambda^4}{3}, \quad A(x_{ij}, \tau) \phi_{\pm1, \pm1} (\cdot) = \frac{\lambda^4}{12}, \]

\[ A(x_{ij}, \tau) \phi_{1,0} (\cdot) = A(x_{ij}, \tau) \phi_{0,1} (\cdot) = \frac{\lambda^2}{2} - \frac{\lambda^4}{6}. \]  

\[ B(x_{ij}, \tau) \phi_{00} (\cdot) = \tau \left( 1 - \frac{2 \lambda^2}{3} + \frac{\lambda^4}{15} \right), \quad B(x_{ij}, \tau) \phi_{1,1} (\cdot) = \frac{\tau \lambda^4}{60}, \]

\[ B(x_{ij}, \tau) \phi_{1,0} (\cdot) = B(x_{ij}, \tau) \phi_{0,1} (\cdot) = \frac{\tau \lambda^2}{6} \left( 1 - \frac{\lambda^2}{5} \right). \]  

Now we can use (9) and (10) to build a new 9-point numerical scheme similar to (34)-(35). However, to avoid writing long expressions, some additional notations will be needed:

\[ \delta^k_{ij}(q_1, q_2) = u^k_{i+q_1, j+q_2} + u^k_{i-q_2, j+q_1} + u^k_{i+q_1, j-q_2} + u^k_{i+q_2, j-q_1} - 4u^k_{ij}, \]

\[ \varepsilon^0_{ij}(q_1, q_2) = v^0_{i+q_1, j+q_2} + v^0_{i-q_2, j+q_1} + v^0_{i+q_1, j-q_2} + v^0_{i+q_2, j-q_1} - 4v^0_{ij}, \]  

\[ k = 0, 1, 2, \ldots. \]  

Thus, the following time-stepping numerical scheme is derived:

1) for the first time-step

\[ u^1_{ij} = u^0_{ij} + \tau v^0_{ij} + \frac{\lambda^2}{2} \left[ \left( 1 - \frac{\lambda^2}{3} \right) \delta^0_{ij}(1,0) + \frac{\lambda^2}{6} \delta^0_{ij}(1,1) \right] + \frac{\tau \lambda^2}{6} \left[ \left( 1 - \frac{\lambda^2}{5} \right) \varepsilon^0_{ij}(1,0) + \frac{\lambda^2}{10} \varepsilon^0_{ij}(1,1) \right]; \]  

2) for the second and next time-steps

\[ u^{k+1}_{ij} = 2u^k_{ij} - u^{k-1}_{ij} + \lambda^2 \left[ \left( 1 - \frac{\lambda^2}{3} \right) \delta^k_{ij}(1,0) + \frac{\lambda^2}{6} \delta^k_{ij}(1,1) \right], \quad k = 1, 2, \ldots. \]  

A von Neumann stability analysis (see, e.g., [13]) provides the stability condition for the above numerical scheme as

\[ \lambda \leq \lambda_{\text{max}} = \frac{\sqrt{3} - \sqrt{3}}{2} \approx 0.796. \]  

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To our knowledge this numerical scheme has not been presented previously in the literature. A conventional explicit nine-point square-shaped scheme (dubbed the isotropic scheme (see, e.g., [14]) has a different form obtained using a 9-point finite difference approximation of the Laplace operator in the two-dimensional space [9]:

\[
  u_{ij}^{k+1} = 2u_{ij}^k - u_{ij}^{k-1} + \lambda^2 \left[ \frac{2}{3} \delta_{ij}^k(1,0) + \frac{1}{6} \delta_{ij}^k(1,1) \right], \quad k = 1, 2, \ldots \quad (51)
\]

Comparing the coefficients in (49) and (51) it is easy to see that the term \( \delta_{ij}^k(1,1) \) is less influential in the new 9-point scheme than in the conventional 9-point scheme (with a coefficient ratio equal to \( \lambda^2 \)). The stability condition for the conventional scheme is less restrictive than for the new one: \( \lambda \leq \lambda_{\text{max}} = \sqrt{3}/2 \approx 0.866 \). On the other hand, the new scheme has some accuracy advantages in comparison with the conventional 9-point approach for \( \lambda \leq 0.796 \) which is shown in the next subsection.

6.2.2. Numerical simulation

We consider simulation results for the proposed 9-point scheme (48)-(49) using initial and boundary conditions generated by the exact solutions of the previous subsection. Let \( c = 1 \). We assume that the unit square \( \Omega = [0,1]^2 \) is used as a space grid region, the time grid interval is \( [0, \lambda] \) with \( n_t = n \). A comparison is made with simulated results on the same grids for the conventional scheme (51). Even though no expression for the first time-step corresponding to the conventional 9-point scheme is presented in [14], the usual approach based on the central difference for approximating the initial condition for \( v \) combined with (51) provides the corresponding expression

\[
  u_{ij}^1 = u_{ij}^0 + \tau v_{ij}^0 + \frac{\lambda^2}{2} \left[ \frac{2}{3} \delta_{ij}^0(1,0) + \frac{1}{6} \delta_{ij}^0(1,1) \right] \quad (52)
\]

which is used for numerical simulation.

In addition, simulation results are provided for the new scheme (49) but using instead of (48) the conventional approach based on the central difference for approximating the initial condition for \( v \). The corresponding first time-step expression has the form

\[
  u_{ij}^1 = u_{ij}^0 + \tau v_{ij}^0 + \frac{\lambda^2}{2} \left[ \left( 1 - \frac{\lambda^2}{3} \right) \delta_{ij}^0(1,0) + \frac{\lambda^2}{6} \delta_{ij}^0(1,1) \right] \quad (53)
\]

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which coincides with (48) if the fourth term in its right-hand side is omitted.

The simulation results are presented in the next two tables and cover both standing wave and trailing wave simulations. We have used two values for the simulation: $\lambda = 0.707$, as in subsection 6.1, and $\lambda = 0.796$, according to the stability condition (50). Relative $L^2$ errors for the schemes (48)$&(49)$, (53)$&(49)$ and (52)$&(51)$ are denoted by $E_{P9}$, $E_{CP9}$ and $E_{C9}$, respectively. According to the simulated data, the new scheme (48)$&(49)$ appears to be more accurate than the other two schemes for both $\lambda = 0.707$ and $\lambda = 0.796$. A demonstrated higher accuracy of the scheme (48)$&(49)$ in comparison with (53)$&(49)$ emphasizes the importance of using the new first time-step procedure instead of the conventional one.

| $n$ | $n_t$ | $\lambda$ | $E_{P9}$   | $E_{CP9}$ | $E_{C9}$   |
|-----|-------|------------|------------|------------|------------|
| 10  | 10    | 0.707      | 3.7058$\cdot$10$^{-2}$ | 8.8235$\cdot$10$^{-2}$ | 1.1741$\cdot$10$^{-1}$ |
| 10  | 10    | 0.796      | 2.9587$\cdot$10$^{-2}$ | 9.6096$\cdot$10$^{-2}$ | 1.1241$\cdot$10$^{-1}$ |
| 20  | 20    | 0.707      | 8.9333$\cdot$10$^{-3}$ | 2.1304$\cdot$10$^{-2}$ | 2.8002$\cdot$10$^{-2}$ |
| 20  | 20    | 0.796      | 8.0697$\cdot$10$^{-3}$ | 2.3410$\cdot$10$^{-2}$ | 2.7523$\cdot$10$^{-2}$ |
| 40  | 40    | 0.707      | 2.3723$\cdot$10$^{-3}$ | 5.2683$\cdot$10$^{-3}$ | 6.8821$\cdot$10$^{-3}$ |
| 40  | 40    | 0.796      | 2.5737$\cdot$10$^{-3}$ | 5.8296$\cdot$10$^{-3}$ | 6.8668$\cdot$10$^{-3}$ |
| 80  | 80    | 0.707      | 7.5573$\cdot$10$^{-4}$ | 1.3119$\cdot$10$^{-3}$ | 1.7084$\cdot$10$^{-3}$ |
| 80  | 80    | 0.796      | 1.0274$\cdot$10$^{-3}$ | 1.4578$\cdot$10$^{-3}$ | 1.7187$\cdot$10$^{-3}$ |

Comparisons of the obtained results with Tables 1 and 2 show that accuracy of the both 9-point schemes in the simulated cases for $\lambda = 0.707$ is much lower than that of the new 5-point scheme.

6.3. A 13-point stencil

The next numerical stencil is based on complete bivariate interpolation polynomials of the fourth degree. Consider the initial segment $\mathcal{M}^*_{\leq 15}$ of $\mathcal{M}^*$:

$$\{1, x_1, x_2, x_1x_2, x_1^2, x_2^2, x_1x_2^2, x_1^2x_2, x_2^2x_1, x_1^3, x_2^3, x_1^2x_2^2, x_1x_2^3, x_2^3x_1, x_1^4, x_2^4\} \quad (54)$$
| $n$ | $n_t$ | $d$ | $\lambda$ | $E_{P9}$ | $E_{CP9}$ | $E_{C9}$ |
|-----|------|-----|---------|--------|--------|--------|
| 10  | 10   | 0.75| 0.707   | 2.6021 $\cdot 10^{-3}$ | 1.3156 $\cdot 10^{-2}$ | 1.5301 $\cdot 10^{-2}$ |
| 10  | 10   | 0.75| 0.796   | 2.8906 $\cdot 10^{-3}$ | 1.7117 $\cdot 10^{-2}$ | 1.8658 $\cdot 10^{-2}$ |
| 20  | 20   | 0.75| 0.707   | 8.9889 $\cdot 10^{-4}$ | 4.3569 $\cdot 10^{-3}$ | 4.9178 $\cdot 10^{-3}$ |
| 20  | 20   | 0.75| 0.796   | 9.4873 $\cdot 10^{-4}$ | 5.5339 $\cdot 10^{-3}$ | 5.9647 $\cdot 10^{-3}$ |
| 40  | 40   | 0.75| 0.707   | 2.9200 $\cdot 10^{-4}$ | 1.2557 $\cdot 10^{-3}$ | 1.3892 $\cdot 10^{-3}$ |
| 40  | 40   | 0.75| 0.796   | 3.4821 $\cdot 10^{-4}$ | 1.5673 $\cdot 10^{-3}$ | 1.6650 $\cdot 10^{-3}$ |
| 80  | 80   | 0.75| 0.707   | 1.0449 $\cdot 10^{-4}$ | 3.3019 $\cdot 10^{-4}$ | 3.6165 $\cdot 10^{-4}$ |
| 80  | 80   | 0.75| 0.796   | 1.4901 $\cdot 10^{-4}$ | 4.0710 $\cdot 10^{-4}$ | 4.2991 $\cdot 10^{-4}$ |

This set includes all the monomials of total degree $\leq 4$. The corresponding index set $Q_{15}$ is presented in Figure 4 where both thirteen solid dots and two empty circles denote interpolation points.

After calculating the corresponding Lagrange basis (see section 4) and using (28)-(29), one can determine that all the coefficients in expressions (9)-(10) related to the two empty circles will disappear. As a result, we get a numerical scheme that involves the 13-point stencil (the solid dots in Figure 4). The notations (47) will be used in presenting the scheme to make the expressions more compact:

1) for the first time-step

$$u_{ij}^{k+1} = u_{ij}^0 + \tau v_{ij}^0 + \frac{\lambda^2}{2} \left[ \frac{4 - 2\lambda^2}{3} \delta_{ij}^0(1,0) + \frac{\lambda^2}{6} \delta_{ij}^0(1,1) + \frac{\lambda^2 - 1}{12} \delta_{ij}^0(2,0) \right]$$

$$+ \frac{\tau \lambda^2}{6} \left[ \left( \frac{4}{3} - \frac{2\lambda^2}{5} \right) \epsilon_{ij}^0(1,0) + \frac{\lambda^2}{10} \epsilon_{ij}^0(1,1) + \left( \frac{\lambda^2}{20} - \frac{1}{12} \right) \epsilon_{ij}^0(2,0) \right]$$

(55)

2) for the second and next time-steps

$$u_{ij}^{k+1} = 2u_{ij}^k - u_{ij}^{k-1} + \frac{\lambda^2}{2} \left[ \frac{4 - 2\lambda^2}{3} \delta_{ij}^0(1,0) + \frac{\lambda^2}{6} \delta_{ij}^0(1,1) + \frac{\lambda^2 - 1}{12} \delta_{ij}^0(2,0) \right]$$

$$+ \lambda^2 \left[ \frac{4 - 2\lambda^2}{3} \delta_{ij}^0(1,0) + \frac{\lambda^2}{6} \delta_{ij}^0(1,1) + \frac{\lambda^2 - 1}{12} \delta_{ij}^0(2,0) \right],$$

$k = 1, 2, \ldots$

(56)
Figure 4: Index set for the 15-point interpolation stencil

Formula (56) for the second and next time-steps completely coincides with that obtained previously [2, 3] using the finite-difference method.

However, expression (55) for the first time-step has not been presented in the literature before. An advantage of using this expression rather than the conventional one (based on the central difference for approximating the initial condition for \( v \)) is shown in Table 5 where simulation results for the standing wave (38) solution are presented. The relative \( L^2 \) errors for the conventional and new approaches are denoted by \( E_{C13} \) and \( E_{P13} \), respectively. For simplicity sake, the periodic boundary conditions have been incorporated in the simulation taking into account that the solution (38) is periodic in both spatial directions. Since the maximal Courant number needed for stability of this scheme is \( 1/\sqrt{2} \), a value of \( \lambda = 0.707 \) was used.

The large values of the error ratio \( E_{C13}/E_{P13} \) demonstrated in Table 5 are explained by a higher accuracy of the new first time-step expression (55) in comparison with the conventional one. On the other hand, it is worth to notice that the relative \( L^2 \) error \( E_{C13} \) (corresponding to the conventional first time-step approach) in Table 5 has almost the same values as the error \( E_{C5} \) in Table 1 despite using a higher degree interpolation stencil in Table 5. That is, an error introduced at the first time-step probably suppresses advantages of using a higher degree interpolation at later time-steps.
Table 5: Wave (38) simulations using the 13-point stencil.

| $n$ | $n_t$ | $\lambda$ | $E_{P13}$     | $E_{C13}$     | $E_{C13}/E_{P13}$ |
|-----|-------|-----------|----------------|----------------|-------------------|
| 10  | 10    | 0.707     | $4.2146 \times 10^{-5}$ | $6.8938 \times 10^{-2}$ | $1.6357 \times 10^3$ |
| 20  | 20    | 0.707     | $6.6004 \times 10^{-7}$ | $1.6636 \times 10^{-2}$ | $2.5205 \times 10^4$ |
| 40  | 40    | 0.707     | $1.1471 \times 10^{-8}$ | $4.1230 \times 10^{-3}$ | $4.0537 \times 10^5$ |
| 80  | 80    | 0.707     | $2.8884 \times 10^{-10}$ | $1.0285 \times 10^{-3}$ | $3.5608 \times 10^6$ |

7. Conclusion

A new method is proposed to build explicit time-stepping stencil computation schemes for the transient 2D acoustic wave equation. The main idea is to use Poisson's formula that provides the exact solution of the initial-value problem through the initial conditions. Implementation of this formula together with polynomial stencil interpolation of the initial conditions (and exact integration) for a particular 2D stencil creates a unified time-marching scheme that combines computation expressions for the first time-step and for the next steps.

Particular explicit stencil computation schemes (with 5, 9 and 13 space points) are derived in the paper. Their stability conditions are determined. All of the obtained first time-step computation expressions are different from those used in conventional finite-difference methods. Simulation comparison results are presented for two benchmark problems that have exact solutions. It is demonstrated by simulation that the proposed computation approach maintains an accuracy advantage in comparison with conventional finite difference schemes which is mostly attributed to the new first time-step computation expressions.

Acknowledgments

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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